General Area Detector Diffraction System (GADDS)

Version 4.1.xx

REFERENCE MANUAL

M86-E01008 4/04

General Area Detector Diffraction System (GADDS) Reference Manual

Version 4.1.xx

M86-E01008 4/04

This manual covers the GADDS software package. To order additional copies of this publication, request the part number shown at the bottom of the page.

Notice

The information in this publication is provided for reference only. All information contained in this publication is believed to be correct and complete. Bruker AXS Inc. shall not be liable for errors contained herein, nor for incidental or consequential damages in conjunction with the furnishing, performance, or use of this material. All product specifications, as well as the information contained in this publication, are subject to change without notice.

This publication may contain or reference information and products protected by copyrights or patents and does not convey any license under the patent rights of Bruker AXS Inc. nor the rights of others. Bruker AXS Inc. does not assume any liabilities arising out of any infringements of patents or other rights of third parties. Bruker AXS Inc. makes no warranty of any kind with regard to this material, including but not limited to the implied warranties of merchantibility and fitness for a particular purpose.

Address comments to: Publications Department
Bruker AXS Inc.
5465 East Cheryl Parkway
Madison, Wisconsin 53711-5373
USA

Revision	Date	Changes
0	12/99	Original release.
1	4/04	Updated all sections.

Table of Contents

1. General Information

The GADDS Software Reference Manual is designed to supplement the GADDS User's Manual and the GADDS Administrator's Manual. Information already contained in these manuals is not duplicated here.

See the GADDS User Manual for:

- General descriptions of the instrument: goniometer, stages, generator, etc.
- General operation of the instrument: power-up, operation, shut-down, etc.
- Theory of analysis
- Geometry conventions
- Typical applications of GADDS to solve common diffraction problems

See the GADDS Administrator's Manual for:

- Pre-installation, installation, alignment, and calibration instructions
- Flood-field, spatial, and beam center instructions
- Software installation and release notes
- Software customization instructions
- Test procedures
- General maintenance
- Bruker service

1.1 Program Overview

GADDS is part of a suite of programs available from Bruker AXS, Inc. for using an Area Detector for powder diffraction problems. In addition to the GADDS software, optional packages are DIFFRAC*plus*, TOPAS P, SAXS, ASTRO, etc.

The functions of these programs are briefly summarized as follows:

- GADDS is the essential instrument control and data acquisition program which controls all hardware functions associated with the multi-wire-based X-ray diffractometer systems. It contains a comprehensive set of online and off-line functions and algorithms for instrument calibration, specimen screening, and frame data acquisition. GADDS also includes an option to display ICDD PDF2 database patterns and search the NIST database of known unit cell dimensions. These features will be described in detail in this manual.
- ASTRO is a supplementary utility program that may be used in conjunction with the GADDS program to optimize data collection strategies for single crystal type applications. Use it to minimize data collection time by collecting only a unique portion of the reflection data or to design custom data collection strategies. This program is described in detail in the ASTRO Technical Reference Manual.
- TOPAS P is a profile fitting program for fundamental parameter and general lineshape fitting of diffraction spectra. This program is described in detail in the PROFILE*plus* Manual.
- DIFFRAC*plus* for GADDS is a complete set of integrated programs for evaluation, search / match, etc. on 1D spectra. Programs included in the DIFFRAC*plus* package include:

  EVA—Graphical evaluation package.

  Diffrac File Exchange—Similar to Raw2Raw utility, but more limited except with UXD file formats.

  PDF Database Maintenance—Utility to view and manipulate PDF database.

  XRD Evaluation Program—Graphical evaluation package with optional search/match algorithm.

  XRD Quantification Program—Graphical quantification package.

These programs are described in detail in the DIFFRAC*plus* Manual.

GADDS may be executed in either online or off-line mode. The online version of GADDS supports a variety of goniometer stages and other instrument configurations including the following hardware options:

- HISTAR detector and dual HISTAR detectors
- D8 Discovery, Platform, Aztalan, or P4 goniometers
- Phoenix (D8) or GGCS (all others) goniometer controllers
- Numerous different goniometer stages
- Watlow temperature controller
- Sealed tube or rotating anode generators
- SMART rotary shutter
- Optical microscope or CCD video camera with zoom control and laser alignment

The online version of GADDS is a powerful and flexible instrument control sample analysis data collection package. The program couples the precise control of the goniometer angles and X-ray shutters (through the GGCS controller) with the operation of two-dimensional, multi-wire X-ray detectors to yield highly accurate and reproducible two-dimensional images (frames) of X-ray diffraction patterns. GADDS includes a wide range of instrument functions (e.g., open/close shutter, drive angles, etc.), calibration routines, sample screening options (e.g., add, rotation, etc.), automatic routines (e.g., scripts) and automated frame data collection. Frame data may be collected in a variety of modes optimized for individual instrument configurations or sample properties.

Examples of typical applications of the GADDS system are:

- Routine data collection on transmission of reflection samples
- Phase ID problems
- Micro-diffraction problems
- Texture analysis
- Stress analysis
- Crystallite size
- Percent crystallinity
- SAXS

1.1.1 Basic GADDS Operation

1. Click on the GADDS icon to execute the online version of GADDS.
2. Verify that the correct project have been loaded.
3. Verify that the appropriate calibration files have been loaded and that the goniometer angles and the values of the distance and X and Y beam centers are correct. Update, if necessary.
4. Select the appropriate level for the experiment (e.g., Level 1 [beginner] or Level 2 [experienced]).
5. Mount the specimen and proceed with the experiment. Individual steps will be described this manual.
6. To exit from the program, drive all angles to zero and click on the File > Exit option. Do not exit from the program by clicking the Windows NT close button—this will cause abnormal termination and loss of configuration data!

1.2 Environment Variables (Logical Names)

Under WNT, logical names are stored as environment variables. Entering environment variables are done through Control Panel's System Applet. You may enter environment variables as either system (available to all users) or as user (available only to the current user).

Logical names which point to directories should end with a colon ":" and the translation should end with the directory separator "\".

Example: Defining the GADDS$FRAMES directory

set GADDS$FRAMES:=C:\FRAMES\

To display a frame, say cor1.001, from the GADDS$FRAMES directory the name to enter in the DISPLAY /NEW panel would then be:

GADDS$FRAMES:cor1.001

If the default working directory in the GADDS Project > New/Edit/Copy panel is defined as GADDS$FRAMES:, you would need to enter only "cor1.001" in the File > Display > New panel.

In order to allow users flexibility in working with multiple products on the same computer (e.g., FRAMBO and GADDS) GADDS supports program-specific logical names (environment variables). The program-specific names are GADDS$SYSTEM:, GADDS$SYSDATA:, and GADDS$FRAMES:, which serve the same purpose as SAXI$SYSTEM: (points to executables and help files), SAXI$SYSDATA: (points to color lookup table directory) and SAXI$FRAMES: (points to directory containing frame and plot data). If the program-specific name exists, its translation is used. If it does not exist, the program attempts to use the corresponding SAXI$ name; thus, the program remains compatible with earlier logical name setups.

GADDS recognizes the following logical names.

GADDS$CALIB:

> This variable translates to the directory which contains area detector calibration files, such as flood-field and spatial tables.

GADDS$FRAMES:

> This variable translates to the root directory which contains area detector frames, calibration files, project files, and 1D spectra (raw files).

GADDS$PROJECT:

> This variable translates to the full pathname of the file to be used as the project database, for example, D:\frames\projects\gadds.prj.

GADDS$SCRIPTS:

> If present, this optional variable translates to the name of the common script directory. Whenever a script file is specified without a

directory, the program will search for the script file in three places: current project directory, system data directory, and common script directory.

GADDS$SYSTEM:

This variable must translate to the name of the directory where the area detector programs, utility programs, new project defaults, and help files reside (e.g., C:\SAXI\GADDSnew\).

GADDS$SYSDATA:

This variable must translate to the name of the directory where the area detector data files (e.g., color lookup tables, calibration files, usertask.ini) reside. (C:\SAXI\GADDSnew\).

GADDS$TEST:

This variable must translate to the name of the directory where the test frames and test command files reside. (e.g., C:\SAXI\GADDSnew\TEST\).

GADDS$CDCODE:

This variable translates to the directory which contains the NIST journal file: CODENS.DAT. If missing, it defaults to GADDS$CDROM:\vaxind\. (e.g., D:\crystal\vaxind\).

GADDS$CDF:

This variable translates to the directory which contains the NIST index file: CRYIDX.BIN. (e.g., C:\saxi\).

GADDS$CDROM:

This variable translates to the directory which contains the NIST database file: CRYSTAL.DAT. (e.g., E:\crystal\).

PROF$SYSTEM:

This optional variable translates to the name of the directory where the profile fitting package resides. (e.g., C:\TopasP\). See Special > Spawn, Section 9.8.

GADDS$PPF

This variable if defined, instructs GADDS to process pole figures in 1.0° resolution using bin integration and to create a partial pole figure ASCII file.

PDF2$IND:

This variable translates to the directory which contains the PDF2 index files. These files should be copied from slow CDROM to the faster hard disk. (e.g., C:\PC-PDF\).

PDF2$KEY:

This variable translates to the directory which contains the PDF2 search indexes: PDF2.S##. (e.g., E:\PDF2\).

PDF2$PDF:

This variable translates to the directory which contains the PDF2 database file: PDF2.DAT. (e.g., E:\PDF2\).

SAXI$ADMODEL

Sets the combination of goniometer and controller assumed for instrument control purposes by GADDS. The environment variable SAXI$ADMODEL, if defined, must translate to:

P3X2000 for 4-circle systems

X2000 for older 3-circle systems (black Aztalan goniometer)

PLATFORM for 3-circle systems

T:1/4-CIRCLE for 3-circle systems with quarter circle in transmission mode.

R:1/4-CIRCLE for 3-circle systems with quarter circle in reflection mode.

D8 for new D8 Discovery systems.

If SAXI$ADMODEL is not defined, PLATFORM (3-circle) is assumed. The model number given here is stored in the header of new frames saved in Bruker format.

SAXI$NAMECHARS

characters in “NAME” part of filename

SAXI$RUNCHARS

characters of “NAME” part used for run#

SAXI$RUNBASE

Numeric base of run # (10 or 36)

SAXI$NUMCHARS

characters in extension, used as frame

SAXI$NUMBASE

Numeric base of frame # (10 or 36)

These names translate to numeric values which establish the initial frame naming parameters, which can be viewed and modified on the Edit > Configure > User settings form. If the configuration has been saved from a previous run of GADDS, the values in the configuration file override these values when GADDS is restarted. Thus, these names are used by GADDS only if there is no existing GADDS._GC file.

SAXI$BIGFONT

When set to a non-zero value, gadds displays the screen using a larger character font.

SAXI$CURSWEIGHT

This name can be defined with an integer value from 2 to 7 to specify the line thickness of the cursors in pixels. This is primarily for use on IRIS systems, where single-

weight lines can look very thin. If SAXI$CURSWEIGHT is undefined or assigned the value 1, the cursors appear as in earlier versions. The cursors drawn in the ZOOM and GRAPH commands are also affected in the same manner.

SAXI$DBGLEVEL

This variable translates to the program debug level that is used to determine which debug statements are sent to the file: stdout.txt. This is only used to debug the program.

0 = off

1 = serial communications, setup messages, correction tables, limits, etc.

2 = header errors, user tasks

3 = echo controller commands, general messages, etc.

4 = echo controller responses, detector messages, raw files, etc.

5 = echo flushed serial characters, sent ASCII codes

6 = timeouts

7 = extended debug output, callbacks, etc.

8 = COM port characters received

SAXI$NOBOXLIM

This optional variable, if defined, will increase the maximum Cursor > Box and Cursor > RBox size limit from 64 to 256 for diagnostic purposes.

SAXI$OLDNAMES

When set to any value, this instructs the program to use the old frame naming conventions when creating new frame files.

SAXI$ON

If non-zero, we continue command file processing regardless of error code. If zero or undefined, command files stop on error code.

SAXI$PKZIP

If defined, it is set to the full pathname of PKZIP for console (version 2.50), which is used in the Project > Backup command.

SAXI$PRINTER

This optional variable points to the default GADDS print queue. A useful trick is to setup a GADDS print queue with typical settings for GADDS printing such as landscape orientation.

SAXI$SITE

The site name given here is stored in the header of frames written in Bruker format.

Under WNT, this defaults to the RegisteredOrganization name in the Registry.

SAXI$SWCHAR

The startup command line switch character can be defined as the translation of this name. By default, SAXI$SWCHAR=/ leading to the default DOS-style parsing. You can set SAXI$SWCHAR=- to change to UNIX-style "-" switches. The command syntax is otherwise the same (only the character which precedes the qualifiers is changed). SAXI$SWCHAR affects interpretation of only the startup command line, not the SLAM command line. We recommend that you retain the "/" switch character setting.

SAXI$USERNAME

The user name given here becomes the default name on the GADDS Edit > Configure > User settings command form. Under WNT, this defaults to the RegisteredOwner name in the Registry.

SAXI$VIDEOFORMAT

Overrides the saving of video images in TIFF format for Coreco or JPEG format for Matrox. Alternate options are:

0	TIFF format stored with *.tif extension (Coreco) or MIL format stored with *.mim extension (Matrox)
1	BMP format stored with *.bmp extension (Coreco or Matrox)
2	TARGA format stored with *.tga extension (Coreco only)
3	JPEG format stored with *.jpg extension (Matrox only)

SAXI$512MAXOVF

Restricts frame file format to contain a maximum overflow table size of 512 bytes (for compatibility with other, older software packages).

1.3 Startup Command Qualifiers

The following qualifiers can additionally be given when starting GADDS. It is assumed that the qualifier switch character has not been changed from its standard value of "/". If it has, substitute the appropriate switch character, e.g., "-".

/AXES=#

Starts GADDS with support for specified axes. By default, GADDS is started with support for 2theta, omega, phi, and chi, of which chi may be fixed at 54.74 degrees. Axes are specified by using an eight bit bitmask with each bit representing the presence (ON) or absence (OFF) of each axis.

Bit	Value	Axis	Bit	Value	Axis
0	1	2Theta	4	16	X
1	2	Omega	5	32	Y
2	4	Phi	6	64	Z
3	8	Chi	7	128	Zoom

/COMMAND

Starts GADDS in command line mode instead of menu mode.

/COMMAND=@<filename> <parm1> <parm2> ...

Starts GADDS and automatically invokes SLAM script file with optional parameters of parm1, parm2, etc.

/CONFIGURATION=<filename>

Causes GADDS to read the initial configuration from <filename> rather than from GADDS._GC.

/DEFAULT=<filename>

Causes GADDS to read the initial configuration from <filename> if the configuration file is either not found or creates a read error or the /NORELOAD switch is used.

/DEFAULT=<filename>

Causes GADDS to read the initial configuration from <filename> if the configuration file is either not found or creates a read error or the /NORELOAD switch is used.

/DUAL

Allow dual detector operations.

/LEVEL1/LEVEL2/LEVEL3

Starts GADDS in requested menu level. Default is 1.

/LOCK

Disables the menu level commands. Useful for individual security situations.

/NOPROJECT

Prevents GADDS from starting in the last project's working directory. Starts in icon's working directory.

/NORELOAD

Prevents GADDS from reading the configuration file: gadds._nc.

/PORT=#

Specifies the goniometer controller com port number. Valid options are 1–4 with 1 being the default.

/PROJECT=<projname>

Specifies GADDS to start in the named project's working directory. This is the project name as defined in the project database. On failure to load requested project, the last project's working directory is used.

/RAXES=#

Instructs GADDS that the goniometer controller is reporting axes that should be ignored and overridden with the GADDS "fixed angles" command. The default is that all reported angles are used (see /AXES=#). This is mainly useful for 2-position chi stages with video option, where /RAXES=8 should be used. Axes are specified by using an eight bit bitmask with each bit representing the presence (ON) or absence (OFF) of each axis.

Bit	Value	Axis	Bit	Value	Axis
0	1	2Theta	4	16	X
1	2	Omega	5	32	Y
2	4	Phi	6	64	Z
3	8	Chi	7	128	Zoom

/TCPORT=#

Specifies the temperature controller com port number. Valid options are 1–4 with 2 being the default.

/THETATHETA

Modifies behavior to theta theta operation.

/X=# /Y=#

Determines GADDS window position offset from upper left corner in screen pixels. A value of -1 (default) will center GADDS in the screen display.

1.4 GADDS Startup Behavior

When GADDS is started, the program goes through many checks to determine the operating state of the program.

1. Command line qualifiers and environment variables are used to override or set the default behavior. All environment variables must be defined prior to starting GADDS.
2. The working directory is defined. By default, GADDS uses the last project's working directory, unless the command line qualifiers, /noproject or /project=projname, are present. If the last project does not exist, not defined, an error occurred, or /noproject was used, then GADDS will prompt the user to define a new project (which includes defining the working directory).
3. The program default settings are defaulted or read. By default the configuration is read from the project's working directory (gadds._nc). If error or /noreload is present, from the GADDS system directory (GADDS$SYSTEM:gaddsdef._nc). On complete failure, the hard coded defaults are used. The names of the normal configuration file and the default configuration file can be changed using /configuration=<filename> and /default=<filename> command line qualifiers.
4. Diffractometer communications with the goniometer controller is initiated. On P4 systems, GADDS confirms the current angle settings.

1.5 Dialog Box and Keyboard Conventions

1.5.1 Dialog Boxes

GADDS has been designed with standard Windows dialog boxes, so you can use standard methods when responding. The action buttons vary depending on the function of the dialog box. The following types of dialogs are used, classified according to type-of-action button:

Message Boxes

These display informational and error messages and have only an OK button. The ENTER key is equivalent to OK.

Yes/No Dialog Boxes

These display a message and request a Yes or No response. Pressing the Y key is equivalent to clicking Yes. The N key is equivalent to No. Pressing ENTER executes whichever button is highlighted. The TAB key moves the highlight between the two buttons.

OK/Cancel Dialog Boxes

These display a message that requires an OK or Cancel response, or they may contain a series of Windows or Motif controls for entering data. Pressing ENTER is equivalent to clicking the currently highlighted action button, which is initially the OK button. Pressing ESC is equivalent to clicking the Cancel button. The TAB and SHIFT+TAB keys move to the next or preceding control in the dialog box, respectively. If the dialog box contains edit fields, you can copy, cut, and paste text within these fields with CTRL+C, CTRL+X, and CTRL+V. These operations use the clipboard, so you can also use these keys to transfer text information among different dialogs or between programs.

Output Dialog Boxes

These display a scrolling multi-line text control; a scroll bar; and OK, Write..., and Print... buttons. The arrow and page keys allow you to scroll the output text, as does the scroll bar. ENTER is equivalent to clicking the highlighted button (initially OK). You can highlight text in the text control with the mouse or shifted arrow keys and copy it to the clipboard with CTRL+C. However, you cannot alter the text in this type of dialog. The Write and Print buttons allow you to send selected text (or all the text, if no selection was made) to a disk file or a printer, respectively.

Edit Dialog Boxes

These display a scrolling multi-line edit control; a scroll bar; and OK, Cancel, Write..., Print..., and Read... buttons. The text in the edit control can be edited according to the normal system conventions. The arrow and page keys allow you to scroll the text, as

does the scroll bar. ENTER is equivalent to clicking the highlighted button (initially OK), and the TAB and SHIFT+TAB keys cycle the highlight (focus) over the edit control and buttons. ESC is equivalent to Cancel. You can highlight text in the text control with the mouse or shifted arrow keys and copy it to the clipboard with CTRL+C, cut to the clipboard with CTRL+X, and paste with CTRL+V. However, ensure that any text you paste into such a dialog is correctly formatted, since format is not checked before a paste. The Write and Print buttons allow you to send selected text (or all the text, if no selection was made) to a disk file or a printer, respectively. The Read button allows you to insert text from a disk file at the current position. As with the paste operation, ensure that text in the file is correctly formatted, since format is not checked before file text is inserted.

1.5.2 Keyboard Conventions

Following are definitions used by Bruker for common keyboard keys and key combinations. Note that the keys used in interactive commands may also be used as menu accelerators. (For example, when the GADDS menu has the focus, CTRL+LEFT ARROW displays the next image in a sequence. But when a cursor command has the focus, the same key moves the cursor left in 10-pixel increments.)

CTRL+BREAK and CTRL+C (NT only)

CTRL+C (SGI only)

Interrupts an operation in progress. Under some workstation environments, CTRL+C is polled, so that to may need to hold the key combination down long enough for the program to detect it.

ESC

Works like the Cancel button in dialogs with a Cancel button. Also works as a soft abort (stop after current frame is finished) in the Acquire > SingleRun, MultiRun, Hemisphere, Quadrant, and Matrix commands.

ENTER

Works like the OK button in OK/Cancel dialogs, or executes the currently highlighted button in most other dialogs.

TAB

Moves to the next field in a dialog box.

SHIFT+TAB

Moves to the preceding field in a dialog box.

UP ARROW and DOWN ARROW keys

Move through items in a menu or multi-line edit control. In most interactive commands, they can also be used to position the cursor as an alternative to the mouse. By default, they move the cursor by 1 pixel in graphic/cursor commands (see PLUS key description below).

LEFT ARROW and RIGHT ARROW keys

Move non-destructively one character left or right when editing text in a dialog; as with up/down arrows, they can position the cursor in interactive cursor commands.

+ plus key

Increases by a factor of 2 the number of pixels that a cursor is moved whenever a cursor key is pressed. Values of 1, 2, and 4 are possible in conjunction with arrow keys, or 10, 20, and 40 in conjunction with CTRL+arrow keys.

- minus key

Decreases by a factor of 2 the number of pixels that a cursor is moved whenever a cursor key is pressed (opposite of the + key, described above).

CTRL+ARROW keys

Move the cursor 10x faster in interactive cursor commands (like Analyze > Cursor, Analyze > Cursor > Box, etc.)

PAGEUP

Move up a page in scrolling text dialogs.

PAGEDOWN

Move down a page in scrolling text dialogs.

INS

Toggles between character insert and overstrike modes when editing a line in a dialog box.

DEL

Deletes forward one character when editing a line in a dialog box. The character under the cursor is deleted.

Backspace

Deletes backward one character when editing a line in a dialog box. The character to the left of the cursor is deleted.

HOME

Moves to beginning of line when editing a line in an input panel.

END

Moves to end of line.

F2, F3, F4

In interactive commands, these are equivalent to left, center, right mouse buttons, respectively

CTRL+C

In a dialog box edit control, copies highlighted text to the clipboard.

CTRL+X

In a dialog box edit control, cuts highlighted text to the clipboard.

CTRL+V

In a dialog box edit control, pastes from the clipboard.

CTRL+P

Prints main GADDS screen to currently selected printer. Under NT, this function does not work when the user is in a dialog box or message box; however, PRTSC will send a copy of the entire screen including GADDS window (or ALT-PRTSC for just active window) to the clipboard.

1.6 GADDS Directory Organization

GADDS's directory organization (as shipped from the factory) is shown below. We recommend that you maintain this directory convention for Bruker-supplied files to minimize the effort required for future software updates. On PCs and workstations, the same logical names are used to point to the programs and data.

Following is the normal directory layout (shown schematically) for GADDS.

C:\ Root directory, containing parent of $SAXI_ROOT system startup files on PC;
Bruker program directories

— C:\SAXI — Bruker-supplied application programs (in the subdirectories).

— C:\SAXI\GADDSnew
GADDS programs, utilities, and help files. The environment variables GADDS$SYSTEM: and GADDS$SYSDATA: by default point to this directory.

— C:\SAXI\GADDSnew\SRCS
Example source files for reading Bruker format data files.

— C:\SAXI\GADDSnew\TEST
Test data for verification of proper installation and setup. The environment variable GADDS$TEST: normally points to this directory.

— C:\SAXI\PVWAVE
Command procedures to import Bruker data files into Precision Visual's Wave program.

— C:\SAXI\VIDEO32
VIDEO executable and help files.

D:\FRAMES
Root of frame data storage. It is recommended that you use a subdirectory under this root as the project working directory for each sample.

— D:\FRAMES\CALIB — Directory where GADDS stores all calibration files for the detector.
The environment variable GADDS$CALIB: by default points to this directory.

— D:\FRAMES\PROJECTS
Directory where GADDS project databases are maintained. Each user should define the environment variable GADDS$PROJECT to point to a project database in this directory.

1.7 Frame Indexes

Frame indexes have been implemented. When a frame name is given in the format:

INDEXNAME#N or INDEXNAME##H

the program looks for a frame index file INDEXNAME (with the extension defaulting to .fin, for Frame INdex). N is a decimal number representing the line number in the index file which contains the filename of the frame; H represents the same, only in base 36. Lines are numbered starting from 0. GADDS will remember the name of the last index specified, so that you can omit INDEXNAME in subsequent references; thus, #N and ##H become valid frame names.

The frame index is an ASCII file in the Harvard format, where each line contains a number (which is ignored by GADDS) followed by the frame name. The default directory for frame index files is the frame directory as specified in the CONFIGURE /EDIT panel.

In the DISPLAY commands, NEXT, PREVIOUS, MOVIE+, and MOVIE-, the auto increment or decrement will be performed on the index line number, not the frame name.

1.8 Special Symbols

Throughout the various input panels, special symbols are reserved for special purposes.

Symbol	Where used	Purpose
$DATA	PEAKS /LOAD	To read the currently loaded peak table
$FRAME	CORRECTIONS DISPLAY FRAME_INFO POLE_FIGURE SPATIAL SMOOTH	To read the currently loaded frame image
$MASK	MASK /VIEW	To read the currently loaded active pixel mask
$NET	(obsolete)	Unused—avoid using $NET in filenames
$NEXT	DISPLAY	Display the next frame in a frame series
$NULL	LOAD MASK /READ MASK /SAVE POLE_FIGURE / SCHEME SAVE	Read or save a null file
$PREV	DISPLAY	Display the previous frame in a frame series
$RUNNEXT	DISPLAY	Displays the next frame in a run series.
$RUNPREV	Display	Displays the previous frame in a run series.
$SCAN	POLE_FIG/ SCHEME	Automatically update the SCAN /EDIT panels for multiple runs
$TITLE	POLE_FIG/ POPLA POLE_FIG/ TEXTUREAT SAVE	When saving a file, keep the original title string

2. Project Management Routines

Project management is the organization of data files into logical groups. Typically, you will create a new project to start a new sample run, a new batch of samples, etc.; when to start a new project is really a user preference or a defined step in a laboratory procedure (for example, an ISO-9000 procedure).

GADDS manages and tracks all projects by using project files (*.prj). All users can share the same projects or each user can have their own unique projects. When GADDS was installed, SETUP created a system wide project file (for all users) and a GADDS administrator project file (for only the account that installed the GADDS software). GADDS locates the project file by translating the environment variable, GADDS$PROJECT, which contains the complete file specification of the project file (for example, D:\frames\projects\gadds.prj). SETUP creates this environment variable in the System Variables space to create the system wide project file. You may override the system wide setting, by creating a user specific project file as follows:

1. Start > Settings > Control Panel > System applet.
2. Click on the Environment tab.
3. Click on a line in the “User Variable for <User>” section.
4. In the Variable: edit box, enter `GADDS$PROJECT`.
5. In the Value: edit box, enter the full file specification. The drive and directory path must already exist. Bruker recommends using our naming convention of D:\frames\projects\GADDS_<username>.prj (you replace <username> with your actual user account name).
6. Click on [Apply].

7. Click on [OK].

Because initially there is no project file, the first time GADDS is started, you will see several messages:

> “Unable to open project database file for reading GADDS$PROJECT.”
>
> “Unable to use last project,”

Each time GADDS is started, the current project database is checked for orphaned projects.

NOTE: Removed orphaned project from database.
D:\frames\20002\Oct\MyProject0\gadds._nc

Then you are automatically sent to the Project > New command (see Section 2.3 Project > New). Enter appropriate values and click [OK]. Inform your GADDS administrator if you get the message:

> “Can't open gaddsdef._nc. Using default settings. You must use Project > Overwrite defaults command.”

When GADDS is started, you are automatically sent to the last project (most recently accessed). You can override this default behavior by modifying the GADDS shortcut with command line qualifiers:

/noproject

> Forces GADDS to always create a new project when it starts.

/project=<projname>

> Forces GADDS to always open into the same project, <projname>.

GADDS prevents offline instances from overwriting the defaults for online operation. When operating in offline mode, GADDS always appends “_offline” to the configuration filename before saving. When reading the configuration, offline GADDS tries to read this offline version, but if missing, GADDS reads the online version. This allows you to operate online GADDS in a directory, while simultaneously running offline GADDS for processing the newly collected frames in the same directory (could be from a different computer using mapped network drives).

2.1 Project > Switch • Change to a different, existing project

Menu Command: Project > Switch

Accelerator: None

User Level: 1

SLAM Syntax: PROJECT /SWITCH $1

Use this command to switch to an existing project. A scrollable, alphabetized list of all known projects will appear. Highlight the project of interest and click [OK].

Before the program switches to the requested project, the message appears:

> "Save the current configuration before changing projects?"

Typically, you click [Yes] as this is the safest option.

The program will switch to the requested project by loading that project's settings, clearing the frame buffer, clearing the displayed frame, and displaying the current project settings. However, if the requested project is no longer valid, the program will display a message, restore the original project settings, and remove the corrupted project from the project database.

2.1.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Select Project) [first in list]

> Enter the existing project name. In menu-mode, a scrollable, alphabetized list of all valid projects appears and you may simply click the requested project. The default is the first project in the list.

2.2 Project > Load • Load a configuration file and create a new project

Menu Command: Project > Load

Accelerator: None

User Level: 2

SLAM Syntax: PROJECT /LOAD $1 (not recommended to use in SLAM mode)

Use this command to create a project from an existing configuration file. You can click the browse button to search for an existing configuration file.

Before the program creates and switches to the requested project, the message appears:

> "Save the current configuration before changing projects?"

Typically, you click [Yes] as this is the safest option.

The program will create and switch to the requested project by loading that project's settings, clearing the frame buffer, clearing the displayed frame, and displaying the current project settings. However, if an error occurs, the program will display a message and restore the original project settings.

Next the program automatically generates a project name and adds the new project to the project database. If the new project name already exists, the message appears:

> "<PROJECT0> is already a project. Replace it?"

Click [Yes] to replace or [No] to generate a different project name (by incrementing the sample number).

2.2.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Configuration Filename) [*._nc]

> Enter the full file specification of an existing configuration file. The default is *._nc which will invoke the file browser.

2.3 Project > New • Create a new project from scratch

Menu Command: Project > New

Accelerator: None

User Level: 1

SLAM Syntax:

> PROJECT /NEW /CNAME=<s>
> $1 /TITLE=<s> /WORKDIR=<s>
> /FORMULA=<s> /MORPH=<s>
> /CCOL=<s> /DENSITY=<s>
> /DENSMETH=<s>

Use this command to create a new project from scratch. Typically, whenever you mount a new sample or a new batch of samples, you want to define a new directory for all your data files.

You must enter information in all the project information parameters. The sample name and sample number are combined to form the project name. If the generated project name is invalid, the message appears:

> "Sample name and number are too long or contain non-alphanumeric characters. Name will be shortened/modified as needed if you continue."

Click [Yes] to continue or [No] to return to dialog input box.

You must enter information in the directory information parameters. You may enter an existing directory, but typically you enter a new directory and the program will create it. You may enter the special value, $PROJECT, which instructs the program to use the directory GADDS$FRAMES:YEAR\MON\<projname>, which is typically defined as D:\frames\2003\Mar\<projname>. The advantage of using $PROJECT is that it automatically generates a directory name that should be unique. If you try to re-use a project directory, the message appears:

> "Working directory already contains a configuration file: gadds._nc. Choose a different directory or use the Project > Load command."

The sample information parameters are all optional. Enter what you know and leave the rest set to "?".

Before the program creates and switches to the requested project, the message appears:

> "Save the current configuration before changing projects?"

Typically, you click [Yes] as this is the safest option.

The program will close any log and auto-script files before creating and switching to the new project.

> "Closing last project's log file…"
>
> "Closing last project's auto-script…"

New project defaults are taken from the system-wide default file create by the Project > Overwrite defaults command. All crystal information is cleared (reflection array list, orientation matrix, and face indices). The new project is created by clearing the frame buffer, clearing the displayed frame, displaying the project settings, and setting all title requests in other menus to the sample title.

If the previous project had either the log or auto-script enabled, you will be prompted to restart those features.

"Start/append log file for new project?"

"Start/append auto-script file for new project?"

2.3.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

/CNAME=<s> .....(Sample Name) [Unknown]

Enter the name of the sample (project name = sample name + number). Default is "Unknown."

$1 .....(Sample Number) [0]

Enter the number of the sample (negative to ignore). Default is 0.

/TITLE=<s> ..... (Title) [?]

Enter a descriptive title for this project (sample). Default is "?".

/WORKDIR=<s>... (Working Directory) [$PROJECT]

Enter the Drive:Directory to make current or the working directory. The program will place all data files in this directory. Or enter "$PROJECT" and the program will generate a project working directory name from the project name and using GADDS$FRAMES: as the root. Default is "$PROJECT".

/FORMULA=<s>... (Chemical Formula) [?]

Enter the chemical formula for this sample or enter "?". Default is "?".

/MORPH=<s>..... (Sample Morphology) [?]

Enter a description of the physical sample or enter "?". Default is "?".

/CCOL=<s> ..... (Sample Color) [?]

Enter a description of the sample color or enter "?". Default is "?".

/DENSITY=<s>..... (Measured Density) [?]

Enter the measured sample density, including units or enter "?". Default is "?".

/DENSMETH=<s>.(Density Method) [?]

Enter a description of the method used to measure the density or enter “?”. Default is “?”.

2.4 Project > Copy • Copy the current project to a new project

Menu Command: Project > Copy

Accelerator: None

User Level: 1

SLAM Syntax:

PROJECT /COPY /CNAME=<s> $1
/TITLE=<s> /WORKDIR=<s>
/FORMULA=<s> /MORPH=<s>
/CCOL=<s> /DENSITY=<s>
/DENSMETH=<s> /CLEAR /RESET

Use this command to create a new project using the current project settings as defaults. You typically use this command when mounting a similar sample on the goniometer or repeating a collect and process operation on the same sample.

Project > Copy differs from Project > New (see Section 2.3) in that:

- The project defaults can be taken from either the system-wide defaults (see Section 2.9 Project > Overwrite defaults) or from the current project settings by using the Clear switch.
- The crystal information may be either cleared or retained from the current project settings by using the Reset switch.
- The project information defaults to stay the same except that the sample number is

incremented; however, you may override these defaults.

2.4.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses: Project > New arguments also apply here (see Section 2.3 for explanations).

/CLEAR .....(Clear Crystal Info?) [No]

Check to clear the crystal face list, reflection array, and orientation matrix. Default is no.

/RESET .....(Reset to Defaults?) [No]

Check to reset program to default settings. Default is no.

2.5 Project > Edit • Edit the current project settings

Menu Command: Project > Edit

Accelerator: None

User Level: 1

SLAM Syntax:

PROJECT /EDIT /TITLE=<s>
/FORMULA=<s> /MORPH=<s>
/CCOL=<s> /DENSITY=<s>
/DENSMETH=<s> /CLEAR /RESET

Use this command to modify the current project settings. Because you are not creating a new project, you cannot change the project's sample name, sample number, or working directory. But you may change the sample's title and the sample information parameters, reset defaults to system-wide default settings, and/or clear the crystal information.

2.5.1 Arguments

Project > New and Project > Copy arguments apply here (see Section 2.3 and Section 2.4 for explanations). Defaults are current settings.

2.6 Project > Backup • Backup all files in the specified project's directories

Menu Command: Project > Backup

Accelerator: None

User Level: 2

SLAM Syntax: PROJECT /BACKUP $1 $2 $3 /NOCALIB /NOWORK

Use this command to backup all files in the project's working directory and/or the current calibration files into a single, compressed, archive file, which you may wish to transfer to tape or CD-R media for archiving purposes.

A scrollable, alphabetized list of all known projects will appear. Highlight the project of interest and click [OK]. Next a dialog of options appears. You must enter a filename for the archive file and enter the directory to place the archive file. Optionally, you may choose to exclude the calibration files or the current working files from the archive; however, typically you backup all your working files, but not the calibration files.

> "Requesting archive file already exists. Update existing archive file?"

Click [Yes] to update, [No] to abort. Updating adds new or updates existing data files in the archive, but does not remove any old data files. If you wish to overwrite an existing archive file, then you must pre-delete the archive (use Windows NT Explorer).

> "No PKZIP file is defined: SAXI$PKZIP"

Your GADDS administrator must configure the console version of PKZIP for use with GADDS. Simply extract the PKZIP files to a directory and define the System Variable, SAXI$PKZIP, to point to the full file specification. GADDS was tested with PKZIP for Console version 2.50.

2.6.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Select Project) [no default]

> Enter the project's name to archive or use $PROJECT for current project. No default.

$2 ..... (Archive Filename) [$PROJECT]

> Enter the filename for the file archive. Default is project name.

$3 ..... (Archive Directory) [GADDS$FRAMES:]

> Enter the directory to store the file archive. Default is GADDS$FRAMES:.

/NOCALIB..... (Exclude Calibration Files?) [Yes]

> Check to exclude all calibration files from the archive. Default is yes.

/NOWORK.....(Exclude Work Files?) [No]

Check to exclude all working directory files from the archive. Default is no.

2.7 Project > Remove • Remove a project from the project database

Menu Command: Project > Remove

Accelerator: None

User Level: 2

SLAM Syntax: PROJECT /REMOVE $1

Use this command to remove the requested project from the project database, but does not delete any data files. A scrollable, alphabetized list of all known projects excluding the current project will appear. Highlight the project of interest and click [OK]. The program will remove the requested project.

NOTE: Because the configuration and data files were not deleted, you could re-add the project using the Project > Load command.

2.7.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Select Project) [no default]

Enter the requested project name to remove from the project database. You cannot remove the current project. No default.

2.8 Project > Delete • Delete all project files and remove from project database

Menu Command: Project > Delete

Accelerator: None

User Level: 2

SLAM Syntax: PROJECT /DELETE $1

Use this command to delete all data files and remove the requested project from the project database. Typically, you perform a Project > Backup command before doing a Project > Delete command.

A scrollable, alphabetized list of all known projects excluding the current project will appear. Highlight the project of interest and click [OK]. The message appears:

> "Delete all files in data directories and try to remove this directory?"

Click [Yes] to continue, [No] to abort. The program will delete all files in the working directory, but not any subdirectories, files in subdirectories, or the calibration files (in the calibration directory), then it will remove the requested project.

2.8.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Select Project) [no default]

> Enter the requested project name to delete working files and remove from the project database. You cannot delete the current project. No default.

2.9 Project > Overwrite defaults • Overwrite the default configuration with the current settings

Menu Command: Project > Overwrite defaults

Accelerator: None

User Level: 3

SLAM Syntax: PROJECT /MAKEDEF

Use this command to define the system-wide default settings for projects. Typically, your GADDS administrator will issue this command whenever he changes the goniometer stage or other hardware option.

Before issuing this command, go through all menu options and define your default settings. The most critical settings are located in the command:

- Edit > Configure > User settings:
- Edit > Configure > Admin settings:
- Collect > Goniometer > All commands:

Double check that these settings are correct.

After issuing the Project > Overwrite defaults command, the message appears:

> "Save the current configuration as default values (for new/copy/edit "reset to defaults" option)?"

Click [Yes] to continue, [No] to abort. The program will save current settings in the GADDS$SYSTEM:gaddsdef._nc system-wide default configuration file. Whenever the reset to defaults option is checked in a Project > New, > Copy, or > Edit command, these system-wide defaults are read.

NOTE: If your GADDS administrator frequently changes goniometer stages, he may wish to create a project for each stage with the appropriate default settings for each stage already preset. Then when he switches stages, he only needs to:

1. Project > Switch: Switch to the project for the new goniometer stage (for example, Fixed-Chi, XYZstage, XYZstageSTRESS, Huber-Cradle, etc., which have already been defined).
2. Project > Overwrite defaults: Save these settings to the system-wide defaults.

2.9.1 Arguments

1. None. Commands execute immediately after confirmation message.

2.10 Project > Exit • Leave program and return to operating system

Menu Command: Project > Exit

Accelerator: None

User Level: 1

SLAM Syntax: EXIT

After saving the current configuration, this command terminates GADDS, returning you to the operating system. You may also exit GADDS by double clicking on the GADDS icon in the upper left, clicking the application close button in the upper right corner, pressing Alt-F4, or with the QUIT command (see Section 12.3 Quit), but these methods do not save the current configuration.

If you choose EXIT from the menu, a box appears with OK and Cancel buttons and the message:

Save current configuration: Are you sure:

Normally, you want the program to save the current settings—press OK. Occasionally, you may wish to ignore your project session and start over—press Cancel. All settings are stored in the project's working directory in the file: gadds._nc, which will be read the next time you start GADDS.

Then, a box appears with OK and Cancel buttons and the message:

EXIT: Are you sure?

The purpose is to provide a safety net in case EXIT was selected by mistake. Click the OK button, or press the ENTER key to exit the program. If you do not wish to exit at this time, click the Cancel button or press Esc, and you'll be returned to the GADDS menu.

In command mode, EXIT terminates GADDS after saving the current configuration, without displaying any prompts.

2.10.1 Arguments

None. Command executes immediately after confirmation message.

3. File Routines

3.1 File > Display > Open • Display a detector frame on the screen

Menu Command: File > Display > Open

Accelerator: Ctrl+D

User Level: 1

SLAM Syntax:

> DISPLAY /NEW $1 /QUADRANT=<n> /LO=<n> /HI=<n> /X=<n> /Y=<n> /MAG=<n> /AUTOINCREMENT /GRAPHICS_SAVE /ORIENTATION /VIDEO /OVERLAY

Use this command to display a specified data file from disk, or to display or redisplay the current contents of the frame accumulation memory.

Up to four different data files can be displayed at the same time using File > Display to place them into separate quadrants. You can also display a region within a frame magnified in a quadrant or in the full image window by setting the input arguments appropriately. While multiple images can be displayed in different quadrants at one time, only the image in the current quadrant is actually in memory. Thus, for example, the Analyze > Cursor functions work only on the image in the current quadrant.

GADDS will read and automatically configure internal parameters for imported Bruker CCD formats (based on the DETTYPE: frame header item and version 9 header items). But whenever the DETTYPE: is “unknown” or “other,” then GADDS tries to read the sub-items: PIXPERCM: and CMTOGRID:. On failure, GADDS must ask for the “Pixels per cm” and “Cm to grid” parameters.

When invoked from the menu, or run from the command line without arguments, File > Display displays a dialog box where you can view/edit

the arguments described below. Pressing the ENTER key or clicking the OK button starts the display. Pressing ESC or the Cancel button returns you to the menu.

Both filenames and filename patterns entered in the input panel are merged with the working directory specified in the Project > New dialog box before GADDS attempts to open the file.

3.1.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input Filename) [$FRAME]

Filename of the frame to be displayed. Input filename defaults to *.gfrm file extension (if missing).The special name $FRAME (the default) refers to the current data in frame accumulation memory. Thus, $FRAME can be used to display the contents of accumulation memory if you've acquired a frame suppressing display, or can be used to redisplay a newly acquired with different lower and upper limits. If you leave this item blank, or specify a wildcard filename pattern, pressing ENTER or clicking the OK button will allow you to choose from a list of the current filenames matching the pattern, after which you will be returned to the input dialog with the selected filename filled in. If you leave this item blank, it is the same as entering a *.* wildcard pattern. Remember that both filenames and patterns entered here are merged with the Project > New working directory, as described above.

/QUADRANT=<n> ..... (Screen Quadrant) [0-full]

Select the quadrant in which the frame is to be displayed. In the dialog box, you can select the quadrant from a drop-down list. While multiple images can be displayed in different quadrants at one time, only the image in the current quadrant is actually in memory; thus, for example, the cursor functions work only on the image in the current quadrant. Quadrants are 0 = full window, 1 = lower left, 2 = lower right, 3 = upper left, and 4 = upper right. Default is 0.

/LO=<n> ..... (Lower Limit) [0]

The number of counts to be mapped to zero in display memory. Pixel values lower than this are truncated to zero on display (although the cursor commands will still read the correct values). The default value is 0; the allowed range is from -255 to +65,535.

/HI=<n> ..... (Upper Limit) [63]

The number of counts to be mapped to the highest display memory value (currently 63; that is, displayed frames are shown with 64 simultaneous colors). Pixel values higher then the specified value are truncated to that value on display (although the cursor commands will still read the correct values).

The special value -1 causes the program to scan the pixel values in the frame and automatically pick reasonable display limits and contrast settings based on the result. The special value -2 directs the program to use whatever the previous limits were. The default value is -1; the allowed range is from -2 to 1,000,000.

/X=<n> .....(X) [256]

X-pixel coordinate to try to center in the specified quadrant. The range is from 0 to 511, 1023, or 2047 (depending on the frame size); the default value is 256. If the magnification is small enough that centering the specified X in the quadrant would leave part of the quadrant blank, the image is translated only far enough to place the edge of the frame at the edge of the quadrant.

/Y=<n> .....(Y) [256]

Y-pixel coordinate to try to center in the specified quadrant. The range is from 0 to 511, 1023, or 2047; the default value is 256. If the magnification is small enough that centering the specified Y in the quadrant would leave part of the quadrant blank, the image is translated only far enough to place the edge of the frame at the edge of the quadrant.

/MAG=<n>..... (Magnification) [1]

The magnification (zoom) factor, to examine a specific area in greater detail. The allowed range is from 1 to 16; the default value is 1.

/AUTOINCREMENT .. (AutoIncrement?) [No]

This allows successive frames to be displayed in different quadrants; for example, when the “MOVIE” option is used. Check this option to increment quadrant 1-4 after display. By default it is unchecked.

/GRAPHICS_SAVE…(Preserve Graphics?) [No]

Specifies whether or not to preserve any overlaid graphics if you clear the screen. Check this option to preserve graphics if clearing screen. By default it is unchecked.

/ORIENTATION…(Use Orientation in Header?) [No]

Normally, you'll want the cursor commands to read out HKL's based on the orientation matrix computed in the last Peaks > Refl. Array > LeastSq command. This is the default setting (unchecked). However, if you display a frame that was stored with its own orientation matrix in Bruker format, you can override GADDS's internal orientation matrix with the one in the frame header, and read HKL's on that frame without having to recompute its orientation matrix. In that case, check this option. Note that this option does not overwrite the matrix from the last

least squares; displaying another frame with this item unchecked, or acquiring a new frame clears the override flag (but does not reset the check box in this dialog — don't leave it inadvertently set!), effectively restoring the matrix from the last Peaks > Refl. Array > LeastSq.

/VIDEO…(Display Associated Video Image?) [No]

Specifies whether to automatically display the associated video image on the video program. The video program must already be running in a separate window. By default it is unchecked.

/OVERLAY.....(Add HKL Overlay?) [No]

This option, when checked, directs the program to draw an overlay of predicted spot positions on top of the image automatically every time a frame is displayed. The parameters given in the File > Display > HKLs dialog are used for these automatic overlays as well. By default, this option is unchecked. The overlay is computed from the current orientation matrix (determined in Peaks > Refl. Array > LeastSq) and takes into account any lattice centering determined in Peaks > Refl. Array > Bravais. You can draw overlays on magnified frames by entering the desired magnification and center in the File > Display panel when the image is displayed (the Edit > Zoom command does not redraw or magnify graphic overlays). Three types of marker characters are used to indicate the difference between the scan angle corresponding to the centroid of the displayed frame and the predicted scan angle of a reflection:

Predicted Scan Angle	Marker
Within scan range of the current frame	Box
Within scan range of a preceding frame	Circle
Within scan range of a subsequent frame	Cross (X)

The circle and cross can be thought of as the tip and tail of an arrow which points from the current frame to the predicted position, assuming a stack of frames with earlier frames positioned in front of the screen and subsequent frames positioned further into the screen.

3.1.2 Display Limits

The translation of pixel values to colors involves two separate translation steps. These steps allow you to view the images with nearly photographic quality and to refine the color mapping in real time, however, this refining makes the mapping process more complicated.

The mapping process is discussed in detail below, specifically with reference to the File > Display command. This command allows you to set both lower and upper display limits, which represents the most general case. Most of the frame acquisition commands also allow you to display the result according to a specified upper display limit exactly equivalent to the upper limit

discussed below. However, these commands fix the lower limit at zero, which works well most of the time. While most commands recognize a few special values for the upper limit (-1 for automatic limit setting, etc.), we ignore these special cases in the following discussion.

The first step is the mapping of pixel values into display memory. Display hardware components differ in the number of color levels available for each pixel. With GADDS, we always assume that the hardware can support at least 64 different values (0-63). The /LO and /HI qualifiers in File > Display let you specify any linear transformation between the pixel values and the values written into the display hardware (with the mapped values clipped to the range 0 to 63, so that values outside this range don't show up in the wrong colors). Thus, if you need fine discrimination within a narrow range of pixel values, you could specify /LO and /HI to cover that range. On the other hand, if wide latitude is more important, you would specify /LO and /HI to cover the whole range of pixel values in the frame.

After the pixel values have been converted and stored into display memory, the display memory values are mapped into colors with a second linear transformation, according to the current limits set in the Edit > Contrast command. Display memory values less than or equal to the lower Edit > Contrast limit are shown in the color at the bottom of the color table (for example, black). And values at or above the upper Edit > Contrast limit are shown in the color at the top of the color table (for example, white). The values in between are linearly mapped into the colors in the color table. Although you enter the contrast limits in terms of pixel value (unless you're using Edit > Contrast interactively, in which case you’re changing the limits in real time without specifying explicit values), Edit > Contrast works internally strictly with the values in display memory.

In general, you don't have to worry much about display limits, since the program takes care of all the pixel-value/display-memory conversion details. For normal data collection, you should usually leave the lower File > Display limit set at zero and the upper limit at 511, or use the “automatic” setting -1 described above. Anyway, powers of two make some internal calculations more precise, so 7, 15, 31, 63, 127, etc. are good general upper limit settings. If your frames look too dark, you can make them brighter by using a smaller File > Display upper limit. If they look too bright, use a larger File > Display upper limit. Since the Edit > Contrast command gives you a lot of extra latitude (and is much faster), use the display limits just for getting your images into the ballpark, then use Edit > Contrast for interactive adjustments.

3.2 File > Display > Next and File > Display > Previous • Display next/previous frame in this series

Menu Command:

File > Display > Next

File > Display > Previous

Accelerator:

Ctrl+RightArrow (next),

Ctrl+LeftArrow (previous)

User Level: 1

SLAM Syntax:

DISPLAY /NEXT

DISPLAY /PREVIOUS

When data frames have been collected as part of a set, these commands provide a convenient means of specifying display of the data frame that comes either just before (File > Display > Previous) or just after (File > Display > Next) the one currently displayed. The next (or previous) sequential name in a series of frames is computed according to the frame naming parameters set in the Edit > Configure > User settings dialog box (see Section 4.1 Edit > Configure > User settings).

The items entered in the File > Display input dialog box remain in effect for the duration of the File > Display Next or File > Display > Previous subcommand, including the display quadrant and autoincrement qualifiers. If the specified quadrant is 1–4 and autoincrement is set, successive frames will be displayed cyclically in the different quadrants.

When invoked from the menu or when run from the command line, File > Display > Next and File > Display > Previous start running immediately without prompting for additional input.

3.2.1 Arguments

None. Command executes immediately.

3.3 File > Display > Movie+ and File > Display > Movie- • Repeatedly display next/previous frame until key is pressed

Menu Command:

File > Display > Movie+

File > Display > Movie-

Accelerator:

Alt+UpArrow (movie+),

Ctrl+DownArrow (movie-)

User Level: 1

SLAM Syntax:

DISPLAY /MOVIE+

DISPLAY /MOVIE-

These commands are used to step through a series of sequentially numbered data frames, displaying them in sequence. Successive frames continue to be displayed until the end of the series (that is, a nonexistent frame) is encountered or until a key or mouse button is pressed. The MOVIE+ option displays the frames in an ascending frame number sequence and the MOVIE- option displays them in descending order.

The display arguments in the File > Display dialog are in effect for the duration of the File > Display > Movie+ or File > Display > Movie- subcommand, including the display quadrant and autoincrement qualifiers. If the specified quadrant is 1–4 and autoincrement is set, successive frames will be displayed cyclically in the different quadrants.

When invoked from the menu or when run from the command line, these commands start immediately (without prompting for additional input).

The next (or previous) sequential name in a series of frames is computed according to the frame naming parameters set in the Edit > Configure > User settings dialog box (see Section 4.1). There is a 0.1 second delay between frame displays.

3.3.1 Arguments

None. Command executes immediately.

3.4 File > Display > HKLs • Overlay predicted HKL pattern on the display

Menu Command: File > Display > HKLs

Accelerator: None

User Level: 2

SLAM Syntax: DISPLAY /HKL $1 $2 $3

These commands allow you to draw an overlay of predicted spot positions onto a displayed frame.

The /OVERLAY option in File > Display also allows you to automatically display the overlay every time a new frame is displayed. The overlay is computed from the current orientation matrix (from the last Peaks > Refl. Array > LeastSq command) and takes into account any lattice centering determined in Peaks > Refl. Array > Bravais. You can draw overlays on magnified frames by entering the desired magnification and center in the File > Display dialog when the image is displayed (the Edit > Zoom command does not redraw or magnify graphic overlays).

3.4.1 Arguments

File > Display > HKLs draws an overlay on the currently displayed frame according to three input arguments. Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Spread) [0.75]

Width in degrees of the predicted pattern. Default is 0.75.

$2 ..... (Lineweight) [1]

Line thickness used for drawing the overlay markers. The drawing routine will constrain the input value to be from 1 to 3. Default is 1.

$3 ..... (Scan Angle) [-9999]

Starting scan angle for pattern prediction, in degrees. The special value -9999 (the default) directs the program to obtain the starting angle from the currently displayed frame. The signed frame width and scan axis (omega or phi) are always obtained from the currently displayed frame. The scan angle range covered by the predicted pattern will be from A1 to A2 calculated as follows:

FRAME_CENTER = SCAN_ANGLE + FRAME_WIDTH/2.

A1 = FRAME_CENTER - SPREAD/2

A2 = FRAME_CENTER + SPREAD/2

The /OVERLAY option in File > Display, when set, directs the program to draw an overlay automatically every time a frame is displayed. The parameters given in the File > Display > HKLs input dialog are used for these automatic overlays as well.

Three types of marker characters are used to indicate the difference between the scan angle corresponding to the centroid of the displayed frame (that is, FRAME_CENTER above) and the predicted scan angle of a reflection.

Predicted Scan Angle	Marker
Within scan range of the current frame	Box
Within scan range of a preceding frame	Circle
Within scan range of a subsequent frame	Cross (X)

The circle and cross can be thought of as the tip and tail of an arrow which points from the current frame to the predicted position, assuming a stack of frames with earlier frames positioned in front of the screen and subsequent frames positioned further into the screen.

3.5 File > Display > Next Run and File > Display > Prev Run

Menu Command: File > Display > Next Run, File > Display > Prev Run

Accelerator: Ctrl+Shift+RightArror (next) Ctrl+Shift+LeftArrow (previous)

User Level: 1

SLAM Syntax: DISPLAY /RNEXT DISPLAY /RPREV

These commands are identical to the File > Display > Next/Prev commands, except that it steps through the run number instead of the frame number.

3.6 File > Display > Movie+ Run and File > Display > Movie- Run

Menu Command: File > Display > Movie+ Run, File > Display > Movie- Run

Accelerator: Ctrl+Shift+UpArror (moview+) Ctrl+Shift+DownArrow (movie-)

User Level: 1

SLAM Syntax: DISPLAY /RMOVIE+ DISPLAY / RMOVIEW-

These commands are identical to the File > Display > Movie +/- commands, except that it steps through the run number instead of the frame number.

3.7 File > Load • Read a frame from disk into frame accumulation memory

Menu Command: File > Load

Accelerator: Ctrl+O

User Level: 1

SLAM Syntax: LOAD $1 $2 /DISPLAY=<n> /SCALE=<n> /OFFSET=<n> /LOGSCALE /USE_CONFIG

The File > Load command copies a data frame from a disk into the 32-bit frame accumulation memory for display and evaluation. The image is also displayed on the screen. You can optionally form a linear combination of two frames, displaying the result. File > Load, followed by a File > Save command, can also be used to convert a frame between the XENGEN 1.3 and Bruker formats, or to replace values in a frame header with the current values in the Edit > Configure panels.

When invoked from the menu or from the command line without arguments, File > Load displays a dialog box where you can view/edit the items described below. If you press ENTER or click the OK button, the load operation starts. Pressing ESC or the Cancel button returns you to the menu without performing the operation.

File > Load is closely related to the File > Display. Typically, File > Display is used much more often than File > Load, since it provides a more

flexible set of display options, for example, for displaying sequential frames in a series or multiple frames in quadrants. However, only File > Load contains options for combining frames and modifying frame headers.

3.7.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input Filename) [no default]

This is the name of the file to be read from disk, or of the first file (of two) to be read when performing a linear combination. The special name $FRAME can be used here to indicate that the first data set in a linear combination is to be the data currently residing in frame accumulation memory, for example, from the last Collect > Add command. If you leave this item blank, or specify a “wildcard” filename pattern, pressing ENTER or clicking the OK button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or clicking OK. You will be returned to the File > Load dialog with the selected filename filled in. If you leave this item blank, it is the same as entering a *.* wildcard pattern. Remember that both filenames and patterns entered here are merged with the project’s working directory.

$2 ..... (Background Filename) [$NULL]

This is the name of a second frame file to be read from disk and linearly combined with the first according to the scale and offset described below. If you leave this field blank, or supply the special name $NULL, only the first file above is read in, and no linear combination is performed. In order to run File > Load without intervention from a command script, you must supply this second filename, and must therefore specify $NULL if you want to load single frame from the command line without intervention. Default is $NULL.

/DISPLAY=<n> ..... (Maximum Display Counts) [-1]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -1; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image

look brighter; larger values make look darker.

/SCALE=<n>.....(Scale Factor) [+n]

If you supply a second filename for the $2 argument described above, the two files are combined pixel-by-pixel according to the equation:

P0 = P1 + P2 * A + B

where P0 is the pixel value in the resulting frame, P1 and P2 are the pixel values in the first and second input frames, A is the scale factor supplied here, and B is the offset, described below. Any resulting P0 values less than zero are clipped to zero. A positive scale factor results in a weighted addition of the two frames while a negative scale factor results in a weighted subtraction of frame 2 from frame 1. If instead of supplying a numeric value for the scale factor, you supply the special characters “+n” or “-n”, the program weights the addition or subtraction according to the acquisition time ratio between the two frames. That is, a value of +n results in a scale factor of t1/t2, and -n results in a scale of -t1/t2, where t1 and t2 are the respective acquisition times of frame 1 and frame 2.

/OFFSET=<n>..... (Offset) [0]

Offset to be added prior to clipping negative values to zero. This corresponds to “B” in the equation given in the scale factor description above. This allows you to quantitatively assess signed differences between two frames. The DIFFER.LUT color table can be useful for viewing signed differences.

While the linear combination capability is useful primarily for background subtraction in general diffraction applications, you can also use it to sum a series of frames to form an oscillation picture. For example, the following SLAM commands generated a sum of 8 myoglobin frames. Note the increase in display level as the sum grows larger:

```
!
! Make oscillation picture from 8 myoglobin frames
!
LOAD swmyo1.002 swmyo1.003 /DISPLAY=32 /SCALE=1.0 /OFFSET=0.0
LOAD $FRAME swmyo1.004 /DISPLAY=64 /SCALE=1.0 /OFFSET=0.0
LOAD $FRAME swmyo1.005 /DISPLAY=96 /SCALE=1.0 /OFFSET=0.0
LOAD $FRAME swmyo1.006 /DISPLAY=128 /SCALE=1.0 /OFFSET=0.0
LOAD $FRAME swmyo1.007 /DISPLAY=160 /SCALE=1.0 /OFFSET=0.0
LOAD $FRAME swmyo1.008 /DISPLAY=192 /SCALE=1.0 /OFFSET=0.0
LOAD $FRAME swmyo1.009 /DISPLAY=224 /SCALE=1.0 /OFFSET=0.0
```

/LOGSCALE.....(Log Scale?) [No]

If checked in the dialog box, or given as /LOGSCALE, the frame image is displayed using a logrithmic scale. By default it is unchecked.

/USE_CONFIG.....(Merge Config into Header?) [No]

If checked in the dialog box, or given as /USE_CONFIG on the command line, this qualifier replaces the following frame header items with the values currently in the Edit > Config dialog. This option always defaults to N (unchecked), regardless of the previous setting.

Header Item	CONFIGURE/EDIT Prompt
USER	User name
DISTANCE	Sample-detector distance
LOWTEMP	Low temp device? (Y/N)
TARGET	X-ray target material
WAVELENGTHS	X-ray source wavelength
SOURCEKV	Source kilovolts
SOURCEMA	Source milliamps
FILTER	Filter / monochromator
CENTER	Direct beam X, Direct beam Y
LUT	Color table filename

You can use this option to update frame header values, then use SAVE to save the frame with the new values. For example, if you took a brass plate image at 18 cm, but the Edit > Config dialog contained the wrong distance, you could avoid having to retake the image as follows:

1. Correct the distance in Edit > Config > User settings.
2. Read in the brass plate with LOAD /USE_CONFIG (or with this option checked in the File > Load input panel).
3. Use File > Save to save the brass plate (so that the disk file is also modified).
4. Use Process > Spatial > Process to compute the spatial correction with the correct distance.

3.8 File > Save • Save a new detector frame to a disk file

Menu Command: File > Save

Accelerator: Ctrl+S

User Level: 1

SLAM Syntax:

SAVE $1 /TITLE=<s> /XENGEN /DISPLAY=<n>

This command copies a data frame from the frame accumulation memory to a specified disk file disk for retention. In the process, it allows you to specify the file format and a title (up to 72 characters) to display with the data frame. (This title is stored in the output frame header.)

The data to be saved must exist in the 32-bit frame accumulation memory. A frame currently displayed as a result of a File > Display, File > Load, Collect Menu, or Process > Spatial > New command can be saved. A few commands will destroy the contents of the accumulation memory. If you need to save a data frame, do so before issuing one of these (destructive) commands:

Edit > Clear (if data/image memory is cleared)

Peaks > Refl. Array > Threshold

If you try to save data that has been overwritten by one of these commands, the program displays a box with the message:

DETECTOR DATA NOT YET TAKEN OR OVERWRITTEN

Because File > Save allows you to write a frame in either Bruker or XENGEN 1.3 format, you can use it to convert a frame from one format to the other. For example, you can use File > Load to read in a Bruker-format frame, followed by SAVE with the XENGEN-format option set to convert a frame from Bruker to XENGEN format. This option is rarely used.

When invoked from the menu, or run from the command line without arguments, File > Save displays a dialog box where you can view/edit the arguments described below. Pressing the ENTER key or clicking the OK button starts the operation. Pressing ESC or the Cancel button returns you to the menu. Upon saving, the program displays the message “SAVING...” on the bottom status line. Saving should be completed within a few seconds. If the output filename starts with the five characters $NULL (case-independent), the output is sent to the null handler and discarded.

If the output file already exists, you are prompted as to whether or not you want to overwrite the file.

3.8.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Output Filename)
[no default]

Enter filename for output frame, the default extension is *.gfrm, unless the old frame naming conventions are being used. The output filename is merged with the frame data directory in the Project > New dialog box. If the output filename starts with the five characters $NULL (case-independent), the output is sent to the null handler (i.e., is thrown away). Note: The special “$NET” is no longer supported by GADDS.

/TITLE=<s> .....(Title) [$TITLE]

Enter title for output frame (72 characters maximum). If you're invoking File > Save from the command line, you must enclose titles containing imbedded blanks in double quotes. The special “$TITLE” will default the title to the current title string. The default is “$TITLE”.

$FILE:<filename> will read up to eight 72 character title lines from an ASCII file and place these title strings into the eight “TITLE” lines in the frame header. The format of the ASCII file is: “R#:<single line of title information>”, where “R#” is the run number, taken from the filename. Repeat up to eight times for each run.

/XENGEN ..... (Xengen Format? (Y/N))
[No]

Check this option to write frame in XENGEN 1.3 (more correctly, in the old PCS computer format). The default is unchecked (Bruker format). This option is rarely used. By default it is unchecked.

/DISPLAY=<n> ..... (Max Displayed Counts)
[0]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -0; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image look brighter; larger values make look darker.

3.9 File > Logfile • Create a new log file and start recording

Menu Command:

File > Logfile

File > Logfile > Enabled

Accelerator: None

User Level: 1

SLAM Syntax:

LOGFILE /NEW $1 /APPEND
LOGFILE [/ON | /OFF]

The File > LogFile commands are used to maintain a record of all of a user's interaction with the system. This record is referred to as the “log file” or “logfile.” Logfiles are standard ASCII text files that can be typed, edited, printed, etc. like any other text file. When you start recording to a log file, you have the option of appending to the file or overwriting it if it already exists.

The File > LogFile > Enabled command toggles the current state of recording to the log file. If logging is enabled, the command disables it. If logging is disabled, the command re-enables it. A check mark is displayed in the menu next to the File > LogFile > Enabled command if logging is currently enabled. From the SLAM command line, LOGFILE /ON and LOGFILE /OFF enable and disable scripting, respectively.

The log file records each command issued, along with its parameter values, a date/time stamp, and any non-graphic command output. For example, the cursor commands write the statistics at the final cursor position to the log file, Analyze > Cursor writes a copy of any 17 x 17 pixel dumps, Process > Stress > Biaxial2D writes a copy of the contents of its scrollable output window, etc. Commands and output are added to the log file until the File > LogFile > Enabled option is turned off or the user switches projects, which will automatically close any open log file.

The File > LogFile > Enabled command does not actually close the log file; it just tells the program to temporarily stop writing output to the file. If you need to access the current log file in another process while GADDS is still running, for example to edit it from another window, you should close the file first. You can close the log file by running File > LogFile with another filename. The program will close the current file before starting a new one.

An example of a log file output for a CURSORS / PIXEL command is:

```
!=====================================================
!11/22/91   15:49:03
CURSORS
      $1=435
      $2=190
      /DUMP=N
      /DELAY=0.0
      /NOERASE=N
!>
!> PIXEL Statistics:  SAXI$TEST:swmyo1.005 11/22/91  15:49:36
!> Xraw, Yraw, Counts:        139       311       596
!> X, Y (Unwarped):        142.68    309.13
!> X, Y (XENGEN):             372       200
!> DX, DY:                -113.00     66.52
!> 2-Theta, Angstroms:     21.333     4.165
!> HKL:                     20.97    -10.98     -2.97
```

Different types of output lines are prefixed with character sequences that make the types easier to separate with editors, text filters, etc. Lines that do not contain command information are prefixed with the comment character “!”. Lines that contain command output are prefixed with “!>”. Note that the cursor was at X,Y = (435,190) when the command started, but the user moved the cursor to a final position of (139,311) before exiting the command.

With scripting enabled, the same command produced the following output script file, containing just one line:

```
CURSORS /PIXEL 139 311 /DELAY=0.0
```

3.9.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its input panel prompt in parentheses:

$1 .....(Log Filename) [frame._lg]

Filename of the log file to which output is directed. By convention, log files have the extension ._lg. If you don't supply a filename extension, the program will add the ._lg extension. If you leave this item blank, or specify a “wildcard” filename pattern, pressing ENTER or clicking the OK button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or clicking the OK button. You will be returned to the File > LogFile dialog with the selected filename filled in. If you leave this item blank, it is the same as entering a *._lg wildcard pattern.

/APPEND .....(Append?) [Yes]

If you check this option, output will be appended to the log file if the file already exists. If the option is unchecked (that is, missing from the command line or unchecked in the dialog box), the output file is overwritten if it already exists.

3.10 File > Scriptfile • Create a new script file and start recording

Menu Command:

File > Scriptfile
File > Scriptfile > Enabled

Accelerator: None

User Level: 2

SLAM Syntax:

LOGFILE /SCRNEW $1 /APPEND
LOGFILE [/SCRON | SCROFF]

File > ScriptFile lets you create/record a script (containing a list of one or more GADDS commands in SLAM format that execute sequentially as a group) as you interactively invoke the commands of your choice. SLAM stands for “Scripting Lexical Analyzer and Monitor” and is the command language used by most Bruker programs. (See more details below under “Command and Script File Conventions” and “@Command.”)

The File > ScriptFile > Enabled command toggles the current state of recording to the script file. If scripting is enabled, the command disables it. If scripting is disabled, the command reenables it. A check mark displays in the menu next to the File > ScriptFile > Enabled command if scripting is currently enabled. From the SLAM command line, LOGFILE /SCRON and LOGFILE /SCROFF enable and disable scripting, respectively.

The File > ScriptFile command can be used to build script files automatically. To do so, toggle the script feature on and operate the system using the exact sequence of commands that you want to appear in the script. To end the script, toggle the scripting feature off. To execute a script file, issue the command “@<filename>” from the GADDS command line, where <filename> represents the name you gave the script file. If you attempt to play back a script just recorded before exiting and restarting GADDS, you must invoke File > ScriptFile with another filename to close the script file before starting playback. File > ScriptFile > Enabled does not close the script file. It only disables recording. For the same reason, in order to access a script file from another process, you should close the script file.

3.10.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Script Filename) [script.slm]

Filename of the script file to which output is directed. By convention script files have the extension *.slm. If you don't supply a filename extension, the program will add the .slm extension. If you leave this item blank, or specify a “wildcard” filename pattern,

pressing ENTER or clicking the OK button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or clicking the OK button. You will be returned to the File > ScrFile dialog with the selected filename filled in. If you leave this item blank, it is the same as entering a *.slm wildcard pattern.

/APPEND .....(Append?) [Yes]

If this option is checked, output will be appended to the script file if the file already exists. If the option is unchecked (that is, missing from the command line or unchecked in the dialog box), the output file is overwritten if it already exists.

3.11 File > Print • Dump screen to printer device or file

Menu Command: File > Print

Accelerator: Ctrl+P

User Level: 1

SLAM Syntax: PRINT $1 /FORMAT=<n> /THRESHOLD=<n> /GREYSCALE

This command prints a copy of the data currently loaded into memory (or on the display) on a designated printer, or to a disk file for later transfer to a printer or into a word processor program.

Under NT, a special “native” format is available to specify using the native operation system's printer drivers. Text and border lines are printed in black, while the frame image is printed in either colors or gray-tones, depending on the selected printer device.

During printing, the black/white or grayscale of the image is approximated by the printer by assigning a minimum threshold for black and then using either white below that value or printing a 25% level grayscale in landscape format. Color scale plots ignore the threshold value and print the screen in 16 colors.

When invoked from the menu, or from the command line without arguments, File > Print displays a dialog box where you can view/edit the following items before performing the print operation. If you press ENTER or click the OK button, printing begins. Pressing ESC or the Cancel button returns you to the menu. Use CTRL+BREAK to interrupt printing in progress.

You can also print the current display screen from just about anywhere in the program by pressing CTRL+P, allowing you to plot screens containing menus, input panels, etc. Don't use CTRL+P during real-time data collection. Timing of real-time operations could be compromised. The parameters on the PRINT input panel affect CTRL+P screen dumps the same way as PRINT command screen dumps. Note: Under NT, the CTRL+P option does not work when GADDS is in either a menu panel or a message box.

3.11.1 Arguments

Each option is listed below by its SLAM command line name, followed by its dialog panel prompt in parentheses:

$1……(Output Device or Filename) [$default]

Enter either the filename or device which is to receive the printout. The default device is SAXI$PRINTER, which you can define as a logical name to point to a file or device if desired. For example, the DOS command SET SAXI$PRINTER=PRN would direct output to a parallel printer. Alternatively, you can just enter the output name directly in the input panel (for example, PRN). If you specify a filename, the system “prints to disk”

creating a file with that filename on the system hard disk which may later be output directly to a printer without having to run GADDS. Under DOS, a command like COPY /B <filename> PRN would copy your output file to a parallel LaserJet printer.

NOTE: You cannot print to a disk file if you use the Native format option.

Under NT, the GADDS printer device is often different than the default print device. Thus it is a good idea to create an unique GADDS print queue with your favorite printer settings and set the environment variable SAXI$PRINTER equal to the “Printer name”. Printing to SAXI$PRINTER will proceed without user intervention. Printing to “$DEFAULT” will default to the NT default printer, but will always display the Print Setup dialog box.

/FORMAT=<n> .....(Format) [-1 native]

Enter the desired output format of the print data. Interactively under NT, valid formats are “native”, “BMP”, “TIFF-color”, “TIFF-grey”, “PostScript-color”, and “PostScript-grey”. Native refers to the native operating system drivers for printers.

In addition to the native NT support, the program supports embedded drivers for certain printers and file formats:

Format	Description
-1	Native NT driver. (default value)
0	PCL4 printers, such as the HP LaserJets.
1	Monochrome TIFF files.
2	Monochrome PostScript files and printers
3	PCL4 color printers, that is, HP PaintJets.
4	Color PostScript Level 2 files and printers, that is, Tektronix Phaser II and HP1200C-PS
5	Color TIFF files.
6	BMP files.
7	Codonics printer.

TIFF and BMP files are printed in portrait orientation, while all other output formats use landscape orientation to make maximum use of the page.

/THRESHOLD=<n>…(Threshold) [16]

Specifies the minimum number of counts to be plotted as black. Higher thresholds cause the printout to look less black; lower thresholds cause it to look more black. Threshold is ignored for color plots.

/GREYSCALE ..... (Highest Resolution) [Yes]

For PCL5 printers, specifies that any counts at or above the threshold are black. Counts between zero and the threshold are printed in a 25% greytone. If absent on the com-

mand line or specified as “N” in the input panel, all counts below the threshold are printed as white.

For color PCL4 printers, specifies to print using 16 colors. If absent on the command line or specified as “N” in the input panel, prints in black/white with all counts below the threshold printed as white. Colors are approximated with the nearest RGB printable color (see your PaintJet manual). For this reason, some greytones are printed in either brown, olive, green, or pink colors.

For PostScript printers, specifies to print using 16 greyscales (FORMAT=2) or 256-colors (FORMAT=4). If absent on the command line or specified as “N” in the input panel, prints in black/white (FORMAT=2) or 16-colors (FORMAT=4).

TIFF files behave similar to monochrome PostScript printers. A “Y” specifies 16 greyscales while “N” signifies black and white TIFF file.

NOTE: To preview a print file without actually printing the file, load the color lookup table with PRINT.LUT (in the Edit > Config > Colors panel), which displays the frame in reverse black/white greyscale.

---

4. Edit Routines

4.1 Edit > Configure > User settings • Edit the current user configuration settings

Menu Command: Edit > Configure > User settings

Accelerator: Ctrl+C

User Level: 1(view/edit), 3 (full edit)

SLAM Syntax:

```
CONFIGURE /EDIT /USER=<s>
/SITE=<s> /CALIBDIR=<s>
/MINCPS=<n> /TIMEOUT=<n>
/NAMECHAR=<n> /RUNCHARS=<n>
/RUNBASE=<n> /NUMCHARS=<n>
/NUMBASE=<n> /LOWTEMP
/TEMP=<n> /XBEAM=<n> /YBEAM=<n>
/FRAMESIZE=<n> /DISTANCE=<n>
```

Edit > Configure > User settings displays a dialog box where you can view/edit certain general setup variables, including the current sample-to-detector distance, beam center coordinates, default calibration data directory, and frame naming conventions. Unless you are the GADDS Administrator, some fields are only viewable: calibration directory, beam center, and detector distance. To change a view-only field, see your GADDS Administrator.

4.1.1 Frame Naming Parameters

Several qualifiers (NAMECHARS, RUNCHARS, RUNBASE, NUMCHARS, NUMBASE) comprise the convention GADDS uses for generating a series of sequential frame names. These naming parameters are used by the Collect > Scan > SingleRun, MultiRun, etc. commands (which collect one or more series of frames), and by File > Display (which can display a frame series in sequence). Thus, to display a series of frames, the naming parameters must be set

appropriately, to match those in effect when the frames were written.

New conventions:

The filename is created with the jobname, an underscore, the run number, an underscore, and then the frame number. Prior to concatenation, the Run # and Frame # are expanded (with leading zeros if required) to the number of characters specified by the Runchars and Numchars parameters. The file extension is .gfrm. For your convenience, GADDS generates and displays an example filename using the current settings.

Old conventions:

If SAXI$OLDNAMES is set, the Run # is appended directly to the Job Name, then the Frame # is added as the filename extension (it is concatenated after pre-pending a dot). Prior to concatenation, the Run # and Frame # are expanded (with leading zeros if required) to the number of characters specified by the Runchars and Numchars parameters. For your convenience, GADDS generates and displays an example filename using the current settings.

4.1.2 Sample-to-Detector Distance and Beam Center Measurement

Your GADDS Administrator should follow the "269-0223xx Detector Distance and Beam Center Calibration for GADDS" procedure (see GADDS Administrator's Manual), to define the true detector distance and beam center parameters. In general, the beam center is stable over long periods of time. However, if you replace or realign the X-ray tube, or realign the goniometer, your GADDS Administrator should repeat this procedure.

NOTE: To process frames collected before these settings were properly set, see the /Use_config argument in Section 3.7.

When you change the detector distance in menu mode, you will be prompted with "Reset to default collision limits for new distance?". Enter "Y" and GADDS will read the default collision limits for 2θ and ω-2θ from the file: GADD$SYSTEM:limits.d (see Collect > Goniometer > Limits, Section 5.15 for more details).

When you change the low temp flag in menu mode on P4 systems, you are informed to set your new collision limits for ω and χ under Collect > Goniometer > Limits (see Section 5.15). Otherwise, you might break your expensive glassware.

4.1.3 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

/USER=<s>.....(User Name) [SAXI$USERNAME]

Enter the user name (default is UNKNOWN). If you define the environment variable SAXI$USERNAME, its translation will be taken as the default value. The name you supply will be stored in the header of any output frames created in Bruker (the normal) format, and in output .p4p files.

/SITE=<s>.....(Site) [SAXI$SITE]

Enter the site name (default is UNKNOWN). If you define the environment variable SAXI$SITE, its translation will be taken as the default value. The name you supply will be stored in the header of any output frames created in Bruker (the normal) format, and in output .p4p files.

/CALIBDIR=<s> ....(Calibration Data Directory) [GADDS$CALIB:]

The directory where calibration data are to be stored, such as flood field and spatial correction files. The default is “GADDS$CALIB:”, which is an environment variable that usually translates to D:\FRAMES\CALIB\. The special symbol, “*:”, means the current directory.

/MINCPS=<n>..... (Minimum Counts per Second) [25]

Enter the minimum counts per seconds on scan frames. Frames collected with fewer cps are automatically recollected up to 3 times. This allows correcting stuck shutter problems. The default is 25 cps. This is automatically deactivated for frames of ten minutes or longer.

/TIMEOUT=<n>.... (Auto/Command Mode Timeout) [10]

Enter the number of seconds that you want the program to wait before proceeding when a prompt or output window displays in SLAM command-line mode. The default is 10 seconds and the valid input range is 0 to 1,000,000 seconds. A value of 0 means no time-out (infinite wait).

/NAMECHARS=<n>…(Characters in Base Frame Name) [28]

The maximum number of characters which can be used in the “base” component of a frame filename. The base component is defined as the filename after removing any node, device, directory, extension, and version components. NAMECHARS should be set to 8 for NT-FAT filenames, or 39 for NT-enhanced FAT or NTFS (or UNIX) filenames. The default is 28.

/RUNCHARS=<n>…(Characters in Run #) [1]

This is the number of characters to be appended to the Job Name as a Set Number or Run Number (that is, the number assigned to a series of frames taken at the same phi,chi setting). The Run Number is padded with leading zeros, if needed to fill RUNCHARS characters; it is not automatically incremented within a scan series unless the Frame Number overflows. It *is* automatically incremented, however, when setting up an EDITRUNS array inside ASTRO. RUNCHARS can usually be left at the default value of 1; however, if you're performing more than RUNBASE runs, make sure that you set RUNCHARS to 2 to prevent wrap-around of the Run Number, otherwise earlier scans could be overwritten by later ones! For example, if RUNCHARS is set to 1 and RUNBASE is 10 (instead of the default value of 36), a Run Number of 10 in the EDITRUNS array will result in a Run Number of 0 in the output filename.

/RUNBASE=<n>…(Base of Run #) [36]

The numeric base of the Run Number. The value must be 10 or 36. If the base is 10, a carry out of each digit is produced when the digit is incremented from a value of 9, and the digit is reset to zero. If the base is 36, the digit is incremented from 9 to A, then to B, etc. A carry is produced when the digit reaches Z, and the digit is reset to zero. RUNBASE should usually be left at the default value of 36.

/NUMCHARS=<n>…(Character in Frame #) [3]

The number of characters to be appended to the filename as an extension representing the number of the frame in the current series. The number is padded with leading zeros if needed to fill NUMCHARS characters. This Frame Number is automatically incremented by one after each frame is collected during an Acquire > SingleRun, MultiRun, Hemisphere, Quadrant, or Matrix command. This value should be left at its default setting of 3 if you're collecting to a FAT-16 formatted disk partition.

A special case occurs when NUMBASE (see below) is set to 10 (the default); the most significant digit only is treated as base-36. Thus, the frame number following .999 will be .a00. This special case allows up to 3600 frames in a series when NUMBASE=10, while maintaining the DOS 8/3 filename convention.

/NUMBASE=<n>…(Base of Frame #) [10]

This value represents the numeric base to be used for the frame number; like RUNBASE, NUMBASE must be 10 or 36. When NUMBASE is 10, the most significant digit in the Frame Number is still treated as base 36, as described above under NUMCHARS.

Base 10 is easier to interpret, but limits the number of frames in a run to 3600 under DOS, which allows, at most, 3 characters in the extension. Base 36 allows a larger number (36^3) of frames per run under DOS. This parameter should usually be left at its default of 10, unless you're performing scans which require single sweeps of more than 3600 frames.

/LOWTEMP.....(Low Temp Device (Y/N) ?) [No]

Check this box if the LT-2 low-temperature device is installed. Specify "N" here (or omit the qualifier in command-line mode) if no low temperature device is installed. This value is stored in the header of output Bruker-format frames. If you enter "Y", GADDS fixes omega at 345° for optical alignment on a 4-circle goniometer (see the Collect > Goniom > Optical command). In addition, during data collection, GADDS rotates phi back and forth by 170° every few frames to help reduce possible sample icing.

/TEMP=<n>.....(Current Temperature) [-1]

Enter current temperature in degrees K (-1 = room temperature or unknown, default value). The Collect > Goniometer > Temperature command (see Section 5.28) can also be used to define this parameter.

/XBEAM=<n> ..... (Direct Beam X) [current value]

Unwarped X-pixel coordinate (0 to frame-size-1) of direct beam center at 2-Theta = 0, in the Bruker coordinate convention with (0,0) at the lower left of a displayed frame. It is important that you enter the correct value here before collecting frames that will be analyzed with the interactive cursor commands used in conjunction with the spatial correction or for determination of crystal orientation with the Reflection Array commands. These commands rely heavily on the value given for the beam center. The value is stored in the output header of Bruker-format frames and in output .p4p files. If you change the value of the FRAMESIZE field, the beam center position will be scaled and converted to the new frame size convention; the display will be updated when you tab out of the FRAMESIZE field.

NOTE: If you save frames in raw (warped) mode, this should be raw X-pixel coordinate.

/YBEAM=<n> ..... (Direct Beam Y) [current value]

Unwarped Y-pixel coordinate (0 to frame-size-1) of direct beam center at 2-Theta = 0, in the Bruker coordinate convention with (0,0) at the lower left of a displayed frame. It is important that you enter the correct value

here before collecting frames that will be analyzed with the interactive cursor commands used in conjunction with the spatial correction or for determination of crystal orientation with the Reflection Array commands. These commands rely heavily on the value given for the beam center. The value is stored in the output header of Bruker-format frames and in output .p4p files. If you change the value of the FRAMESIZE field, the beam center position will be scaled and converted to the new frame size convention; the display will be updated when you tab out of the FRAMESIZE field.

NOTE: If you save frames in raw (warped) mode, this should be raw Y-pixel coordinate.

/FRAMESIZE=<n>…(Size of Created Frames) [1024]

Enter the linear frame dimension (512 or 1024) for newly created frames. Subsequent frames created by commands in the Collect menu will have this size. If you change the value of the FRAMESIZE field, the beam center position will be scaled and converted to the new frame size convention; the display will be updated when you tab out of the FRAMESIZE field. Storage requirements per 512 x 512 frames range from 256K bytes (8 bits per pixel) to 1 Mbyte (32 bits per pixel). GADDS automatically compresses frames; this compression results in no data loss and usually results in storage close to 256K bytes, or close to 512K bytes if enough diffraction lines are high enough that it cannot be contained in 8 bits/pixel. 1024 x 1024 frames require four times this amount of storage. Acquiring and processing larger frames is slower, but will improve integration results, so it is highly recommended to use 1024 frames for power diffraction work.

/DISTANCE=<n>…(Sample-Detector Distance) [current value]

Enter current nominal sample-to-detector distance in centimeters. The default setting is 12.00 cm. It is important that you enter the correct value here whenever you change the detector distance. The value is stored in the header of any output frames created in Bruker format, and is used by the flood-field and spatial corrections, the interactive cursor commands, integration commands, and all the Reflection Array commands that deal with crystal orientation. The distance is also written to output .p4p files.

On systems with a motorized delta axis, use the Collect > Goniometer > Det. Stage command to move the detector distance.

4.2 Edit > Configure > Admin settings • View/edit the current administrator configuration settings

Menu Command: Edit > Configure > Admin settings

Accelerator: None

User Level: 2 (view), 3 (edit)

SLAM Syntax:

CONFIGURE /ADMIN /TARGET=<s>
/WAVELENGTH=<n> /ALPHA1=<n>
/ALPHA2=<n> /BETA=<n> /UNITS=<s>
/KV=<n> /MA=<n> /STANDBYKV=<n>
/STANDBYMA=<n>
/STANDBYIDLETIME=<n>
/STANDBYNOEXCLUDE
/MONOCHROMATOR=<s>
/OFFSET=<n>

Edit > Configure > Admin settings displays a dialog box where you can view/edit certain instrumental setup variables, including the x-ray source, generator, and optics. Unless you are the GADDS Administrator, all fields are only viewable. To change a view-only field, see your GADDS Administrator.

Whenever a GADDS configuration file is read (starting GADDS, switching projects, etc.), the program checks the Preferred generator settings against the current settings and if different, displays the message:

Warning: Current high-voltage generator settings are different than user values.

When you invoke a command from the menu (or the command line without arguments), a dialog box appears. View or edit its contents (or type text). Then:

- Press ENTER or click the OK button to save your entry.
- Press ESC or click the Cancel button to return to the menu without saving your last entry.

4.2.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

/TARGET=<s> ..... (X-ray Target Material) [Cu]

Enter the standard 2-letter chemical symbol for the source target material (Cu, Mo, etc.), if applicable. Otherwise enter a short description of the radiation source. The default target selection is Cu. If you enter one of the recognized target types (Cu, Mo, Ag, Fe, Cr, or Co), the X-ray wavelengths in the following fields will be updated automatically. The value is stored in the header of output Bruker-format frames and in output .p4p files.

/WAVELENGTH=<n>…(X-ray Source Wavelength) [1.541838]

Enter the weighted-average X-ray wavelength in Angstroms. The default value is based on the default target (Cu) and is set at 1.541838 Å. This value is automatically updated when the target is re-entered if the target is one of the known types (Cu, Mo, Ag, Fe, Cr, or Co). It is important that you update this entry whenever the source wavelength is changed. The value is stored in the header of any output frames created in Bruker format and in output .p4p files. It is also used by the interactive cursor commands, all the Reflection Array commands that deal with crystal orientation, Peaks commands, and Stress commands.

/ALPHA1=<n> .....(Alpha-1) [1.54056]

Enter the Ka1 X-ray wavelength in Angstroms. The default value is based on the default target (Cu) and is set at 1.54056 Å. This value is automatically updated when the target is re-entered if the target is one of the known types (Cu, Mo, Ag, Fe, Cr, or Co). It is important that you update this entry whenever the source wavelength is changed. The value is stored in the header of any output frames created in Bruker format and in output .raw files. It is also used by the interactive cursor commands, all the Peaks commands, and the Stress commands.

/ALPHA2=<n> ..... (Alpha-2) [1.54439]

Enter the Ka2 X-ray wavelength in Angstroms. The default value is based on the default target (Cu) and is set at 1.54439 Å. This value is automatically updated when the target is re-entered if the target is one of the known types (Cu, Mo, Ag, Fe, Cr, or Co). It is important that you update this entry whenever the source wavelength is changed. The value is stored in the header of any output frames created in Bruker format and in output .raw files. It is also used by the interactive cursor commands, all the Peaks commands, and the Stress commands.

/BETA=<n> ..... (Beta) [1.39222]

Enter the Kb X-ray wavelength in Angstroms. The default value is based on the default target (Cu) and is set at 1.39222 Å. This value is automatically updated when the target is re-entered if the target is one of the known types (Cu, Mo, Ag, Fe, Cr, or Co). It is important that you update this entry whenever the source wavelength is changed. The value is stored in the header of any output frames created in Bruker format and in output .raw files. It is also used by the interactive cursor commands and all the Peaks commands.

/UNITS=<s> .....(Units) [angstroms]

Enter the wavelength units as either Angstroms (conventional and US standard) or nanometers (new European standard). The default value is Angstroms. This value only affects displaying wavelengths within the GADDS program. All wavelengths within data files are always stored in Angstroms.

/KV=<n> .....(Preferred Settings: Voltage) [50]

Enter the preferred X-ray generator kV setting (default is 50 kV). This value is stored in output .p4p and .raw files and in the header of output Bruker-format frames. If you use Goniom > Generator to set the X-ray generator voltage, this value will default to the current generator setting.

/MA=<n> .....(Preferred Settings: Current) [40]

Enter the preferred X-ray generator milliamps setting (default is 40 ma). This value is stored in output .p4p and .raw files and in the header of output Bruker-format frames. If you use Goniom > Generator to set the X-ray generator current, this value will default to the current generator setting.

/STANDBYKV=<n>…(Standby settings: Voltage) [20]

Enter the standby X-ray generator kV setting (default is 20 kV). GADDS will automatically reduce the generator settings to standby mode whenever the program has been idle for 10 minutes and the time is not between 8a.m. and 5 p.m. on a weekday. (This feature fails after 16-Jan-2038).

/STANDBYMA=<n>…(Standby settings: Current) [5]

Enter the standby X-ray generator milliamps setting (default is 5 ma). See above /STANDBYKV.

/STANDBYIDLETIME=<n>…(Standby settings: Idle time) [30 min]

Enter the standby idle time after which the generator is set to standby values.

/STANDBYNOEXCLUDE…(Standby settings: Don't exclude weekdays 8AM to 5 PM) [No]

Check “Y” to allow standby to occur during normal working hours.

/MONOCHROMATOR=<s>…(Filter / Monochromator) [parallel, graphite]

Enter a short description of filter or monochromator (default is “parallel, graphite”). Currently this value has no effect on the operation of the program, but it is stored in the header of output Bruker-format frames.

/OFFSET=<n>..... (2-Theta Offset) [0.0]

This only affects dual detector systems. On Master frame buffer, enter 0.0. On Slave

frame buffer, enter the slave's detector 2θ offset in degrees from the goniometer's 2θ setting.

4.3 Edit > Configure > Read • Read a new configuration from a disk file

Menu Command: Edit > Configure > Read

Accelerator: None

User Level: 2

SLAM Syntax: CONFIGURE /READ $1

Use this command to restore current program settings from a specified disk file. These configuration files, which have file extensions of ._nc, contain the current flood file correction, spatial correction, and current values of nearly all input panel items for nearly all the GADDS commands (a few exceptions).

4.3.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1……..(Configuration Filename) [gadds._nc]

Enter the filename where the configuration is to be saved (or read). The default file is gadds._nc. If you omit the file extension, *._nc is assumed.

4.4 Edit > Configure > Write • Save the current configuration to a disk file

Menu Command: Edit > Configure > Write

Accelerator: None

User Level: 2

SLAM Syntax: CONFIGURE /WRITE $1

Use this command to save current program settings to a specified disk file for later read-in using the Edit > Configure > Read command. Typically, you would use these commands to save a good configuration, play around with the program, and if something fails, restore the good configuration.

These configuration files, which have file extensions of ._nc, contain the current flood file correction, spatial correction, and current values of the input panel items for nearly all the GADDS commands (a few exceptions).

On startup, GADDS normally reads its configuration from a file called gadds._nc in the current project's working directory. You can override this startup behavior with a startup command line qualifier. (See Section 1.3, for details.) On exiting, GADDS normally saves its configuration file into a file called gadds._nc in the current project's working directory.

CAUTION

These commands are active and do not prompt before performing an operation (i.e., overwriting an existing file).

4.4.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1……...(Configuration Filename) [gadds._nc]

Enter the filename where the configuration is to be saved (or read). The default file is gadds._nc. If you omit the file extension, *._nc is assumed.

4.5 Edit > Configure > Show model • Display the current goniometer and controller type

Menu Command: Edit > Configure > Show model

Accelerator: None

User Level: 1

SLAM Syntax: CONFIGURE /SHOWMODEL

Use this command to display the current goniometer model type, maximum frame size, current frame size, current flood correction, current spatial correction, project working directory, and calibration directory.

Normally, the goniometer type is defined when the software is installed, but occasionally, when one changes the goniometer stage, you must also change the goniometer type as follows:

X100	Obsolete setting
X200	Obsolete setting
P3X1000	Obsolete setting
P3X2000	HI-STAR on P4 goniometer
X1000	Obsolete setting
X2000	HI-STAR on Aztalan goniometer
PLATFORM	HI-STAR on PLATFORM goniometer
¼-CIRCLE	Obsolete setting, use T:¼-CIRCLE
T:¼-CIRCLE	PLATFORM ¼-circle in transmission mounting
R:¼-CIRCLE	PLATFORM ¼-circle in reflection mounting
D8	HI-STAR on D8 DISCOVER goniometer

4.5.1 Arguments

None. Command executes immediately.

4.6 Edit > Configure > Colors • Edit the current color configuration settings

Menu Command: Edit > Configure > Colors

Accelerator: None

User Level: 1

SLAM Syntax:

CONFIGURE /COLORS $1 /WINBG=<n> /WINFG=<n> /CURSOR=<n> /HIGHLIGHT=<n> /BORDER=<n> /GRAPH=<n> /OVERLAY=<n> /MATCH1=<n>

This command displays a dialog box where you can view or edit the colors used for the windows displayed by the program and the color scheme (called a “color table” or “color lookup table”) used to display detector frame pixel values.

Each window color (WINBG, WINFG, CURSOR, HIGHLIGHT, and BORDER) is specified as a 9-digit decimal integer. The first three digits correspond to the red level, the second three to the green level, the last three to the blue level. The range for each color is 0-255. Thus, the number itself has a range from 000000000 to 255255255 (RRRGGGBBB). For example, the value 255000000 is bright red, 000255000 is bright green, 255255000 is bright yellow, 255255255 is white, 050000050 is dark purple, 000000000 is black, and 080080080 is gray.

The simplest way to select a color is to enter an asterisk (*) and let the program display a color table map, where you can click on any color and have the RGB value calculated.

When you invoke a command from the menu (or the command line without arguments), a dialog box appears. View or edit its contents (or type text). Then:

- Press ENTER or click the OK button to save your entry.
- Press ESC or click the Cancel button to return to the menu without saving your last entry.

GADDS displays the angle status in the following color scheme:

- Non-controllable axes in border color.
- Moving axes in highlight color.
- Stationary and controllable axes in foreground color.
- Axes in collision state in reverse video: background on highlight color.

4.6.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(Color Table Filename) [bb.lut]

Enter name of the color lookup table to be used for frames. This entry does not affect the colors used for menus, windows, screen background, etc. Color tables are assumed to be located in the directory pointed to by GADDS$SYSDATA:, and a .lut filename extension is assumed if you don't specify one. The following color tables are supplied with the program. In addition, you can supply the special value, $DEFAULT, which refers to a table similar to bb.lut below, which is not disk-resident but, rather, is hard-wired into the program code.

BB.LUT	The default color table generated using a blackbody radiation model. Intensities are monotonically increasing, but color provides better discrimination than a straight monochrome scheme.
CUSTOM.LUT	Arbitrary multicolor scheme
DIFFER.LUT	Red/green color table useful in viewing frames that are built from differences (for example a subtraction of one frame from another)
MONO.LUT	Monochrome grayscale color table
PRINT.LUT	Reverse monochrome grayscale color table. Useful for previewing monochrome hardcopy screen dumps
V16.LUT	16-level color table, using a scheme similar to the defaults on older PCS systems
V8.LUT	8-level color table, using a scheme similar to the defaults on older PCS systems
V8SYM.LUT	Like V8, but with colors symmetrically distributed about the center display memory value
VIDEO.LUT	Another arbitrary multicolor scheme

When using the Edit > Config > Colors dialog, you can select the lookup table name from a list of available filenames by specifying a "wildcard" pattern in the COLOR TABLE FILENAME entry or by leaving the entry blank, and pressing ENTER or the left mouse button. The default filespec used to

search for available lookup tables is GADDS$SYSDATA:*.lut.

/WINBG=<n> .....(Window Background Color) [000000050]

Specifies the window background color as a 9-digit number in RRRGGGBBB format (see above). This is the color of the background outside of the image area when the program is started. By default, it is dark blue (000000050).

/WINFG=<n>.....(Window Foreground Color) [255255255]

Specifies the window foreground color as a 9-digit number in RRRGGGBBB format (see above). This is the color of the screen text you see in the status areas, menus, and panels. By default, it is white (255255255).

/CURSOR=<n> .....(Cursor Color) [000255255]

Specifies the color of the cursors that appear in the interactive cursor commands as a 9-digit number in RRRGGGBBB format (see above). This same color is used to draw graphic overlays (for example, X-Y plots). By default, it is cyan (000255255).

/HIGHLIGHT=<n>…(Highlight Color) [210000000]

Specifies the background color of “highlighted” text as a 9-digit number in RRRGGGBBB format (see above). Text which is highlighted includes window title bars, and prompts, warnings and error messages displayed on the bottom status line. By default, it is read (210000000).

/BORDER=<n>..... (Border Color) [064192200]

Specifies the color of the line drawn around windows and panels as a 9-digit number in RRRGGGBBB format (see above). By default, it is light cyan (064192200).

/GRAPH=<n> ..... (Raw Graph Color) [255255255]

Specifies the color of the graphs drawn in the Peaks commands as a 9-digit number in RRRGGGBBB format (see above). By default, it is white (255255255).

/OVERLAY=<n> ... (Peak Overlay Color) [000255000]

Specifies the color of the peak overlays drawn in the Peaks commands as a 9-digit number in RRRGGGBBB format (see above). By default, it is green (000255000).

/MATCH1=<n>..... (Match #1 Overlay Color) [000255255]

Specifies the color of the second graph drawn in the Peaks commands as a 9-digit number in RRRGGGBBB format (see above). By default, it is cyan (000255255).

4.7 Edit > Clear • Erase the data array and/or the display screen

Menu Command: Edit > Clear

Accelerator: Ctrl+Del

User Level: 1

SLAM Syntax: CLEAR $1 /QUADRANT=<n> /GRAPHICS_SAVE /IMAGE_SAVE

Analyze > Clear erases a specified region of the display and/or frame buffer memory. Clearing of the screen can be confined to just image data (retaining any overlaid graphics) or just graphic overlays (retaining the underlying image).

When invoked from the menu, or from the command line without arguments, Analyze > Clear displays a dialog box where you can view/edit the arguments described below. Pressing the ENTER key or clicking the OK button starts the operation. Pressing ESC or the Cancel button returns you to the menu.

4.7.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(Screen, Data, or All?) [ALL]

Selects either the screen, the frame buffer accumulation memory (data) or both are to be cleared. “SCREEN” = erase display, “DATA” = erase accumulation memory, “ALL” = erase both. The default value is “ALL”.

/QUADRANT=<n>…(Screen Quadrant) [0]

Specifies the targeted display quadrant(s), to be cleared. The selection criteria are: 0 = all (the entire image area), 1 = first quadrant (lower left), 2 = second quadrant (lower right), 3 = third quadrant (upper left), and 4 = fourth quadrant (upper right). The default value is 0 (clears everything).

/GRAPHICS_SAVE…(Preserve Graphics (Y/N) ?) [No]

Specifies whether or not to preserve the graphics if you clear the screen. Enter “Y” to erase just the displayed image and retain any overlaid graphics, “N” otherwise. The default value is “N”.

/IMAGE_SAVE ..... (Preserve Image (Y/N) ?) [No]

Specifies whether or not to preserve the image if you clear the screen. Enter “Y” to erase only the overlaid graphics and retain the underlying image, “N” otherwise. The default value is “N”.

4.8 Edit > Contrast • Change the screen brightness and contrast

Menu Command: Edit > Contrast

Accelerator: Ctrl+T

User Level: 1

SLAM Syntax: CONTRAST /LO=<n> /HI=<n>

This command performs real-time linear mapping of frame pixel values into the colors in the color lookup table currently loaded. (See Edit > Colors for more about color lookup tables.) Based on the current mouse position (or the specified LO and HI values if invoked from the command line), Edit > Contrast computes a lower and upper limit. All pixel values at or below lower limit show up as lowest color in the color table (for example, black). Those at or above upper limit appear as highest color (for example, white). Pixel values in between are linearly mapped to colors in the table.

When you invoke this command from the menu, or from the command line with no arguments, you can change the lower and upper limit with the mouse or arrow keys. Horizontal motion changes the width of the contrast window. Motion to the left brings the lower and upper limits closer together (increasing contrast) and motion to the right moves the upper and lower limits farther apart (reducing contrast and increasing latitude). Horizontal motion is, thus, analogous to a contrast control or choosing a type of film according to the desired latitude. Vertical motion raises or lowers the upper and lower limits together and is analogous to a brightness control or to selecting the length of exposure of a film.

When you're using the arrow keys to modify contrast, you can press CTRL simultaneously with an arrow key to jump in intervals ten times larger than the arrow key alone.

To exit and save your changes to the color mapping, press ENTER or the left mouse button. To exit and reset the mapping to default (wide-open) levels, press ESC or the right button. When invoked from the command line with both the arguments shown below, the mapping is changed to the specified lower and upper limits, and control returns immediately to the command line.

SLAM arguments follow:

/LO=<n> ..... [0]

The number of counts to be mapped to the lowest display color. The default value is 0. The valid range is -255 to 65535.

/HI=<n> ..... [255]

The number of counts to be mapped to the highest display color. The default value is 255. The valid range is -255 to 65535.

4.9 Edit > Zoom • Magnify a specified square area on the display

Menu Command: Edit > Zoom

Accelerator: Ctrl+Z

User Level: 1

SLAM Syntax: ZOOM $1 $2 $3

Analyze > Zoom displays the pixels surrounding a specified center point as a magnified image. Magnification is performed by pixel replication, with the replication factor a power of 2 from 1 to 16, where 1 corresponds to the normal, unmagnified display. If the specified X or Y center would leave part of the image area blank, the image is translated only far enough to place the edge of the frame at the edge of the image area.

No arguments are prompted for when ZOOM is invoked from the menu. ZOOM displays a full-screen crosshair; the zoom center is selected with the crosshair, which can be dragged with the mouse (or cursor keys). Once the zoom center is selected, press ENTER or release the left mouse button to display the following pop-up menu, from which you can choose the desired magnification factor:

Exit

1X

2X

4X

8X

16X

Select the EXIT option to exit and return to the menu.

Cursor commands that return pixel values and positions can be used on zoomed images. Positions are reported relative to the original image; for example, if the magnification factor is 16, you would need to press the left arrow key 16 times in Analyze > Cursor to change from one X-pixel coordinate to another (assuming you start at the edge of an unmagnified pixel).

When invoked from the command line interpreter mode, the ZOOM command accepts three arguments.

$1 ..... (X) [255]

Enter X-pixel to try to center on screen. The range is from 0 to framesize-1.

$2 ..... (Y) [255]

Enter Y-pixel to try to center on screen. The range is from 0 to framesize-1.

$3 ..... (Magnification) [1]

Enter the magnification (zoom) to examine a specific area in greater detail. The allowed range is from 1 to 16.

4.10 Edit > Frame info • View a frame header

Menu Command: Edit > Frame info

Accelerator: Ctrl+F

User Level: 1

SLAM Syntax: FRAME_INFO $1

Edit > Frame Info allows you to view the header of the currently displayed frame, or that of a specified frame file (very useful for detective work for data collection parameters).

When invoked from the menu, or run from the command line without arguments, Edit > Frame Info displays a dialog box where you enter the name of the frame whose header is to be viewed. After entering the filename, pressing ENTER or clicking the OK button displays the header in a scrollable window; pressing ESC or clicking the Cancel button returns you from the dialog to the menu without displaying the header.

When viewing the header, pressing the ENTER key or clicking the OK button terminates the scrollable window and returns you to the menu bar. You can click the Write.. button to write the currently selected header text (or the entire header, if nothing is selected to an ASCII text file, or click the Print... button to send the header text to a printer.

See Appendix A: Area Detector Frame Format: Headers for more information.

4.10.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Frame Filename) [$FRAME]

Filename of the frame whose header is to be displayed. The special name $FRAME (the default) refers to the currently displayed frame. If you leave this item blank on the input panel, or specify a “wildcard” filename pattern, pressing ENTER or clicking the OK button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or scroll bars and mouse, then pressing ENTER or clicking OK. You will be returned to the input panel with the selected filename filled in. If you leave this item blank, it is the same as entering a *.* wildcard pattern. Remember that both filenames and patterns entered here are merged with the Crystal > New Project data directory (see Crystal > New Project for details).

See the Appendix A, Bruker Area Detector Frame Data Format, for details on the frame header.

5. Collect Routines

5.1 Collect > Detector > Cu bias • Set PDC to Cu (low) bias setting

Menu Command: Collect > Detector > Cu bias

Accelerator: Ctrl+Shift+C

User Level: 1

SLAM Syntax: DETECTOR /CU

Use this command to place the PDC and detector at the Cu (low) bias setting. The action is performed immediately, with no prompt for additional input. The DETECTOR item in the goniometer status area at the lower right of the display is updated to reflect the new bias status.

NOTE: For the GADDS software to be able to change the detector bias, the PDC (position decoding circuit) must be in
Detector Bias - On Source Select - Auto.

If the bias setting is incorrect when invoking either a Process > Flood > New, a Process > Spatial > New, or any Collect > Scan command, GADDS will prompt the user to switch to the correct bias setting before collecting the data. Fe, high, bias is used by Flood and Spatial, while Cu, low, bias is used for Scan commands.

5.1.1 Arguments

None. Command executes immediately.

5.2 Collect > Detector > Fe Bias • Set PDC to Fe (high) bias setting

Menu Command: Collect > Detector > Fe bias

Accelerator: Ctrl+Shift+F

User Level: 1

SLAM Syntax: DETECTOR /FE

Use this command to place the PDC and detector at the Fe (high) bias setting. The action is performed immediately, with no prompt for additional input. The DETECTOR item in the goniometer status area at the lower right of the display is updated to reflect the new bias status.

NOTE: For the GADDS software to be able to change the detector bias, the PDC (position decoding circuit) must be in
Detector Bias - On Source Select - Auto.

If the bias setting is incorrect when invoking either a Process > Flood > New, a Process > Spatial > New, or any Collect > Scan command, GADDS will prompt the user to switch to the correct bias setting before collecting the data. Fe, high, bias is used by Flood and Spatial, while Cu, low, bias is used for Scan commands.

5.2.1 Arguments

None. Command executes immediately.

5.3 Collect > Detector > Y vs. X • Set PDC for normal positional display

Menu Command: Collect > Detector > Y vs. X

Accelerator: none

User Level: 1

SLAM Syntax: DETECTOR /YVSX

Use this command to place the PDC and detector into normal X-Y position display. The action is performed immediately, with no prompt for additional input.

5.3.1 Arguments

None. Command executes immediately.

5.4 Collect > Detector > E vs. E • Set PDC for energy versus energy for bias calibration

Menu Command: Collect > Detector > E vs. E

Accelerator: none

User Level: 1

SLAM Syntax: DETECTOR /EVSE

Use this command to place the PDC and detector into energy versus energy for bias calibration. The action is performed immediately, with no prompt for additional input.

5.4.1 Arguments

None. Command executes immediately.

5.5 Collect > Detector > Add • Accumulate a frame with temporary linear flood field

Menu Command: Collect > Detector > Add

Accelerator: none

User Level: 1

SLAM Syntax:

DETECTOR /ADD $1 /CLEAR
/PATTERN /COUNTS=<n>
/DISPLAY=<n> /REALTIME
/RESET=<n> /SHUTTER

Use this command to collect a single “still” frame of data at a fixed goniometer position using a linear flood field. Data is continuously acquired until either a specified amount of time has elapsed or a specified number of counts is reached, whichever occurs first.

You can optionally display the accumulated frame after it has been acquired, or update the display immediately as each count is recorded (referred to as “real-time display”). If you elect one of the display options, ADD also updates the current frame status information displayed at the upper right of the screen.

The frame remains in the frame buffer's accumulation memory; it is not written directly to disk. Use the SAVE command to save the data to disk.

5.5.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(Max. Seconds) [30]

This is the maximum count time (in seconds). The default value is 30; the range is from 1 to 65,535 seconds. Times can be entered in decimal seconds or in HH:MM:SS.SS (hours, minutes and seconds) format. Data collection ends when the specified time has elapsed, or when the maximum count limit (see MAX COUNTS below) has been reached.

/CLEAR .....(Pre-Clear?) [Y]

This qualifier, when set, clears memory before the new data frame is collected. If it is not set, the new data are added to the image already in the frame accumulation memory (for example, an image left over from a previous ADD, LOAD, or SCAN command).

/PATTERN .....(Test Pattern?) [N]

This qualifier, when present, draws a test grid into the frame accumulation memory prior to collecting data. The test grid is used for factory alignment and consists of grid lines on a 64-pixel spacing; two circles, one with a 270-pixel radius and one with a 280-pixel radius; and two crosses rotated to 45 degrees, one linear cross, and one passed through the current flood field correction.

/COUNTS=<n>..... (Max. Counts) [10,000,000]

This qualifier sets an upper limit on how many counts may occur before data collection is terminated. When the specified number is reached the system ends the data collection, saving the data frame. The default value is 10,000,000 counts, with a range from 0 to 10^{37} counts. Data collection will also be terminated if MAX SECONDS is reached before MAX COUNTS.

/DISPLAY=<n> ..... (Max Displayed Counts) [7]

0 = no display, otherwise # counts corresponding to white on the display. The initial default is 7; the allowed range is from 0 to 10^{6}.

/REALTIME..... (Real-time Display) [Y]

This qualifier, when present, displays data as it is being collected. The display does require additional processing time, and will limit the maximum rate at which counts can be accumulated. If the MAX DISPLAYED COUNTS qualifier is given a non-zero value, the frame will be automatically displayed at the end of the ADD if real-time display is off. This latter display method has no effect on observed data rate.

If you're not sure whether real-time display will affect the observed data rate signifi-

cantly at your current incident count rate, check the late counts in the frame header of a representative frame with the FRAME_INFO command. If the late counts are more than a few percent of the total counts, your data collection will be more efficient if real-time display is turned off. In general, you should be able to use real-time display for set-up and sample evaluation, but you should disable it during collection of frame series which will be used as input to data reduction (see the similar SCAN command display options).

/SHUTTER .....(Open & Close Shutter?) [N]

This qualifier, if present, causes the shutter to open at the start of the ADD, and to close at the end. Otherwise, the shutter stays in its current state for the duration of the ADD.

/RESET=<n>.....(Bar-Graph Hold Time) [0.0]

This qualifier specifies the number of seconds before repetitive auto-clear of frame memory (0 = do not clear). The default value is 0; the range is from 1 to 65,535 seconds. This parameter is useful in conjunction with real-time display if you're looking for a change in intensity over time. For instance, if you're driving the goniometer manually to look for or maximize the intensity of a reflection, it helps to clear the screen frequently, for example every 1 second by setting the reset interval to 1.

5.6 Collect > Detector > Reset • Reset to x-position vs. y-position, Cu bias

Menu Command: Collect > Detector > Reset

Accelerator: Ctrl+Shift+R

User Level: 1

SLAM Syntax: DETECTOR /DETRESET

Use this command to place the PDC and detector at the Cu (low) bias setting and into normal X-Y position display. The action is performed immediately, with no prompt for additional input. The DETECTOR item in the goniometer status area at the lower right of the display is updated to reflect the new bias status.

NOTE: For the GADDS software to be able to change the detector bias, the PDC (position decoding circuit) must be in
Detector Bias - On Source Select - Auto.

If the bias setting is incorrect when invoking either a Process > Flood > New, a Process > Spatial > New, or any Collect > Scan command, GADDS will prompt the user to switch to the correct bias setting before collecting the data. Fe, high, bias is used by Flood and Spatial, while Cu, low, bias is used for Scan commands.

5.6.1 Arguments

None. Command executes immediately.

5.7 Collect > Detector > X-E vs. X • Set PDC for X preamp calibration

Menu Command: Collect > Detector > X-E vs. X

Accelerator: none

User Level: 2

SLAM Syntax: DETECTOR /XEVSX

Use this command to place the PDC and detector for X preamp calibration. The action is performed immediately, with no prompt for additional input.

5.7.1 Arguments

None. Command executes immediately.

5.8 Collect > Detector > Y-E vs. X • Set PDC for Y preamp calibration

Menu Command: Collect > Detector > Y-E vs. X

Accelerator: none

User Level: 2

SLAM Syntax: DETECTOR /YEVSX

Use this command to place the PDC and detector for Y preamp calibration. The action is performed immediately, with no prompt for additional input.

5.8.1 Arguments

None. Command executes immediately.

5.9 Collect > Detector > Custom • Enter values to be loaded into PDC setup registers

Menu Command: Collect > Detector > Custom

Accelerator: none

User Level: 3

SLAM Syntax: DETECTOR /PDCCUSTOM $1 $2 $3

Use this command to place the PDC and detector into a custom configuration. Useful for testing purposes only.

5.9.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 ..... (X-ADC Source) [0]

Enter 0 for X-position, 1 for X-energy, 2 for Y-position, or 3 for Y-energy.

$2 ..... (Y-ADC Source) [2]

Enter 0 for X-position, 1 for X-energy, 2 for Y-position, or 3 for Y-energy.

$3 ..... (Bias) [0]

Enter 0 for Cu, low BIAS, 1 for Fe, high bias.

5.10 Collect > Goniometer > Drive • Move goniometer angles to specified positions

Menu Command: Collect > Goniometer > Drive

Accelerator: Ctrl+Shift+D

User Level: 1

SLAM Syntax:

GONIOMETER /DRIVE $1 $2 $3 $4 $5 $6 $7 $8
or
GONIOMETER /DRIVE $1 $2 $3 $4

Use this command to drive the goniometer angles and axes to a specified position. The default settings are the current angles/positions, so you only change the axes that you wish to drive. The minimum and maximum allowed values are taken from the current software collision limit settings (see Collect > Goniometer > Limits settings, Section 5.15), but on a ¼-circle system, the extended limits (see Collect > Goniometer > ExtLimits, Section 5.16) can restrict goniometer motion and detector XYZ limits (see Collect > Goniometer > XYZ stage, Section 5.27) can further restrict goniometer motion.

When in the panel, pressing the ESC key or clicking Cancel button returns you to the main menu-menu. Pressing the ENTER key or clicking OK button initiates the drive command.

GADDS checks the specified angles against the current collision limits and extended limits and displays an error message if the requested angles/positions are not allowed. Otherwise, GADDS begins moving the goniometer to the specified angles/positions. During the drive the message appears on the bottom status line:

DRIVING—PRESS ANY KEY TO STOP...

You can halt the drive by pressing a keyboard key (for example, ENTER or the space bar).

On completion, the program updates the current goniometer angles displayed in the goniometer status area at the lower right of the screen.

Collect > Goniometer > Drive will try to drive any angle to the specified destination by the shortest path, unless the collision limits specifically prevent it from doing so. In that case, the longer path will be taken. On 1/4-circle systems, Collect > Goniometer > Drive will drive around obstacles in omega-chi space as defined by the Goniometer /Extlimits command, which may take several drives to reach the final destination.

5.10.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(2-Theta) [current setting]

$1 .....(THETA1) [current setting]

Enter the destination 2θ angle in degrees (or the theta-tube angle for θ-θ systems) in degrees. Default is current setting.

$2 .....(Omega) [current setting]

$2 .....(THETA2) [current setting]

Enter the destination ω angle in degrees (or the theta-detector for θ-θ systems) angle in degrees. Default is current setting.

$3 .....(Phi) [current setting]

Enter the destination ϕ angle in degrees. Default is current setting.

$4 .....(Chi) [current setting]

Enter the destination χ angle in degrees. Default is current setting.

$5 .....(X) [current setting]

Enter the destination X position in mm. Default is current setting.

$6 .....(Y) [current setting]

Enter the destination Y position in mm. Default is current setting.

$7 ..... (Z) [current setting]

Enter the destination Z position in mm. Default is current setting.

$8 ..... (Aux1) [current setting]

Enter the destination aux position in aux units. Default is current setting. Typically, this axis is used for the video zoom option, thus its units are magnification factor in the range 1.0 to 7.0.

5.11 Collect > Goniometer > Manual • Control goniometer from manual box

Menu Command: Collect > Goniometer > Manual

Accelerator: Ctrl+Shift+M

User Level: 1

SLAM Syntax:

GONIOMETER /MANUAL $1 $2 $3 $4 $5 $6 $7 $8
or
GONIOMETER /MANUAL $1 $2 $3 $4 $5
also
RATEMETER $1 /RESET=<n> /SHUTTER

Use this command to operate the goniometer motors using the manual control box. While the manual control is activated, the program control is suspended.

When in the panel, pressing the ESC key or clicking Cancel button returns you to the main menu-menu. Pressing the ENTER key or clicking OK button initiates the manual command. The goniometer is said to be in “manual mode” when in this state. During manual mode, the following message appears on the bottom status line:

MANUAL MODE. ESC=EXIT, S=SHUTTER, T=ATTENUATOR, A=ADD, C=COUNT, L=LASER.

Pressing ESC (or CTRL+G) exits manual mode, closing the shutter (if open), and returns you to the main menu. Pressing the S key toggles the state of the X-ray shutter open/closed. Its status is updated in the goniometer status area at the lower right of the screen. Pressing the T key performs the same function for the incident beam attenuator on systems equipped with an attenuator. Similarly, pressing the L key will toggle the state of the laser, on systems equipped with a laser.

Pressing the A key displays the Collect > Add input dialog. After you edit the items in this dialog, pressing ENTER or clicking the OK button begins a Collect > Add operation, during which the goniometer remains under control of the manual box. This feature is most useful in conjunction with Collect > Add's /REALTIME real-time display option, with or without the /RESET periodic redisplay option, to observe changes in the X-ray pattern as the goniometer angles are changed. If you want to terminate the acquisition early, use CTRL+BREAK, which returns you to manual mode (as will the ESC key or Cancel button pressed while in the ADD input panel). (See Collect > Add, Section 5.47).

Pressing the C key displays the RATEMETER input panel. If you supply values for the items in this panel, pressing the ENTER key or left mouse button begins a RATEMETER operation, during which the goniometer remains under control of the manual box. This is most useful during instrument alignment, with or without the

/RESET option, to observe changes in the x-ray pattern in real-time as the goniometer angles are changed. If you want to terminate the RATEMETER early, use the CTRL-BREAK key combination, which returns you to manual mode (as will the ESC key or right mouse button pressed while in the RATEMETER input panel).

While you're controlling the goniometer manually, the setting angles displayed in the goniometer status area on the lower right of the screen are not updated in real time. However, if you press the ENTER on Phoenix controller's or AXIS PRINTOUT button on the GGCS controller's manual control box, the values on the screen will be updated to reflect the current angles (VIDEO will also be updated with new zoom and XYZ values). On the Phoenix controller, you can also press the ACVAL key to display the current angles on the manual control box's LCD. The display is also updated automatically when you exit manual mode.

To operate the manual control box on the Phoenix controller (D8-Discover systems), press SHIFT-F1, then select the requested axis by pressing 1 for 2θ, 2 for ω, 3 for ø, 4 for χ, 5 for X, 6 for Y, 7 for Z, 8 for Aux1. Select drive speed by pressing + for fast or – for slow. To drive the axis, press and hold the down arrow for reverse or up arrow for forward. Release the arrow to stop the drive.

NOTE: The D8 controller will drive for 120° and stop; this is normal. To display axes angles and positions, press the ACVAL (actual values) button.

NOTE: If angles are dashes, you need to initialize the drive with a home command.

To operate the manual control box on the GGCS controller (Platform and earlier systems), select the requested axis by pressing the button. If a non-controllable axis is selected, then the message appears:

Bad button combination.

The buttons are labeled A, B, C, and D (also labeled: φ, χ, 2θ, and ω). Multiple button presses are required to control the additional axes: A+B for X, A+C for Y, A+D for Z, and C+D for Aux1.

To drive the selected axis, press and hold the fast forward, slow forward, fast reverse, or slow reverse button. To stop the drive, release the drive button.

NOTE: On R:1/4-circle platform goniometers, the chi axis will drive in the opposite direction, that is the forward buttons will drive chi in the reverse direction.

While the Collect > Goniometer > Manual dialog allows you to modify the base goniometer angles used for optical alignment, they are not actually used in the course of this command. (See Collect > Goniometer > Optical, Section 5.12 for more information about the base angles).

5.11.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(Base 2-Theta) [varies]

$1 .....(Base Theta1) [varies]

Enter the “home” 2θ or θ1 value in degrees for optical alignment. On most goniometers, this is the swing angle to which the goniometer is driven to begin optical alignment. On θ-θ systems, this is the generator tube axis. Default is current setting. Typically, this value is 0° or -60°, which will drive the detector to an out-of-the-way position.

$2 .....(Base Omega) [varies]

$2 .....(Base Theta2) [varies]

Enter the “home” omega or θ2 value in degrees for optical alignment. Default is current setting. On most goniometers, the microscope is mounted to the goniometer base at a fixed angle from the collimator. On D8-Discover system, this angle is user settable. On Platform systems, this was -30° (use 330°). On Aztalan systems this was -90° (use 270°). On 4-circle goniometers, the microscope is mounted to the circle and one uses 0° or 330° for these systems, but if the LT device is attached, 345° is recommended (to avoid glassware breakage).

$3 ..... (Base Phi) [varies]

Enter the “home” phi value in degrees for optical alignment. Default is current setting. Typically, one uses 0° or for 4-circle systems, 30°.

$4 ..... (Base Chi) [varies]

Enter the “home” chi value in degrees for optical alignment. Default is current setting. Typically, one uses the fixed chi value of 54.74° (45° on Aztalan) or for T:1/4-circle systems, -54.74°; for R:1/4-circle systems, 54.74; or for 4-circle systems, 330°.

$5……(2T/OM/PH/CH Fast:Slow Ratio) [14]

Enter the slew speed to slow speed ratio for manual control box. Default is 14. The manual control box allows driving at two speeds. The fast speed for each axis corresponds to the speed set in Collect > Goniometer > Speeds. The slow speed will be that of the fast speed divided by this number. The ratio used is the same for each axis. This parameter has no effect on Phoenix controllers (D8 Discovery systems) which has a fixed slow speed.

$6 .....(X/Y Fast:Slow Speed Ratio) [14]

Enter the slew speed to slow speed ratio for manual control box. Default is 14. This parameter has no effect on Phoenix controllers (D8 Discovery systems) which has a fixed slow speed.

$7 .....(Z Fast:Slow Speed Ratio) [14]

Enter the slew speed to slow speed ratio for manual control box. Default is 14. This parameter has no effect on Phoenix controllers (D8 Discovery systems) which has a fixed slow speed.

$8 .....(Aux Fast:Slow Speed Ratio) [14]

Enter the slew speed to slow speed ratio for manual control box. Default is 14. This parameter has no effect on Phoenix controllers (D8 Discovery systems) which has a fixed slow speed.

5.12 Collect > Goniometer > Optical • Perform/check optical centering of sample

Menu Command: Collect > Goniometer > Optical

Accelerator: Ctrl+Shift+O

User Level: 1

SLAM Syntax:

GONIOMETER /OPTICAL $1 $2 $3 $4 $5 $6 $7 $8
or
GONIOMETER /OPTICAL $1 $2 $3 $4 $5

Use this command to drive the goniometer between a few useful pre-defined positions to minimize the effort required to center the sample crystal mounted on a goniometer head as viewed through the sample microscope or video microscope mounted on the goniometer base. These pre-defined positions are relative to a specified starting position, whose setting angles are referred to as the “base angles.” The program contains suitable default values for the base angles for D8 3-circle, Platform 3-circle, older Aztalan (black) 3-circle, and 4-circle goniometers; however, these base angles can also be modified from the input panel here, if necessary. The base angles should place the phi axis normal to the microscope axis and one set of

goniometer head adjustments normal to the microscope axis.

It is important that the environment variable SAXI$ADMODEL be defined correctly for your goniometer type, since the alignment philosophy is different between D8 3-circle, Platform 3-circle, 4-circle and old 3-circle systems. You also need to make sure that any configuration files you read in correspond to the correct goniometer type, since the values in the configuration file will be transferred to GADDS and the goniometer controller on program startup. (See Edit > Configuration > Show Model, Section 4.5, for more information). 4-circle systems use settings at the base chi and base chi + 180 for estimating sample height. 3-circle systems use the base omega and base omega + 180.

When in the panel, pressing the ESC key or clicking Cancel button returns you to the main menu-menu. Pressing the ENTER key or clicking OK button initiates the optical command. The goniometer is said to be in “manual mode” when in this state. During manual mode, the message appears on the bottom status line:

> MANUAL MODE. ESC=EXIT, S=SHUTTER, T=ATTENUATOR, A=ADD, C=COUNT, L=LASER.

The Optical command enables the manual control box for interactive control of the goniometer but, unlike the Collect > Goniometer > Manual command, it assigns a different functions to the ENTER button on the Phoenix’s manual control box and to the AXIS PRINTOUT button on the GGCS’s manual control box.

On the Phoenix’s manual control box, press SHIFT-F2, then 1 for 2θ, then press ENTER to drive the goniometer to the base angles. Additional presses of ENTER will drive phi by 180°. If you select one of the other axis buttons instead of 2θ, certain fixed angles are added to the base position, as listed in the table below. As with the 1 (2θ). Additional presses of the ENTER button when in one of these other positions will drive phi by 180°.

On the GGCS’s manual control box, depress the 2-THETA axis button on the manual box (all three others should be up), then press AXIS PRINTOUT to drive the goniometer to the base angles. Additional presses of AXIS PRINTOUT will drive phi 180°. If you depress one of the three other axis buttons instead of 2-THETA, certain fixed angles are added to the base position, as listed in the following table:

Axis Button	**Position (4-Circle)**	**Position (3-Circle)**
2-THETA	Base Position	Base Position
OMEGA	+ 90 in phi	+ 90 in phi
PHI	+ 180 in chi	+ 180 in omega
CHI	+ 180 in chi + 90 in phi	+ 180 in omega + 90 in phi

As with the 2-THETA button, additional presses of the AXIS PRINTOUT button when in one of these other positions drive phi 180°.

While the Collect > Goniometer > Optical dialog box allows you to modify the fast:slow speed ratio used by Collect > Goniometer > Manual, it is not used here. The slow speed is instead fixed at 30 degrees/minute. (See Collect > Goniometer > Manual, Section 5.11, for more information about the speed ratio).

5.12.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 to $8

See Collect > Goniometer > Manual (Section 5.11).

NOTE: This command is designed to work only on stages with a goniometer head.

5.13 Collect > Goniometer > Flatsample • Perform/check flat sample plane on XYZ stage

Menu Command: Collect > Goniometer > Flatsample

Accelerator: Ctrl+Shift+W

User Level: 1

SLAM Syntax:

GONIOMETER /FLATSAMPLE /X1=<n> /Y1=<n> /Z1=<n> /X2=<n> /Y2=<n> /Z2=<n> /X3=<n> /Y3=<n> /Z3=<n>

On systems equipped with an XYZ stage, it is possible to collect scans at multiple target locations. On flat samples such as wafers, one frequently wishes to take scans on target positions laid out on a rectangular grid. Instead of manually determining the Z axis position of each target on the grid, one can pre-determine the flat sample plane, then lay out the target locations using Collect > Scan >GridTargets (see Section 5.41) which will automatically calculate the correct Z axis value from the flat sample plane.

FLATSAMPLE works on the simple principle that 3 points determine a flat plane. Initially, these points are defaulted to form a small triangle about the current goniometer position in XYZ. For greater accuracy, the user should enlarge this triangle of points.

Next, the user will be given the option to drive to each point on the triangle. The program will pre-drive to the selected point, then allow the user to manually drive X, Y and Z. Remember that Z is aligned only when the laser is positioned within the video cross-hairs. When all three points have been positioned, the flat sample plane is fully defined.

5.13.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

/X1.....(X VALUE FOR POINT 1)

/Y1.....(Y VALUE FOR POINT 1)

/Z1.....(Z VALUE FOR POINT 1)

Enter the (X,Y,Z) coordinates for the top vertex of imaginary triangle on the sample.

/X2.....(X VALUE FOR POINT 2)

/Y2.....(Y VALUE FOR POINT 2)

/Z2.....(Z VALUE FOR POINT 2)

Enter the (X,Y,Z) coordinates for the second vertex of imaginary triangle on the sample.

/X3.....(X VALUE FOR POINT 3)

/Y3.....(Y VALUE FOR POINT 3)

/Z3.....(Z VALUE FOR POINT 3)

Enter the (X,Y,Z) coordinates for the third vertex of imaginary triangle on the sample.

5.14 Collect > Goniometer > Update • Enter observed goniometer angles

Menu Command: Collect > Goniometer > Update

Accelerator: none

User Level: 2

SLAM Syntax:

GONIOMETER /UPDATE $1 $2 $3 $4 $5 $6 $7 $8 $9
or
GONIOMETER /UPDATE $1 $2 $3 $4

This command is used to reset the goniometer controller's (Phoenix's or GGCS's) memory to the correct goniometer position. That is, if the readings on the goniometer's angular scales are different from those reported by the program, use this command to enter the readings from the angular scales to the nearest 0.5°. The program then sends these readings to the goniometer controller, which very accurately maintains the current positions modulo 1 degree but must rely occasionally on this type of user input for the coarse absolute position.

On 4-circle, P3, style goniometers, all angles are entered to the nearest 0.5 degree. The program then sends these readings to the goniometer controller, which very accurately maintains the current positions modulo 1 degree, but must rely occasionally on this type of user input for the coarse absolute position.

On all other goniometers (for example D8, Platform, or Aztalan), all angles and positions are entered with full fractional values. Rarely, if ever, does one know the exact axis setting, so typically, one performs a Collect > Goniometer > Home (see Section 5.25) command after updating an axis to accurately position the axis.

When invoked from the menu, or run from the command line without arguments, Collect > Goniometer > Update displays a dialog box where you can view/edit the arguments described below. Pressing the ENTER key or clicking the OK button updates the angles. Pressing ESC or clicking the Cancel button exits without updating the angles. On successful completion, the program also updates the current goniometer angles displayed in the goniometer status area at the lower right of the screen.

NOTE: To change the settings of non-controllable axes, see the Collect > Goniometer > Fixed axes command, Section 5.24.

5.14.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(2-Theta) [current value]

$1 .....(Theta1) [current value]

The current 2-Theta (swing) angular reading from the goniometer, to the nearest 0.5 degree. On θ-θ systems, this is the Theta1, tube axis.

$2 .....(Omega) [current value]

$2 .....(Theta2) [current value]

The current omega angular reading from the goniometer, to the nearest 0.5 degree. On θ-θ systems, this is the Theta2, detector axis.

$3 .....(Phi) [current value]

The current phi angular reading from the goniometer, to the nearest 0.5 degree

$4 .....(Chi) [current value]

The current chi angular reading from the goniometer, to the nearest 0.5 degree (leave this field alone if you're connected to a 4-circle goniometer).

$5 .....(X) [current value]

The current X positional reading from the goniometer, to the nearest 0.5 mm.

$6 ..... (Y) [current value]

The current Y positional reading from the goniometer, to the nearest 0.5 mm

$7 ..... (Z) [current value]

The current Z positional reading from the goniometer, to the nearest 0.5 mm

$8 ..... (Aux1) [current value]

The current AUX angular/positional reading from the goniometer, to the nearest 0.5 degree/mm.

$9 ..... (Aux1) [current value]

The current delta position reading from the goniometer. This is only available on systems with a motorized delta axis.

5.15 Collect > Goniometer > Limits • Enter software collision limits

Menu Command: Collect > Goniometer > Limits

Accelerator: none

User Level: 2

SLAM Syntax:

GONIOMETER /LIMITS $1 $2 $3 $4 $5 $6 $7 $8 $9 $0
or
GONIOMETER /LIMITS $1 $2 $3 $4 $5 $6 $7 $8 $9 $0 /XMAX=<n> /XMIN=<n> /YMAX=<n> /YMIN=<n> /ZMAX=<n> /ZMIN=<n> /AMAX=<n> /AMIN=<n> /DMIN=<n> /DMAX=<n>

This command is used to specify the software collision limits for the goniometer axes. They are particularly useful if special devices (for example, a He beam path) are being used or the detector distance has been changed from the factory default and you do not wish to use the preprogrammed defaults.

When invoked from the menu, or run from the command line without arguments, this command displays a dialog box where you can view/edit the arguments described below. Pressing the ENTER key or clicking the OK button stores the limits you've entered. Pressing ESC or clicking the Cancel button exits without modifying the limits.

Ensure that the environment variable SAXI$ADMODEL is defined correctly for your goniometer type, since the default limits are different between 4- and 3-circle systems. Also, ensure that any configuration files you read in correspond to the correct goniometer type, since the limits in the file will be transferred to both the GADDS program and the goniometer controller program.

On three-axis systems, you might see the message: "Warning: Possible omega cable wrap issue when both omega and omega-2theta limits are not used. Recommend using omega-2theta limits of -269 to 89."

Also, you cannot enter a limit range equal to or exceeding 360 degrees. Obviously if you have 360 degrees of unrestricted movement, then you have unlimited movement and you should enter 0.0, 0.0 for both limits.

Finally, whenever the detector distance setting is changed (see Edit > Configure > User settings, Section 4.1), the program will asked:

> Reset to default collision limits for new distance? [yes] [No].

Answer yes and GADDS will read the ASCII file, GADDS$SYSTEM:limits.d for new collision limits based on the goniometer type, stage, video option, and detector distance for the 2θ, ω, and ω-2θ (or $\theta1$, $\theta2$, and $\theta1+\theta2$) limits. Your GADDS administrator may wish to edit this file for your particular system.

5.15.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt and default values in degrees. (Note that a positive limit is a limit on drives which proceed in the positive direction. A negative limit limits drives in the negative direction. If both the positive and negative limit for any angle or axis are zero, the program considers its motion unlimited).

Table 5.1 – D8 DISCOVER Goniometers

		Defaults	
Parameter	**Input Prompt**	**D8** θ–θ	**D8**
$1	Positive 2-Theta limit		90.00
	Positive Theta1 limit	80.00	
$2	Negative 2-Theta limit		-90.00
	Negative Theta1 limit	-10.00	
$3	Positive Omega limit		180.00
	Positive Theta2 limit	80.00	
$4	Negative Omega limit		-180.00
	Negative Theta2 limit	-10.00	
$5	Positive Omega – 2-Theta limit		60.00
	Positive Theta1 + Theta2 limit	0.00	
$6	Negative Omega - 2-Theta limit		-240.00
	Negative Theta1 + Theta2 limit	0.00	
$7	Positive Phi limit (both 0=none)	0.00	0.00
$8	Negative Phi limit (both 0=none)	0.00	0.00
$9	Positive Chi limit (both 0=none)	0.00	0.00
$0	Negative Chi limit (both 0=none)	0.00	0.00

Table 5.2 – PLATFORM Goniometers

		Defaults	
Parameter	**Input Prompt**	**Platform**	**¼-Circle**
$1	Positive 2-Theta limit	90.00	90.00
$2	Negative 2-Theta limit	-90.00	-90.00
$3	Positive Omega limit	180.00	180.00
$4	Negative Omega limit	-180.00	-180.00
$5	Positive Omega - 2-Theta limit	60.00	40.00
$6	Negative Omega - 2-Theta limit	-240.00	-40.00
$7	Positive Phi limit (both 0=none)	0.00	0.00
$8	Negative Phi limit (both 0=none)	0.00	0.00
$9	Positive Chi limit (both 0=none)	0.00	0.12 / 90.12 *
$0	Negative Chi limit (both 0=none)	0.00	-90.12 / -0.12 *

*First number is for transmission mounting, second is for reflection mounting of ¼-circle stage.

Table 5.3 – Other Older Goniometers

		Defaults	
Parameter	**Input Prompt**	**4-Circle**	**3-Circle**
$1	Positive 2-Theta limit	110.00	30.00
$2	Negative 2-Theta limit	-110.00	-85.00
$3	Positive Omega limit	58.00 / 45.00	180.00
$4	Negative Omega limit	-58.00 / -55.00	-180.00
$5	Positive Omega – 2-Theta limit	58.00	60.00
$6	Negative Omega – 2-Theta limit	-58.00	-240.00
$7	Positive Phi limit (both 0=none)	0.00	0.00
$8	Negative Phi limit (both 0=none)	0.00	0.00
$9	Positive Chi limit (both 0=none)	0.00 / 40.00 / 93.00	0.00
$0	Negative Chi limit (both 0=none)	0.00 / -90.00 / -93.00	0.00

Second numbers are for LT attachment in co-axial mode. Third for LT in 30° offset mode.

Table 5.4 – All Goniometers with X, Y, Z, or Aux axes

Parameter	Input Prompt	Defaults
/XMAX=<n>	Positive X limit (both 0=none)	90.00
/XMIN=<n>	Negative X limit (both 0=none)	-90.00
/YMAX=<n>	Positive Y limit (both 0=none)	90.00
/YMIN=<n>	Negative Y limit (both 0=none)	-90.00
/ZMAX=<n>	Positive Z limit (both 0=none)	90.00
/ZMIN=<n>	Negative Z limit (both 0=none)	-90.00
/AMAX=<n>	Positive Aux1 limit (both 0=none)	7.00 / 7.02
/AMIN=<n>	Negative Aux1 limit (both 0=none)	1.00 / 0.98
/DMAX=<n>	Maximum Delta limit (both 0=none)	30.0
/DMIN=<n>	Minimum Delta limit (both 0=none)	6.0

Second numbers are for D8 Discovery systems (Phoenix controllers).

5.16 Collect > Goniometer > Extlimits • Display extended software collision limits

Menu Command: Collect > Goniometer > Extlimits

Accelerator: none

User Level: 2

SLAM Syntax: GONIOMETER /EXTLIMITS

This command is used to graphically draw the extended software collision limits between the omega and chi axes. Mainly used for the 1/4-circle stage where when chi is at -90 degrees, omega is restricted such that the stage will not drive into the collimator.

GADDS$SYSTEM:limits_4.* P3 systems

GADDS$SYSTEM:limits_r.* Reflection 1/4-circle

GADDS$SYSTEM:limits_t.* Transmission 1/4-circle

The extended map limits are read from the various files depending upon which goniometer model is active. To change the limits, you must manually edit this file. Some important considerations are:

- The first and last points must be identical (to form a closed loop).
- Omega ranges of -180 to +180 degrees are special case -> no limit.
- Valid drive range is INSIDE the graphed region.
- These extended limits are used in addition to normal limits.

Any system without a controllable chi circle is unaffected by the extended limits command.

It is important that the environment variable SAXI$ADMODEL is defined correctly for your goniometer type, since the default limits are different between 4-circle and 1/4-circle systems. See Edit > Configure > ShowModel, Section 4.5, for more information.

5.16.1 Arguments

None. Command executes immediately.

5.17 Collect > Goniometer > Speeds • Enter slew drive speeds of axes

Menu Command: Collect > Goniometer > Speeds

Accelerator: none

User Level: 2

SLAM Syntax:

GONIOMETER /SPEEDS $1 $2 $3 $4 $5 $6 $7 $8 $9

or GONIOMETER /SPEEDS $1 $2 $3

or GONIOMETER /SPEEDS $1 $2

This command is used to set the maximum drive speeds for the goniometer axes. These speeds are also used as the “fast” drive speeds in manual mode (see Collect > Goniometer > Manual, Section 5.11).

When invoked from the menu, or run from the command line without arguments, Collect > Goniometer > Speeds displays a dialog box where you can view/edit the arguments described below. Pressing the ENTER key or clicking the OK button updates the drive speeds. Pressing ESC or clicking the Cancel button exits without changing the speeds.

Ensure that the environment variable SAXI$ADMODEL is defined correctly for your goniometer type, since the speed conventions are different among Platform, 4-circle, and older Aztalan (black) 3-circle systems. Also ensure that any configuration files you read in correspond to the correct goniometer type, since the values in the file will be transferred to GADDS and the goniometer controller program. See Edit > Configure > Show model, Section 4.5, for more details.

5.17.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses. The conventions are different for Platform 3-circle, 4-circle, and older Aztalan 3-circle systems and are listed separately with all values in degrees/minute or mm/minute, except for delta that is in cm/min.

Table 5.5 – D8 DISCOVER Multi-Axes Systems

Parameter	Dialog Box Prompt	Default	Maximum Allowable
$1	(2-THETA SPEED)	600.00	1000.00
or $1	(THETA1 SPEED)	600.00	1000.00
$2	(OMEGA SPEED)	600.00	1000.00
or $2	(THETA2 SPEED)	600.00	1000.00
$3	(PHI SPEED)	3600.00	3600.00
$4	(CHI SPEED)	600.0	600.0
$5	(X SPEED)	150.0	1600.0
$6	(Y SPEED)	150.0	1600.0
$7	(Z SPEED)	150.0	1600.0
$8	(AUX SPEED)	50.0	300.0
$9	(DELTA SPEED)	100.0	1000.0

NOTE: On PHOENIX controllers, the maximum allowable speeds are read from the DEVICE.INI configuration file.

Table 5.6 – PLATFORM (beige) Multi-Axes Systems

Parameter	Dialog Box Prompt	Default	Maximum Allowable
$1	(2-THETA SPEED)	600.00	1000.00
$2	(OMEGA SPEED)	600.00	1000.00
$3	(PHI SPEED)	3600.00	3600.00
$4	(CHI SPEED)	600.0	600.0
$5	(X SPEED)	150.0	1600.0
$6	(Y SPEED)	150.0	1600.0
$7	(Z SPEED)	150.0	1600.0
$8	(AUX SPEED)	50.0	300.0

Table 5.7 – PLATFORM (beige) 3-Circle Systems

Parameter	Dialog Box Prompt	Default	Maximum Allowable
$1	(2-THETA SPEED)	1000.00	1000.00
$2	(OMEGA SPEED)	1000.00	1000.00
$3	(PHI SPEED)	3600.00	3600.00

Table 5.8 – 4-Circle Systems

Parameter	Dialog Box Prompt	Default	Maximum Allowable
$1	(2-THETA, OMEGA SPEED)	234.375	600.00
$2	(PHI, CHI SPEED)	600.00	600.00

Table 5.9 – Older Aztalan (black) 3-Circle Systems

Parameter	Dialog Box Prompt	Default	Maximum Allowable
$1	(2-THETA SPEED)	150.00	150.00
$2	(OMEGA, PHI SPEED)	600.00	600.00

CAUTION

Although the software's valid range for speeds is up to the "Maximum Allowable" values (specified above), increasing the slew speeds to above what the goniometer can handle, will result in lost axis position. Heavy stages, or samples, will result in a slower, reliable slew speed for the omega axis. If you increase the speeds above the default, please test the drives for reliability.

5.18 Collect > Goniometer > Zero • Drive all angles to home position (zero degrees)

Menu Command: Collect > Goniometer > Zero

Accelerator: Ctrl+Shift+Z

User Level: 1

SLAM Syntax: GONIOMETER /ZERO

Use this command to quickly drive the goniometer to the “zero” position. The zero position is defined as either:

- All angles to zero degrees (non-XYZ systems)
- XYZ angles to zero degrees
- All angles to zero degrees, except omega to 180 (omega restricted by collision from 0)

When invoked from the menu, this command displays one of the following prompts in a Yes/No message box:

> DRIVE ALL AXES TO ZERO: ARE YOU SURE?
>
> DRIVE XYZ STAGE TO ZERO: ARE YOU SURE?
>
> DRIVE ALL AXES TO ZERO & OMEGA to 180: ARE YOU SURE?

Pressing the Y key, ENTER key, or clicking the Yes button will drive all the goniometer axes to their zero position. Pressing N, the ESC, or the No button will return you to the menu without driving the axes.

In command line mode, the action is the same, except that the program does not prompt before driving the axes to zero.

5.18.1 Arguments

None. Command executes immediately after confirmation prompt.

5.19 Collect > Goniometer > Attenuator • Insert/remove attenuator

Menu Command: Collect > Goniometer > Attenuator

Accelerator: Ctrl+Shift+N

User Level: 1

SLAM Syntax: GONIOMETER /ATTENUATOR

When invoked from the menu, or run from the command line, Collect > Goniometer > Attenuator immediately toggles the status of the hardware beam attenuator on those systems equipped with an attenuator. If the attenuator is currently not inserted, the program opens the shutter (if not already open) and inserts the attenuator. If the attenuator is inserted, the program removes the attenuator from the beam (and must briefly close the shutter to do so). The SHUTTER item in the goniometer status area at the lower right of the display is updated to reflect the new attenuator status.

5.19.1 Arguments

None. Command executes immediately.

5.20 Collect > Goniometer > Shutter • Open/close x-ray shutter

Menu Command:

Collect > Goniometer > Shutter

or Collect > Shutter

Accelerator: Ctrl+Shift+S

User Level: 1

SLAM Syntax:

GONIOMETER /SHUTTER

or SHUTTER

When invoked from the menu, or run from the SLAM command line, Collect > Goniometer > Shutter toggles the status of the X-ray shutter (that is, if the shutter is currently closed, the program opens it and, if it is open, the program closes it). The action is performed immediately, with no prompt for additional input. The SHUTTER item in the goniometer status area at the lower right of the display is updated to reflect the new shutter status.

GADDS supports an optional high-precision rotary shutter. This shutter is intended for use with rotating anodes and synchrotron sources. The normal Bruker shutter on sealed tube systems is perfectly adequate for acquiring high-quality data as is. However, in the case where the high-precision shutter is added to a sealed tube system with existing shutter, GADDS con-

trols both shutters. When shutter open/close commands are issued from GADDS, both shutters are operated, except in the cases of Collect > Add, Collect > Scan > commands (SingleRun, MultiRun, Rotation, etc.), Process > Flood > New, Process > Spatial > New. In these cases, the safety (old) shutter is pre-opened at the start of the command and is closed when the command has been completed. Operations performed between these two events (for example, collection of a frame series) open and close only the high-precision shutter.

5.20.1 Arguments

None. Command executes immediately.

5.21 Collect > Goniometer > Laser • Turn on/off the laser

Menu Command: Collect > Goniometer > Laser

Accelerator: Ctrl+Shift+L

User Level: 1

SLAM Syntax: GONIOMETER /LASER

When invoked with the LASER option from the master menu or when run from the command line GONIOMETER /LASER immediately toggles the status of the hardware laser beam, on those systems equipped with a laser.

5.21.1 Arguments

None. Command executes immediately.

5.22 Collect > Goniometer > Generator • Control the high voltage generator: kv and ma settings

Menu Command: Collect > Goniometer > Generator

Accelerator: Ctrl+Shift+G

User Level: 1

SLAM Syntax: GONIOMETER /GENERATOR $1 $2 /WAIT

When invoked from the menu or when run from the command line without arguments, Collect > Goniometer > Generator displays a dialog box where you can view/edit the desired generator settings. The values in the dialog default to the current generator settings. When in the panel, pressing the ENTER key or clicking the OK button sends the entered generator settings to the Bruker K710D generator. Pressing ESC or clicking the Cancel button in the dialog returns you to the menu without changing the generator settings. The new generator settings are displayed in the goniometer status window.

5.22.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (kV) [current setting or 0]

Enter the desired kV setting for the X-ray generator.

$2 ..... (mA) [current setting or 0]

Enter the desired mA setting for the X-ray generator.

WAIT ..... (Wait Y/N) [No]

Check this option to wait for the generator to reach the desired settings, or leave it unchecked to return to the GADDS menu immediately after sending the new settings to the generator.

5.23 Collect > Goniometer > Det. Stage • Drive delta axis

Menu Command: Collect > Goniometer > Det. Stage

Accelerator: none

User Level: 3

SLAM Syntax: GONIOMETER /DETECTOR $1

Use this command to operate the delta axis (detector distance) on systems with a motorized delta axis. Only Phoenix controllers support a delta axis. The minimum and maximum values are taken from the current software collision limit settings (see Collect > Goniometer > Limits, Section 5.15).

5.23.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(Delta) [current setting]

Enter the destination delta axis (detector distance) in cm.

5.24 Collect > Goniometer > Fixed axes • Set reported settings for non-controllable axes

Menu Command: Collect > Goniometer > Fixed axes

Accelerator: none

User Level: 2

SLAM Syntax: GONIOMETER /FIXEDAXES $1 $2 $3 $4 $5 $6 $7 $8

Use this command to defined the current angles/positions of the fixed, non-controllable axes. Collect > Goniometer > Fixedaxes displays an input panel where you can view/modify the desired destination angles. The values in the input panel default to the current goniometer position. When in the panel, pressing the ENTER key or left mouse button, the program updates the current goniometer angles displayed in the goniometer status area at the lower right of the screen.

NOTE: To change the settings of controllable axes, see the Collect > Goniometer > Update command, Section 5.14.

5.24.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(2-Theta) [current setting]

$1 .....(THETA1) [current setting]

The destination 2-Theta (swing) angle in degrees. Or theta1 (tube) axis.

$2 .....(Omega) [current setting]

$2 .....(THETA2)[current setting]

The destination Omega angle in degrees. Or theta2 (detector) axis.

$3 .....(Phi) [current setting]

The destination Phi angle in degrees.

$4 .....(Chi) [current setting]

The destination Chi angle in degrees.

$5 .....(X) [current setting]

The destination X position in mm.

$6 .....(Y) [current setting]

The destination Y position in mm.

$7 .....(Z) [current setting]

The destination Z position in mm.

$8 .....(Aux1) [current setting]

The destination AUX position in aux units.

5.25 Collect > Goniometer > Home axis • Home goniometer axis

Menu Command: Collect > Goniometer > Home axis

Accelerator: none

User Level: 2

SLAM Syntax: GONIOMETER /HOME $1 $2

When a goniometer controller is first powered up or power-cycled, the setting angle positions may be different from those reported by the controller. While the Collect > Goniometer > Update command allows you to make sure the reported angles agree with those you read from the angular scales on the goniometer, it's difficult to tell if the reported position is off by a small amount. Collect > Goniometer > Home Axis allows a specified axis to be driven to an internal fiducial mark and its position to be updated so that the reported position is exactly consistent from power-up to power-up. In the case of a Platform goniometer, absolute fiducial marks are available (typically at +30.00° in 2-theta and -30.00° in omega), and the axis will seek the fiducial mark when homed. (Some systems, such as micro-diffraction systems have a modified 2-theta fiducial position.) In the case of a P4, the axis seeks the degree mark nearest its current location.

When invoked from the menu, or run from the command line without arguments, Collect > Goniometer > Home Axis displays a dialog box where you can view/edit the input arguments. Pressing the ENTER key or clicking the OK button initiates the “homing” of the requested axis. The goniometer 2-theta or omega axis is driven to within 3° of the home position and a 6-degree search for the home mark is initiated. Phi and chi axes have a home mark every degree.

During the drive, the following message displays:

DRIVING — PRESS ANY KEY TO STOP...

You can halt the drive by pressing a keyboard key (for example, ENTER or the space bar). Pressing ESC or clicking Cancel in the input dialog returns you to the menu without performing the homing operation. On completion of homing, the program updates the current goniometer angles displayed in the goniometer status area at the lower right of the screen.

CAUTION

Aborting homing in the middle of a drive may result in loss of the current angle position. Should you abort homing, you MUST update the current angle and re-home the axis.

5.25.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Axis Number) [1]

This is the number of the axis to be homed, either 1 for 2-theta/theta1, 2 for omega/theta2, 3 for phi, 4 for chi axis, 5 for X, 6 for Y, 7 for Z, 8 for zoom, 9 for delta (detector distance).

$2 .....(Velocity) [250]

Velocity to drive during home search in steps/degree. Range 1 to 1024. On D8 systems, this parameter is ignored.

5.26 Collect > Goniometer > Park XYZ • Park large XYZ stage (OM=0, X=far right, Z=back)

Menu Command: Collect > Goniometer > Park XYZ

Accelerator: none

User Level: 1

SLAM Syntax: GONIOMETER /PARK

Use this command to park the XYZ stage in an out of the way position. When invoked with the PARK option from the GONIOMETER submenu GONIOMETER /PARK displays the following prompt on the bottom status line:

PARK XYZ STAGE: ARE YOU SURE?

Pressing the Y key, ENTER key, or left mouse button will drive the XYZ stage to the “PARK” or lock-down position. First, the Z-axis is driven back to the current negative Z collision limit (see GONIOMETER /LIMITS). Then, both omega and X are driven to 0.0 and far right limit, respectively. The user can then lock down the large XYZ stage by turning the lock screw.

Pressing N, the ESC key, or right mouse button will return you to the GONIOMETER submenu without driving the axes.

In command line mode, the action is the same, except that the program does not prompt before driving the axes to “park.”

5.26.1 Arguments

None. Command executes immediately after confirmation prompt.

5.27 Collect > Goniometer > XYZ collision • Avoid XYZ stage collision with detector

Menu Command: Collect > Goniometer > XYZ collision

Accelerator: none

User Level: 2

SLAM Syntax: GONIOMETER /XYZ $1 $2 $3 $4

Use this command to define the corners of the detector and XYZ stage to avoid collisions between the two units when attempting a drive operation.

When invoked with the XYZ option from the GONIOMETER submenu or when run from the command line without arguments, GONIOMETER /XYZ displays an input panel where you can view/modify the desired settings.

5.27.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Detector Distance) [current distance in mm]

The detector distance, in mm., is measured from the center of the goniometer to the physical face of the detector. It is the same detector distance which is entered in CON-

FIGURE /EDIT menu, except in mm, not cm. This value defaults to the current detector distance.

$2 .....(Detector Half-Width) [115 mm]

The detector half-width, in mm., is measured from the center of the 2-theta arm to the edge of the detector housing.

$3 .....(XYZ Stage/Sample Half-Width) [76 mm]

The sample half-width is measured from center of the XYZ stage to the edge of the sample which can approach the detector face. This value is always entered as positive.

$4 .....(XYZ/Stage Depth Reference) [0 mm]

The sample depth reference, is the Z offset which when added to the current Z axes setting will give zero when the plane of the sample face touches the center of the goniometer. This value is SIGNED.

5.28 Collect > Goniometer > Temperature • Watlow Series 988 Temperature Controller

Menu Command: Collect > Goniometer > Temperature

Accelerator: Ctrl+Shift+T

User Level: 1

SLAM Syntax: GONIOMETER /TEMP $1 /RAMP=<n> /HOLD=<n> /WAIT

Operate a temperature controller using the secondary COM port, which defaults to COM2:, but can be specified with the command line argument: /TCPORT=#, where # is the com port number (1–4). Currently supported temperature controllers are:

- Watlow Series 988
- AntonPAAR KHR
- EuroTherm 800 series
- EuroTherm 905
- DHS-900/DCS-350 (Eurotherm 2600/2700)

Connection to the TC is only established upon entering the GONIOMETER /TEMP command and is always disconnected upon exiting this command. This permits a more elaborate TC control program to be run from either the SYSTEM command or as a separate and independent program task; however, the GONIMOETER /TEMP command will not function if the TC port is already in use or allocated by another program. You must terminate any TC control program before executing the GONIOMETER / TEMP command.

All temperature parameters are stored in subsequently created frame headers. You may override waiting for the either the ramp up to temperature, the hold time, or both with either the <Enter> or <Lf-button> and the temperature parameters will still be stored in newly created frame headers. Interrupting with <Ctrl-Break> will not store the new temperature settings.

5.28.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Set Point) [22.0]

Enter the requested temperature in degrees C.

/RAMP=<n>..... (Ramp Rate) [100.0]

Enter requested ramping rate in degrees C per minute.

/HOLD=<n> ..... (Hold Time) [0.0]

Enter hold time for stabilizing in seconds. Whenever this value is non-zero, the program will pause until the temperature has been held at the requested set point for the required amount of time.

/WAIT .....(Wait) [Y]

"Y" to wait for ramping up to requested temperature setting. If the hold time is non-zero, waiting for ramping up to temperature set point is automatically performed.

5.29 Collect > Goniometer > Encoders • Adjust encoder zero offsets

Menu Command: Collect > Goniometer > Encoders

Accelerator: none

User Level: 3

SLAM Syntax:

GONIOMETER /ENCODERS $1 $2 $3 $4

or GONIOMETER /ENCODERS $1 $2 $3 $4 $5 $6 $7 $8 $9

This command allows you to access the Phoenix AV or GGCS EZ command without leaving GADDS. Because this command changes the zero positions of the goniometer angles, it is recommended that only the person in charge of your system (for example, system manager) or Bruker service personnel use this command. This command subtracts the specified amount to the encoder zero of the specified axis. For example, entering a value of 0.05 for omega will add 0.05 to all subsequent observed omega values.

The refined values for the omega and chi encoder zeros provide a general indication when encoder zeros need to be adjusted, BUT BE VERY CAREFUL. Because of the large number of parameters refined in the unit cell

least squares and the potential for coupling among parameters. DON'T CHANGE ENCODER ZEROS BASED ON THE RESULT OF A SINGLE LEAST SQUARES. Over time, you'll get a general feeling whether your data sets, for example, all tend to indicate that the omega zero is high; make adjustments based on average results accumulated over time. The least squares zero adjustments are values that should be added to the angle zero, so negate the value determined from least squares before entering it here.

5.29.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

$1 .....(2-Theta) [0.00]

$1 .....(Theta1) [0.00]

Enter the 2-theta encoder zero offset in degrees to be added to subsequent 2-theta values reported by the controller. Or theta1 axis (tube).

$2 .....(Omega) [0.00]

$2 .....(Theta2) [0.00]

Enter the omega encoder zero offset in degrees to be added to subsequent omega values reported by the controller. Or theta2 axis (detector).

$3 ..... (Phi) [0.00]

Enter the phi encoder zero offset in degrees to be added to subsequent phi values reported by the controller.

$4 ..... (Chi) [0.00]

Enter the chi encoder zero offset in degrees to be added to subsequent chi values reported by the controller.

$5 ..... (X) [0.00]

Enter the X encoder zero offset in mm to be added to subsequent X values reported by the controller.

$6 ..... (Y) [0.00]

Enter the Y encoder zero offset in mm to be added to subsequent Y values reported by the controller.

$7 ..... (Z) [0.00]

Enter the Z encoder zero offset in mm to be added to subsequent Z values reported by the controller.

$8 ..... (Aux1) [0.00]

Enter the Aux1 encoder zero offset in units to be added to subsequent Aux values reported by the controller.

$9 .....(Delta) [0.00]

Enter the Delta encoder zero offset in cm to be added to subsequent Delta values reported by the controller.

5.30 Collect > Scan > SingleRun • Perform a single scan series— Resume an interrupted SingleRun

Menu Command: Collect > Scan > SingleRun

Accelerator: Ctrl+Shft+F1

User Level: 1

SLAM Syntax:

SCAN /SINGLERUN $1 [/2THETA=<n> | /THETA1=<n>] [/OMEGA=<n> | /THETA2=<n>>] /PHI=<n> /CHI=<n> /X=<n. /Y=<n> /Z=<n> /AUX=<n> /AXIS=<n> /WIDTH=<n> /SCANTIME=<n> /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n> /NAME=<s> /RUN=<s> /FRAMENO=<s> /DISPLAY=<n> /REAL TIME /CLEAR /OLDXENGEN /MODE=<n> /ROTATE /VIDEO /OSCILLATE=<s> /AMPLITUDE=<n> /AUTOZALIGN

Additional SLAM Syntax for dual detector mode:

… /SNAME=<s> /SRUN=<n> /SFRAME=<s>

Collect > Scan > SingleRun allows you to collect a scan series comprising one or more contiguous frames of data starting at specified goniometer setting angles. Normally, Collect > SingleRun stores frames as an unwarped image, after applying the spatial correction

table. It also applies the flood-field (intensity uniformity) correction as the counts are received.

When you invoke the command from the menu (or the command line without arguments), a dialog box appears where you can view/edit the arguments described below as follows:

- press ENTER or click the OK button to start scanning.
- press ESC or click the Cancel button to return to the menu.

You can interrupt a scan as follows:

- press ESC to stop after finishing collecting the current frame.
- press CTRL+BREAK to interrupt the scan.
- press CTRL+S to temporarily stop after finishing collecting the current frame (press CTRL+Q to resume).

NOTE: Unlike the Collect > Scan > MultiRun command, an interrupted SingleRun scan cannot be restarted with the Collect > Scan > Resume command. Instead, the SingleRun parameters are automatically decremented after each frame is saved. Thus, you can simply reissue a SingleRun command to resume where it left off. Also, Collect > Scan > SingleRun does not precheck the scan range for potential collision the way Collect > Scan > MultiRun does. If you need these capabilities, use Collect > Scan > MultiRun (which can perform a single series if desired).

When you interrupt a scan with CTRL+BREAK, the goniometer returns to the starting scan angle of the current scan. This repositioning is performed by backing up to the starting position minus one frame width (or +/-0.5° maximum), then driving forward to the starting position. The same positioning technique is used when driving to the first scan in a new series, which makes the positioning extremely repeatable but does require you to allow for an extra scan width at the beginning of the series when you're starting close to the goniometer collision limits.

The current configuration is saved in the current default configuration file (usually gadds._nc) before starting the first scan, which makes recovery easier in the event of a power failure, etc.

The filename of the first frame is generated from the Job Name, Run# and Starting Frame# (listed below) as defined in Edit > Configure > User settings: Frame Naming Parameters (see Section 4.1.1).

Because, one typically starts a scan and walks away from the instrument, GADDS will precheck that the available disk space is sufficient for storing the requested number of frames in 8-bit mode. However, if the frames are stored in 16-bit mode, you may still run out of disk space during the requested scan operation.

The CPU intensive VIDEO program is always set to frozen mode at the start of all scan commands.

5.30.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses.

$1 .....(# rames) [1]

The number of frames to be acquired in this series. Ensure that the generated filename of the last frame in the series is a valid filename with regard to the frame naming parameters in the Edit > Configure > User settings dialog.

/2THETA=<n> .....(2-Theta) [0.00]

/THETA1=<n> .....(Theta1) [0.00]

The detector swing angle (goniometer 2-theta setting angle), in degrees, at which GADDS positions the goniometer at the start of the frame series. Valid values are -180° to 180°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering “@” will be automatically replaced with current angle setting. On θ-θ systems, this is the θ1 angle (tube).

/OMEGA=<n>..... (Omega) [0.00]

/THETA2=<n>..... (Theta2) [0.00]

The omega angle, in degrees, at which GADDS positions the goniometer at the start of the frame series scans. If you specify a scan axis (see /AXIS=<n> below) of 2, omega will be scanned as each frame is taken. Otherwise, omega remains fixed throughout the frame series. Valid values are -360° to 360°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering “@” will be automatically replaced with current angle setting. On θ-θ systems, this is the θ2 angle (detector).

/PHI=<n>..... (Phi) [0.00]

The phi angle, in degrees, at which GADDS positions the goniometer at the start of the frame series scans. If you specify a scan axis (see /AXIS=<n> below) of 3, phi will be scanned as each frame is taken. Otherwise, phi remains fixed throughout the frame series. Valid values are -360° to 360°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering “@” will be automatically replaced with current angle setting.

/CHI=<n>.....(Chi) [0.00]

The chi angle, in degrees, at which GADDS positions the goniometer at the start of the frame series. A Platform goniometer is fixed at CHI=54.74°. An older Aztalan (black) 3-circle goniometer is fixed at CHI=45°. Valid values are -360° to 360°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering "@" will be automatically replaced with current angle setting.

/X=<n> .....(X) [0.00]

The X-axis position, in mm, at which GADDS positions the goniometer at the start of the frame series. Entering "@" will be automatically replaced with current axis position setting.

/Y=<n> .....(Y) [0.00]

The Y-axis position, in mm, at which GADDS positions the goniometer at the start of the frame series. Entering "@" will be automatically replaced with current axis position setting.

/Z=<n>.....(Z) [0.00]

The Z-axis position, in mm, at which GADDS positions the goniometer at the start of the frame series. Entering "@" will be automatically replaced with current axis position setting.

/AUX=<n>..... (Aux) [1.00]

The Aux1 axis position, in units, at which GADDS positions the goniometer at the start of the frame series. Entering "@" will be automatically replaced with current setting. Typically, this axis is used for the video zoom lens and is entered as a magnification factor in the range 1.0 to 7.0.

/AXIS=<n>..... (Scan Axis #) [2]

The number of the axis to be scanned, as follows: 2 for omega scans, 3 for phi scans, 4 for chi, 5 for X, 6 for Y, or 7 for Z, N=None, C=Coupled, or T=Tube (on theta-theta systems). Note that while SAINT can reduce phi scans taken at any chi angle, some data reduction programs (XENGEN) may not be able to reduce phi-scan data unless it was taken at CHI=0. When using a restrictive data-reduction package, you must perform omega scans on both the Platform goniometer and the older Aztalan (black) 3-axis.

/WIDTH=<n> ..... (Frame Width) [-0.25]

The scan width, in degrees (either positive or negative), of each frame to be acquired. Thus, the starting scan angle for the Nth frame in the series (where the first frame is N=0) is OMEGA+N*WIDTH if the axis (above) is 2, or PHI+N*WIDTH if the axis (above) is 3 (where WIDTH, OMEGA, and PHI are the values given on the same line of the array). The intensity within a frame is

uniformly distributed with respect to scan angle over the range WIDTH specified here (unless 3-circle frames are taken by oscillation, in which case the ends of the range have slightly higher weight, and there may be some overlap or underlap of successive frames; oscillation can however compensate for other sources of error such as intensity fluctuation due to an unstable source).

/SCANTIME=<n>…(Seconds/Frame) [1:00.00]

The accumulation time, in seconds, during which each frame is to be acquired. You can enter time in decimal seconds or in the format HH:MM:SS.SS (where HH represents hours, MM minutes, and SS.SS decimal seconds). Valid values are 0.05 to 32,767 seconds. The default value is 60.

/TITLE=<s> .....(Title) [Scan frame]

Enter a title for the output frames (80 characters maximum). The default entry is the sample title from the Project > New/Copy/Edit dialog box (or “Scan Frame”). If you invoked this command from the command line, you must enclose any title containing blanks in double quotes.

$FILE:<filename> will read up to eight 72-character title lines from an ASCII file and place these title strings into the eight “TITLE” lines in the frame header. The format of the ASCII file is: “R#:<single line of title information>”, where “R#” is the run number, taken from the filename. Repeat up to eight times for each run.

/SAMPLE=<s>..... (Sample Name) [Corundum]

Enter sample name, to be stored in frame header. If no name is specified, the default name of “Corundum” will be entered.

/NUMSAMPLE=<s>…(Sample Number) [0]

Enter sample number, to be stored in frame header. The permitted range is from 0 to 32,767, with a default setting at 0.

/NAME=<s>..... (Job Name) [NEWFRAM]

Enter the base filename for the output frames. The filenames for each series of output frames are generated by adding the series RUN# and an extension built from the series starting FRAME# to the end of this base name. For example, if the Job Name is LYS, the Run Number is 04, and the starting Frame Number is 000 (assuming that the number of characters in a Run Number is set to 2 and the number of characters in a Frame Number is set to 3 in the Edit > Config dialog), the data files would be named (in sequence) LYS04.000, LYS04.001, LYS04.002, and so forth. For more information, see Section 4.1.1, Edit > Configure > User settings: Frame Naming Conventions.

The default name if none is specified is NEWFRAM.

The Job Name can contain an NT drive and directory name, if desired, but you should use the project data directory instead. The output filename is merged with the project's working directory defined in the Project > New|Copy|Edit dialog prior to creating the output frame. If you specify $NULL as the Job Name, the frames are sent to the null handler and discarded. (Note: $NET is NOT supported under GADDS, please do not use.)

/RUN=<s> .....(Run #) [0]

This is the Run Number of the series. This is not actually a number, but is rather taken as RUNCHARS characters of ASCII text. Also, all characters must be valid characters to be used with filenames because the Run Number becomes part of the generated output filename. Basically, the Run Number is formatted and appended to the output base filename before the file extension. See Frame Naming Conventions, Edit > Configure > User settings command, and Collect > Scan > MultiRun command for more details.

/FRAMENO=<s>…(Frame #) [000]

This is the starting frame number for the series. Like the Run Number, this is actually taken as text of length NUMCHARS rather than as a numeric value. The text specified here will be used as the extension of the first output frame in the series and will be incremented according to the frame naming parameters to form the extensions of subsequent frames. See Frame Naming Conventions, Edit > Configure > User settings command, and Collect > Scan > MultiRun command for more details.

/DISPLAY=<n> ..... (Max Display Counts) [31]

Enter the number of counts to be mapped to the highest display memory value (that is, to set the display for acquiring frames). This value is usually white on the screen. The valid value range is -2 to 1,000,000. However, Three special values are defined as follows: 0 suppresses display of frames as they are acquired; -1directs the program to pick a reasonable value; and -2 directs the program to use the current level. The default value is 31.

/REAL TIME ..... (Real-time Display?) [Yes]

This qualifier, when present, displays data as it is being collected. The display does require additional processing time, and will limit the maximum rate at which counts can be accumulated. If the MAX DISPLAYED COUNTS qualifier is given a non-zero value, the frame will be automatically displayed at the end of each scan if real-time display is off. This latter display method has no effect on observed data rate. Unless your data rate is very low, it is better NOT to use real-

time display in the course of a SCAN command, even though the default here is “Y”. Note: Real-time is not permitted whenever display _ 0.

While real-time display is active, you can change the upper display limit using the plus key to increase or the minus key to decrease the current limit by a factor of two. (Range is 7 to 524287). Modify the contrast using the left and right arrow keys. Modify the brightness using the up and down keys. Holding the control key down in combination with any arrow key results in a greater change of contrast or brightness.

/CLEAR .....(Pre-Clear?) [Yes]

This parameter specifies whether or not the memory will be cleared before the new data frame is collected. If clearing is not performed, each successive frame in the series will be added to the counts accumulated before is collection is begun (effectively producing a rotation picture). Enter “Y” to clear the memory, “N” otherwise. The default value is Y (clear).

/OLDXENGEN .....(Xengen Output Format?) [No]

Check this option to write frame in XENGEN 1,3 format (more correctly, in the old PCS computer format). The default, is unchecked (Bruker format).

/MODE=<s>…(Mode (Step/Scan/Oscillate)) [Scan]

Selects either a scan, oscillate, or stepping (between frames of a series) of the requested drive along the drive axis.

Perform sample oscillation (3-circle goniometer only). Normally, scans are taken by continuously (actually in 0.0005 deg steps) driving the specified scan axis of the goniometer as the data are accumulated. This provides a very uniform distribution of collection time versus scan angle, as well as very good contiguity between successive frames. If the /MODE qualifier is set to oscillate, the scan angle is driven back and forth between the starting position and starting position plus the frame width approximately once per second. AN INTEGRAL NUMBER OF OSCILLATIONS IS ALWAYS PERFORMED IN THIS MODE -- the collection time per frame is adjusted as necessary to accommodate an integral number of ~1 s oscillations. The default is “Scan.”

In general, oscillation is not recommended. Drawbacks are that the ends of the scan range have anomalously high weight (since the goniometer must stop and restart at the end of each oscillation), and there may be some overlap or underlap of successive frames. Oscillation can however compensate for some sources of error such as

intensity fluctuation due to an unstable source, and is therefore an option.

/ROTATE.....(Rotate Sample?) [No]

Perform sample rotation in phi. When used in conjunction with /MODE=OSCILLATE, an integer number of rotations are performed during each oscillation. Use of both the /MODE=OSCILLATE and /ROTATE arguments are designed for micro- diffraction applications, where a “random” sample is desired.

/VIDEO.....(Capture Video Image?) [No]

Capture vide image of sample with same name and .TIF extension. Requires a system equipped with the video option. The video capture program must be running in a separate window.

Only on dual detector systems are additional parameters for control of the Slave frame buffer.

/OSCILLATE=<s>..(Sample Osc) [None]

Select the axes to oscillate during data collection. Valid entries are: “None”, “X”, “XY”, “XYZ”, “Y”, “YZ”, or “Z.”

/AMPLITUDE=<n> (Amplitude) [0.0]

Enter the half amplitude of the oscillations in range 0 to +25 mm. Oscillation occurs between the starting position minus amplitude and the starting position plus amplitude and uses a speed of half the maximum drive speed for that axis.

/AUTOZALIGN..... (Auto Z Align) [No]

Check “Yes” to perform automatic sample height alignment using laser spot imaging. This feature requires VIDEO 1.3.02 or later. If Zoom is 1.0, you must enter a starting Z value that is within 3.5 mm of the true sample height. At Zoom of 7.0, starting Z must be within 0.5 mm of true position.

/SNAME=<s> ..... (Slave Job Name) [NEWFRA2]

Job name for frames collected on Slave frame buffer.

/SRUN=<s> ..... (Slave Run #) [0]

Run number for frames collected on Slave frame buffer.

/SFRAME=<s> ..... (Slave Frame #) [000]

Starting frame number for frames collected on Slave frame buffer.

5.31 Collect > Scan > EditRuns • Edit parameters for MultiRun scans

Menu Command: Collect > Scan > EditRuns

Accelerator: Ctrl+Shft+F2

User Level: 1

SLAM Syntax: SCAN /EDITRUNS (interactive command only)

Use this command to create, read, or edit a run list (often called an array) of scans that you wish to acquire in multiple-run fashion (where one or more series of contiguous frames are collected without intervention).

Upon entering a Collect > Scan > EditRuns command, GADDS displays a run list with current settings. (A typical list follows.) Each run list is identical in format to that in ASTRO, allowing you to transfer run lists between GADDS and ASTRO. (Use the [READ...] button in the dialog box to import the run list written by ASTRO.) On ASTRO list with an extra DeltaD column, only those lines with DeltaD=0.0 are read.

Typical run list:

Run#	Frame#	2-Theta	Omega	Phi	Chi	Axis	Width	#Frames	Time
0	001	-28.00	-28.00	0.00	54.74	2	-0.300	606	10.00
1	001	-28.00	-28.00	90.00	54.74	2	-0.300	435	10.00
2	001	-28.00	-28.00	180.00	54.74	2	-0.300	230	10.00
3	001	-28.00	-28.00	0.00	54.74	2	-0.300	50	10.00

Each line of a run list defines one contiguous scan series. When entering the individual run arguments, keep in mind the following special considerations:

- The RUN#, FRAME#, and #FRAMES must conform to the frame naming parameters. (See Edit > Configure > User settings command.)
- The number of runs (or lines) must not exceed the maximum number of runs allowed by RUNCHARS and RUNBASE (see Edit > Configure > User settings command). The default maximum number of runs is 36. The absolute maximum is 51.
- All generated filenames must be valid and should not create duplicate names (explained later in this section).

With these considerations in mind, we recommend that you always configure the frame naming conventions as follows:

- For 36 or fewer runs, set the “Base of Run #” (in the Edit > Configure > User settings dialog) to base 36, which will prevent the run number from wrapping from 9 to 0. The “Characters in Run #” should be 1. These are the default settings.
- For greater than 36 runs, you must set the “Characters in Run #” (in the Edit >Configure > User settings dialog) to 2 characters. The “Base of Run #” can be base 10, if you find it more convenient.

Each line of a run list contains the following items:

RUN#

This is the Run Number of the series. This is not actually a number, but is rather taken as RUNCHARS characters of ASCII text. Also, all characters must be valid characters to be used with filenames because the Run Number becomes part of the generated output filename. Basically, the Run Number is formatted and appended to the output base filename before the file extension. See Frame Naming Conventions, Edit > Configure > User settings command, and Collect > Scan > MultiRun command for more details.

FRAME#

This is the starting frame number for the series. Like the Run Number, this is actually taken as text of length NUMCHARS rather than as a numeric value. The text specified here will be used as the extension of the first output frame in the series and will be incremented according to the frame naming parameters to form the extensions of subsequent frames. See Frame Naming Conventions, Edit > Configure > User settings command, and Collect > Scan > MultiRun command for more details.

2-THETA (Swing)
THETA1 (Tube)

The detector swing angle (goniometer 2-theta setting angle), in degrees, at which GADDS positions the goniometer for the frame series scans. Valid values are -180° to 180°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering "@" will be automatically replaced with current angle setting. On θ-θ systems, this is θ1 (tube).

OMEGA
THETA2 (detector)

The omega angle, in degrees, at which GADDS positions the goniometer at the start of the frame series scans. If you specify a scan axis (below) of 2, omega will be scanned as each frame is taken. Otherwise, omega remains fixed throughout the frame series. Valid values are -360° to 360°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering "@" will be automatically replaced with current angle setting. On θ-θ systems, this is θ2 (detector).

PHI

The phi angle, in degrees, at which GADDS positions the goniometer at the start of the frame series scans. If you specify a scan axis (below) of 3, phi will be scanned as each frame is taken. Otherwise, phi remains fixed throughout the frame series. Valid values are -360° to 360°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering "@" will be automatically replaced with current angle setting.

CHI

The chi angle, in degrees, at which GADDS positions the goniometer for this frame series. A Platform goniometer is fixed at CHI=54.74°. An older Aztalan (black) 3-circle goniometer is fixed at CHI=45°. Valid values are -360° to 360°, but are typically reduced by the current software collision limits as defined in Collect > Goniometer > limits command. Entering "@" will be automatically replaced with current angle setting.

AXIS

The number of the axis to be scanned, as follows: 2 for omega scans, 3 for phi scans, 4 for chi, 5 for X, 6 for Y, 7 for Z, or -1 for coupled. Note that while SAINT can reduce phi scans taken at any chi angle, some data reduction programs (XENGEN) may not be able to reduce phi-scan data unless it was taken at CHI=0. When using a restrictive data-reduction package, you must perform

omega scans on both the Platform goniometer and the older Aztalan (black) 3-axis.

WIDTH

The scan width, in degrees (either positive or negative), of each frame to be acquired. Thus, the starting scan angle for the Nth frame in the series (where the first frame is N=0) is OMEGA+N*WIDTH if the axis (above) is 2, or PHI+N*WIDTH if the axis (above) is 3 (where WIDTH, OMEGA, and PHI are the values given on the same line of the array). The intensity within a frame is uniformly distributed with respect to scan angle over the range WIDTH specified here (unless 3-circle frames are taken by oscillation, in which case the ends of the range have slightly higher weight, and there may be some overlap or underlap of successive frames; oscillation can however compensate for other sources of error such as intensity fluctuation due to an unstable source).

#FRAMES

The number of frames to be acquired in this series. Ensure that the generated filename of the last frame in the series is a valid filename with regard to the frame naming parameters in the Edit > Configure > User settings dialog.

TIME

The accumulation time, in seconds, during which each frame is to be acquired. You can enter time in decimal seconds or in the format HH:MM:SS.SS (where HH represents hours, MM minutes, and SS.SS decimal seconds). Valid values are 0.05 to 32,767 seconds.

When you invoke this command (> EditMulti), GADDS displays a scrollable editing window, listing all scan series currently in the corresponding array. You can add to, delete from, or reorganize the list as desired using the appropriate screen-editing functions (see Section 1.5, Dialog Box and Keyboard Conventions).

When you invoke the multirun scan command (Collect > Scan > MultiRun), each series will be acquired in the order they appear in the corresponding array. GADDS generates output filenames for each frame from the Job Name (in the Collect > Scan > MultiRun dialog box). GADDS also generates the Run Number (given for the series in the array), the starting Frame# (given for the series in the array), the Frame# being collected, and the frame naming parameters (defined in the Edit > Configure > User settings input panel). The first and last generated filenames in each frame series must be valid. Also, the generated filenames between frame series should not overlap. Always check the bottom status line when you first start a new Collect > Scan > MultiRun to ensure that filenames are being synthesized the way you want, to avoid duplication of filenames during data collection (which will overwrite the previous file).

The EditRuns command is an interactive command, meaning that you can invoke it from the command line, but it will not proceed without user intervention. And it has no built-in command-mode time-out as with other scrolling output windows. Additionally, the Collect > Scan > MultiRun does not work well from script files, as you cannot define the run list in command mode. Thus, we recommend using the equivalent SCAN/SINGLERUN script commands instead.

5.31.1 Arguments

None. Command executes immediate for interactive editing.

5.32 Collect > Scan > MultiRun • Perform several series, as setup in the EditRuns form

Menu Command: Collect > Scan > MultiRun

Accelerator: Ctrl+Shft+F3

User Level: 1

SLAM Syntax:

SCAN /MULTIRUN $1 /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n> /DISPLAY=<n> /REAL TIME /CLEAR /OLDXENGEN /STARTRUN=<n> ENDRUN=<n> /MODE=<n> /ROTATE /VIDEO /OSCILLATE=<S> /AMPLITUDE=<n>

Additional SLAM Syntax for dual detector mode:

… /SNAME=<s>

NOTE: As one cannot load the run list in command mode, we recommend using the equivalent SCAN /SINGLERUN commands in script mode.

This command allows you to collect multiple scan series, each containing one or more contiguous frames of data starting at specified goniometer setting angles. Normally, Collect > Scan > MultiRun stores frames as an unwarped image, after applying the spatial correction table. It also applies the flood-field (intensity uniformity) corrections as the counts are received.

Before invoking Collect > Scan > MultiRun, you must set the parameters that are unique from series to series. (See Section 5.31, Collect > Scan > EditRuns command, for details on these settings and the generation of filenames.) Then use Collect > Scan > MultiRun to define those parameters that are the same for all the different scan series to be performed and start the scans.

When you invoke the command from the menu (or the command line without arguments), a dialog box appears where you can view/edit the arguments described below as follows:

- press ENTER or click the OK button to start scanning.
- press ESC or click the Cancel button to return to the menu.

You can interrupt a scan as follows:

- press ESC to stop after finishing collecting the current frame (soft abort).
- press CTRL+BREAK to interrupt the scan (hard abort or immediate abort).

During actual frame data collection, a small summary file is written and updated after each frame is collected. This file contains the current status of data collection, including the current run and frame number, current angle settings, and elapsed data collection time. This file is

used to resume a data set that has been interrupted.

To resume acquiring data where the scan operation was interrupted (even by power failure), use the Collect > Scan > ResumeRuns command. (See Section 5.33 for more details.)

When you interrupt a scan with CTRL+BREAK, the goniometer returns to the starting scan angle of the current scan. This repositioning is performed by backing up to the starting position minus one frame width (or +/- 0.5° maximum), then driving forward to the starting position. The same positioning technique is used when driving to the first scan in a new series, which makes the positioning extremely repeatable but does require you to allow for an extra scan width at the beginning of the series when you're starting close to the goniometer collision limits.

The current configuration is saved in the current default configuration file (usually gadds._nc) before starting the first scan, which makes recovery easier in the event of a power failure, etc.

The filename of the first frame is generated from the Job Name, Run# and Starting Frame# (from the appropriate line in the run list) as defined in Edit > Configure > User Settings: Frame Naming Parameters (see Section 4.1.1).

Because, one typically starts a scan and walks away from the instrument, GADDS will pre-check that the available disk space is sufficient for storing the requested number of frames in 8-bit mode. However, if the frames are stored in 16-bit mode, you may still run out of disk space during the requested scan operation(s).

5.32.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses. These arguments are the same as the similar singlerun type scans and are, thus, explained in Section 5.30. See that section for explanations.

$1 ..... (Job Name) [NEWFRAM]

See /NAME=<s> in Section 5.30.

/TITLE=<s> ..... (Title) [Scan Frame]

/SAMPLE=<s>..... (Sample Name) [Corundum]

/NUMSAMPLE=<n>(Sample Number) [0]

/DISPLAY=<n> ..... (Max Display Counts) [31]

/REAL TIME ..... (Real-time Display?) [Y]

/CLEAR ..... (Pre-Clear?) [Y]

/OLDXENGEN..... (Xengen Output Format?)[N]

See Section 5.30.

/STARTRUN=<n>…(Sequence # of Starting Run) [1]

You can collect just a specified range of the scan series set up in the run list using STARTRUN and ENDRUN. With STAR-

TRUN you enter the first line number (not the RUN#) in the run list for which data collection is to be performed. The lines are numbered 1–50. The default is 1, and the valid range is 1–50.

/ENDRUN=<n> .....(Sequence # of Ending Run) [9999]

You can collect just a specified range of the scan series set up in the run list using STARTRUN and ENDRUN. With ENDRUN you enter the line number (not the RUN#) in the run list after which data collection is to be terminated. The lines are numbered 1–50. The default is 9999 (which works the same as 50), and the valid input range is 1–32767.

/MODE=<s> .....(Mode (Scan / Oscillate / Step)) [Scan]

/ROTATE.....(Rotate Sample?) [No]

/VIDEO.....(Capture Video Image?) [No]

/OSCILLATE=<s>..(Sample Osc) [None]

/AMPLITUDE=<n> (Amplitude) [0.0]

See Section 5.30.

Only on dual detector systems are additional parameters for control of the Slave frame buffer.

/SNAME..... (Slave Job Name) [NEWFRA2]

See Section 5.30.

Collect > Scan > MultiRun checks for possible collision at the extremes of all scans before beginning the first run. If the first or last frame in a run is outside the set limits, the program displays a box with the message:

PROBABLE COLLISION IN 1ST SCAN OF EDITRUNS LINE <line #>

or

PROBABLE COLLISION IN LAST SCAN OF EDITRUNS LINE <line #>

Here, <line #> represents the number of the line (starting at 1) in the run list which produced the message. You can continue with the scans or quit (to re-edit the run list) and try again.

The current program configuration is saved in the current default configuration file (usually gadds._nc) before starting the first scan, which makes recovery easier in the event of a power failure, etc.

For single crystal type applications, you can use Collect > Scan > MultiRun collect multiple scan series, which covers a little more than half the entire Ewald sphere. This strategy allows you to obtain the full amount of coverage needed to solve the structure, regardless of unit cell size or Laue class, without any need for preplanning with ASTRO.

The default hemisphere runs require about 7.5 hours for full data collection (with 10-seconds-per-frame scan time) and comprise 3 runs totaling about 1250 frames. They are set up assuming a sample-to-detector distance of about 6 cm, which provides full coverage out to better than 0.93 Å (45° with Mo radiation). These default hemisphere runs provides the best redundancy, which improves the quality of the data and absorption corrections. For high-symmetry Laue groups, it's possible to collect a full data set in less time (typically about 4 hours, 750 frames). However, the default hemisphere runs will probably produce a higher quality data set.

In addition, ASTRO is available for preplanning a data collection strategy that minimizes data collection time for a single asymmetric unit or asymmetric unit plus Bijvoet pairs. With this approach, you can often collect enough data for structure solution in 2 or 3 hours on crystals with orthorhombic or higher symmetry (again, sacrificing redundancy).

Before invoking Collect > Scan > MultiRun, you can view/edit the runs to be performed (as needed) with Collect > Scan > EditRuns, although the default runs supplied should be satisfactory in most cases (unless you are using more restrictive collision limits).

GADDS retrieves the defaults for multirun scans from the gadds._nc file (located in the project directory). The defaults for new projects are taken either from the current settings or the gaddsdef._nc file (located in the GADDS system directory). Should you need to change between 3-circle and 4-circle runs, here are the currently used defaults for you to enter:

Table 5.10 – Default 3-circle Hemisphere Runs

Run#	Frame#	2-Theta	Omega	Phi	Chi	Axis	Width	#Frames	Time
0	001	-28.00	-28.00	0.00	54.70	2	-0.300	606	10.00
1	001	-28.00	-28.00	90.00	54.70	2	-0.300	435	10.00
2	001	-28.00	-28.00	180.00	54.70	2	-0.300	230	10.00
3	001	-28.00	-28.00	0.00	54.70	2	-0.300	50	10.00

Table 5.11 – Default 4-circle Hemisphere Runs

Run#	Frame#	2-Theta	Omega	Phi	Chi	Axis	Width	#Frames	Time
0	001	28.00	28.00	0.00	30.00	3	.300	1250	10.00
1	001	28.00	43.00	0.00	280.00	2	-.300	100	10.00
2	001	28.00	43.00	90.00	280.00	2	-.300	100	10.00
3	001	28.00	43.00	180.00	280.00	2	-.300	100	10.00
4	001	28.00	43.00	270.00	280.00	2	-.300	100	10.00

Before performing a scan with the above runs, ensure that they agree with the collision limits (see Collect > Goniometer > Limits) for your particular system.

These runs are valid for both Mo and Cu radiation. However, Cu data will be complete to a lower resolution. For a Platform goniometer, a good strategy for collecting higher resolution shells is to swing the detector out farther and interleave the higher resolution scans approximately 45° in chi relative to the low resolution scans (putting them in the “cusps” at the outer edges of the low resolution scans). You will have to modify this strategy a little (for example, by trial and error in ASTRO) due to potential omega-2theta collisions.

5.33 Collect > Scan > ResumeRuns • Resume interrupted MultiRun scans

Menu Command: Collect > Scan > ResumeRuns

Accelerator: None

User Level: 1

SLAM Syntax:

```
SCAN /RESUMERUNS
$1  /TITLE=<s> /SAMPLE=<s>
/NUMSAMPLE=<s>/DISPLAY=<n>
/REAL TIME /CLEAR /OLDXENGEN
/STARTRUN=<n> /ENDRUN=<n>
/MODE=<n> /ROTATE /VIDEO
/OSCILLATE=<s> /AMPLITUDE=<n> $2
/SNAME=<s> [/2THETA=<n> |
/THETA1=<n>] [/OMEGA=<n> |
/THETA2=<n>] /PHI=<n> /CHI=<n>
/X=<n> /Y=<n> /Z=<n> /AUX=<n>
/AXIS=<n> /WIDTH=<n>
/SCANTIME=<n> /RUN=<s>
/FRAMENO=<s> $3
```

This command will restart a scan sequence (interrupted manually, with CTRL+BREAK or ESC, or by power failure) where it left off. The command applies to scans acquired by Collect > Scan > MultiRun, but not those by Collect > Scan > SingleScan.

GADDS updates the scan parameters in a disk file (RESUME._TM) at the start of each scan. The updating procedure explicitly closes the file to ensure that the information is written to the disk drive. GADDS uses this updated parameter information in resume._tm to restart the sequence.

When invoked from the menu, or run from the command line without arguments, Collect > Scan > Resume displays a dialog box where you can view/edit the arguments described below. The displayed defaults in this panel are read from the RESUME._TM file and should correspond to the state of the system when scanning was interrupted (that is, they should correspond to the first incomplete frame). You should review (edit if necessary) these values before restarting data collection. Pressing ENTER or clicking the OK button resumes data collection. Pressing ESC or the Cancel button exits the dialog and returns you to the menu.

When invoked from the command line, SCAN /RESUMERUNS can take the arguments shown in the SLAM syntax description above (where <n> represents a numeric value and <s> represents a string value). The first 13 arguments correspond to those that were specified in the Acquire > MultiRun, Hemisphere, or Quadrant input dialog. The next 15 represent the values obtained from the run list for the interrupted scan.

5.33.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses.

$1 .....(Job Name)
[from resume._tm]

/TITLE<s> .....(Title) [from resume._tm]

/SAMPLE<s> .....(Sample Name)
[from resume._tm]

/NUMSAMPLE<s> (Sample Number)
[from resume._tm]

/DISPLAY=<n>.....(Max Display Counts)
[from resume._tm]

/REAL TIME.....(Real-time Display?)
[from resume._tm]

/CLEAR.....(Pre-Clear?)
[from resume._tm]

/OLDXENGEN .....(Xengen Output Format?)
[from resume._tm]

/STARTRUN=<n>..(Sequence # of Starting Run) [from resume._tm]

/ENDRUN=<n> .....(Sequence # of Ending Run)
[from resume._tm]

/MODE=<n>.....(Mode (Scan/Oscillate/Step)) [from resume._tm]

/ROTATE.....(Rotate Sample?)
[from resume._tm]

/VIDEO. ..... (Capture Video Image?)
[from resume._tm]

/OSCILLATE=<s>. (Sample Osc)
[from resume._tm]

/AMPLITUDE=<n> (Amplitude)
[from resume._tm]

/SNAME..... (Slave Job Name)
[from resume._tm]

See Section 5.30, Section 5.31, and Section 5.32.

$2 ..... (# Frames) [from resume._tm]

Enter the number of frames remaining to be collected in the current scan series.

/2THETA=<n>..... (2-Theta) [from resume._tm]

/THETA1=<n>..... (Theta1) [from resume._tm]

Enter the detector swing angle in degrees at which the remaining frames in the current scan series are to be collected. On θ-θ systems, this is the θ1 angle (tube).

/OMEGA=<n>..... (Omega)
[from resume._tm]

/THETA1=<n>..... (Theta1)
[from resume._tm]

Enter the omega angle, in degrees, at which the goniometer will be positioned at the start of this frame series. If you specify a scan axis number (see /AXIS=<n> below) of 2,

omega will be scanned as each frame is taken. Otherwise, omega remains fixed throughout the frame series. On θ-θ systems, this is the θ2 angle (detector).

/PHI=<n>.....(Phi) [from resume._tm]

Enter the phi angle, in degrees, at which the goniometer will be positioned at the start of this frame series. If you specify a scan axis number (see /AXIS=<n> below) of 3, phi will be scanned as each frame is taken. Otherwise phi remains fixed throughout the frame series.

/CHI=<n> .....(Chi) [from resume._tm]

Enter the goniometer chi setting angle, in degrees, at which the remaining frames in the current scan series are to be collected. A Platform goniometer is fixed at CHI=54.74°. An older Aztalan (black) 3-circle goniometer is fixed at CHI=45°.

/X=<n> .....(X) [from resume._tm]

Enter the goniometer chi setting angle, in degrees, at which the remaining frames in the current scan series are to be collected.

/Y=<n> .....(Y) [from resume._tm]

Enter the goniometer chi setting angle, in degrees, at which the remaining frames in the current scan series are to be collected.

/Z=<n>..... (Z) [from resume._tm]

Enter the goniometer chi setting angle, in degrees, at which the remaining frames in the current scan series are to be collected.

/AUX=<n>..... (Aux) [from resume._tm]

Enter the goniometer chi setting angle, in degrees, at which the remaining frames in the current scan series are to be collected.

/AXIS=<n>..... (Scan Axis #) [from resume._tm]

Enter the number of the axis to be scanned, either 2 (for omega scans) or 3 (for phi scans). Remember that some data reduction programs cannot reduce phi-scan data unless it was taken at CHI=0. A Platform goniometer is fixed at CHI=54.74°. An older Aztalan (black) 3-circle goniometer is fixed at CHI=45°. SAINT can reduce phi scans taken at nonzero chi.

/WIDTH=<n> ..... (Frame Width) [from resume._tm]

Enter the scan width of each frame to be acquired in degrees. This value can be either positive or negative. Thus, the starting scan angle for the Nth frame in the series (where the first frame is N=0) is OMEGA+N*WIDTH if AXIS above is 2, or PHI+N*WIDTH if AXIS above is 3, where WIDTH, OMEGA, and PHI are the values given here on this line of the array.

/SCANTIME=<n> ..(Seconds/Frame) [from resume._tm]

Enter the time, in seconds, for which each frame is to be acquired. You can optionally specify long times in the format HH:MM:SS.SS where HH represents hours; MM, minutes; and SS.SS decimal seconds.

/RUN=<s> .....(Run #) [from resume._tm]

Enter the RUN# of the interrupted scan series. Make sure it matches the current RUNBASE and RUNCHARS defined in the Edit > Config dialog.

/FRAMENO=<s> ...(Frame #) [from resume._tm]

Enter the Frame Number of first incomplete frame in the interrupted scan series. Make sure it matches the current NUMBASE and NUMCHARS defined in the Edit > Config dialog.

$3 .....(Interrupted Run# to Resume) [from resume._tm]

Enter run (line#) to resume (0 if no run in progress).

5.34 Collect > Scan > Rotation • Take a phi rotation picture

Menu Command: Collect > Scan > Rotation

Accelerator: Ctrl+Shft+F4

User Level: 1

SLAM Syntax:

SCAN /ROTATION $1 /TTZERO /PHI=<n> /CHI=<n> /DISPLAY=<n> /REAL TIME /RESET=<n>

Collect > Scan > Rotation allows you to collect a rotation “photo” of a sample or crystal by rotating the sample in phi while exposing it to the X-ray beam.

When invoked from the menu, or run from the command line without arguments, Collect > Scan > Rotation displays a dialog box where you can view/edit the arguments described below. Pressing the ENTER key or clicking the OK button starts the operation. Pressing ESC or Cancel button stops the operation and returns you to the menu.

You can interrupt the operation by pressing CTRL+BREAK. Upon interruption, the goniometer stays at the position where the rotation was interrupted.

5.34.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses.

$1 ..... (Exposure Time) [36.0]

Enter the requested exposure time in seconds. The valid range is from X to 65535 seconds, where the minimum is calculated from the maximum phi speed and the default value is 36.

/CLEAR ..... (Pre-Clear?) [Yes]

See Section 5.30 for an explanation of this argument.

/TTZERO ..... (Zero 2-Theta, Omega (Y/N)) [No]

/TTZERO ..... (Zero Theta-1, Theta-2 (Y/N)) [No]

If you check this option, 2-theta and omega are driven to zero before the rotation is acquired. Otherwise, these setting angles are left at their current position. The default is “Y” (checked). On θ-θ systems, this drives θ1 and θ2 to zero.

/PHI=<n> ..... (Starting Phi) [0.00]

Enter starting phi for photo in degrees. The allowed range is from 0 to 360, with a default setting of 0.

/CHI=<n>.....(Starting Chi) [0.00]

Enter goniometer chi for photo in degrees. The allowed range is from 0 to 360, with a default setting of 0.

/DISPLAY=<n>.....(Mzx Displayed Counts) [15]

See Section 5.30 for an explanation of this argument.

/REAL TIME.....(Real-time Display?) [Yes]

See Section 5.30 for an explanation of this argument.

/RESET=<n>.....(Reset Interval) [0]

This qualifier specifies the number of seconds before repetitive auto-clear of frame memory (0 = do not clear). The default value is 0; the range is from 1 to 65,535 seconds. This parameter is useful in conjunction with real-time display if you're looking for a change in intensity over time.

When you start collecting a rotation frame, if you checked the option to zero 2-theta and omega, GADDS drives the two angles to zero, otherwise the goniometer 2-theta and omega setting angles stay at their current position. Chi moves to the value specified on the input panel (a 3-circle goniometer is fixed at chi=54.74° or chi=45°, depending on the type) and phi moves to the starting angle specified on the input panel. After these goniometer movements, GADDS opens the shutter, performs a full rotation of phi, while acquiring a frame. The shutter closes once the exposure has been completed, then GADDS displays the unwarped frame. The speed of rotation depends on the collection time requested in the input panel. The requested time adjusts as needed to make a full phi rotation. Since the maximum rotation speed is 3600 degrees/minute (for Platform), 24 seconds is the shortest actual rotation exposure time (600 degrees/minute, for P4, 36 seconds).

A rotation photo taken at a detector swing angle (2-theta setting angle) of zero provides the best method for estimating the direct beam center. Usually, you'll need a strongly diffracting crystal to see a good pattern. The rotation photo will contain a center of symmetry at the direct beam position. You can place the origin and endpoint of a vector cursor (see Analyze > Cursor > Vector) on two spots related by the center of symmetry and obtain the direct beam coordinates from the displayed vector midpoint values.

5.35 Collect > Scan > HKL • Reciprocal space scan from starting HKL to ending HKL

Menu Command: Collect > Scan > HKL

Accelerator: Ctrl+Shft+F5

User Level: 1

SLAM Syntax:

SCAN /HKL $1 $2 $3 /SCANTIME=<n>
/TITLE=<s> /SAMPLE=<s>
/NUMSAMPLE=<n> /NAME=<s>
/RUN=<s> /FRAMENO=<s>
/DISPLAY=<n> /REAL TIME

SCAN /HKL will collect a frame series for later processing with GRAPH /HKL.

When invoked from the command line, SCAN / HKL can take the following arguments (where <n> represents a numeric value and & indicates continuation on the next line):

5.35.1 Arguments

Each argument is listed below by its command line name, followed by its input panel prompt in parentheses:

$1 ..... (Starting HKL) [-.5 1.5 1.5]

Enter starting hkl value. May be reals.

$2 ..... (Ending HKL) [.5 2.5 2.5]

Enter ending hkl value. May be reals.

$3 ..... (# Frames) [101]

Number of frames to be acquired in this series. Make sure it doesn't exceed the number permitted by FRAME# above in conjunction with the frame naming parameters in the CONFIGURE /EDIT panel.

/SCANTIME=<n> . (Seconds/Frame) [1:00.00]

Time in seconds for which each frame is to be acquired. You can optionally specify long times in the format HH:MM:SS.SS where HH represents hours; MM, minutes; and SS.SS decimal seconds.

/TITLE=<s> ..... (Title) [Scan/HKL frame]

Enter title for output frames, 80 characters maximum. The default entry is “Scan Frame.” If you invoked this command from the command line, you must enclose any title continuing embedded blanks in double quotes.

$FILE:<filename> will read up to eight 72-character title lines from an ASCII file and place these title strings into the eight “TITLE” lines in the frame header. The format of the ASCII file is: “R#:<single line of title information>”, where “R#” is the run number, taken from the filename. Repeat up to eight times for each run.

/SAMPLE=<s> .....(Sample Name) [YLID]

Enter sample name, to be stored in frame header. If no name is specified, the default name of “Lysozyme” will be entered.

/NUMSAMPLE=<n>(Sample Number) [0]

Enter sample number, to be stored in frame header. The permitted range is from 0 to 32,767, with a default setting at 1.

/NAME=<s>.....(Job Name) [HKLFRAM]

Enter the base filename for the output frames. The filenames for each series of output frames are generated by adding the series RUN# (see below) window) and an extension built from the series starting FRAME# (see below) to the end of this base name. For example, if the Job Name is LYS, the Run Number is 04, and the starting Frame Number is 000 (assuming that the number of characters in a Run Number is set to 2 and number characters in a Frame Number is set to 3 in the CONFIGURE /EDIT panel), the data files are named in sequence as: LYS04.000, LYS04.001, LYS04.002, etc.). See the description “FRAME NAMING CONVENTIONS” for more information. The default name if none is specified is NEWFRAM.

The Job Name for frames stored locally can contain a DOS drive and directory name if desired. The output filename is, except in the special cases discussed below, merged with the default frame directory defined in the CONFIGURE /EDIT panel prior to creating the output frame. See CONFIGURE /EDIT for a description of how this is done.

There are two special Job Name cases. The first, $NET is NOT supported under GADDS. The second special Job Name is $NULL. In this case, the frames are not output -- they are thrown away.

/RUN=<s>..... (Run #) [0]

The Run Number of the series. This is not actually a number, but is rather taken as /RUNCHARS characters of ASCII text (where /RUNCHARS is defined in the CONFIGURE /EDIT input panel) to be used as the last /RUNCHARS characters of the output base filename (i.e., the last /RUNCHARS characters before the extension). Make sure that these values, and the frame naming parameters in CONFIGURE /EDIT are set the way you want before starting to scan, as described above.

/FRAMENUM=<s> (Frame #) [000]

This is the starting frame number for the series defined by this line of the array. Make sure it conforms to the frame naming parameters currently set in CONFIGURE /EDIT. Like the Run Number, this is actually taken as text rather than a numeric value. The text specified here will be used as the extension of the first output frame in the series, and will be incremented according to the frame naming parameters to form the extensions of subsequent frames.

/DISPLAY=<n>.....(Max Display Counts) [31]

0 = no display, otherwise # counts corresponding to white on the display. SAVE will optionally display the data being saved using this value as the upper display limit (see DISPLAY /NEW for more details). The default value is 16; the allowed range is from 0 to 10^6 counts.

/REAL TIME .....(Real-time Display?) [Yes]

This qualifier, when present, displays data as it is being collected. The display does require additional processing time, and will limit the maximum rate at which counts can be accumulated. If the MAX DISPLAYED COUNTS qualifier is given a non-zero value, the frame will be automatically displayed at the end of each scan if real-time display is off. This latter display method has no effect on observed data rate. Unless your data rate is very low, it is better NOT to use real-time display in the course of a SCAN command, even though the default here is “Y.”

While real-time display is active, you can change the upper display limit using the plus key to increase or the minus key to decrease the current limit by a factor of two (the range is 7 to 524287). Modify the contrast using the left and right arrow keys. Modify the brightness using the up and down keys. Holding the control key down in combination with any arrow key results in a greater change of contrast or brightness.

5.36 Collect > Scan > Psi • Take a Psi scan of 360° around reciprocal vector

Menu Command: Collect > Scan > Psi

Accelerator: Ctrl+Shft+F6

User Level: 1

SLAM Syntax:

SCAN /PSI $1 $2 /SCANTIME=<n> /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n> /NAME=<s> /RUN=<s> /FRAMENO=<s> /DISPLAY=<n> /REAL TIME

SCAN /PSI will collect a frame series for later processing with GRAPH /PSI.

When invoked from the command line, SCAN /PSI can take the following arguments (where <n> represents a numeric value and & indicates continuation on the next line).

5.36.1 Arguments

Each argument is listed below by its command line name, followed by its input panel prompt in parentheses:

$1 ..... (HKL) [022]

Enter the hkl position for psi scan.

$2 ..... (#Frames) [180]

Enter the number of frames to collect (determines the step size).

/SCANTIME=<n> . (Seconds/Frame) [1:00.00]

Time in seconds for which each frame is to be acquired. You can optionally specify long times in the format HH:MM:SS.SS where HH represents hours; MM, minutes; and SS.SS decimal seconds.

/TITLE=<s> ..... (Title) [Scan/psi frame]

Enter title for output frames, 80 characters maximum. The default entry is “Scan Frame.” If you invoked SCAN /SINGLERUN from the command line, you must enclose any title continuing embedded blanks in double quotes.

$FILE:<filename> will read up to eight 72-character title lines from an ASCII file and place these title strings into the eight “TITLE” lines in the frame header. The format of the ASCII file is: “R#:<single line of title information>”, where “R#” is the run

number, taken from the filename. Repeat up to eight times for each run.

/SAMPLE=<s> .....(Sample Name) [YLID]

Enter sample name, to be stored in frame header. If no name is specified, the default name of “Lysozyme” will be entered.

/NUMSAMPLE=<s>(Sample Number) [0]

Enter sample number, to be stored in frame header. The permitted range is from 0 to 32,767, with a default setting at 1.

/NAME=<s> .....(Job Name) [PSIFRAM]

Enter the base filename for the output frames. The filenames for each series of output frames are generated by adding the series RUN# (see below) window) and an extension built from the series starting FRAME# (see below) to the end of this base name. For example, if the Job Name is LYS, the Run Number is 04, and the starting Frame Number is 000 (assuming that the number of characters in a Run Number is set to 2 and number characters in a Frame Number is set to 3 in the CONFIGURE /EDIT panel), the data files are named in sequence as: LYS04.000, LYS04.001, LYS04.002, etc.). See the description “FRAME NAMING CONVENTIONS” for more information. The default name if none is specified is NEWFRAM.

The Job Name for frames stored locally can contain a DOS drive and directory name if desired. The output filename is, except in the special cases discussed below, merged with the default frame directory defined in the CONFIGURE /EDIT panel prior to creating the output frame. See CONFIGURE /EDIT for a description of how this is done.

There are two special Job Name cases. The first, $NET is NOT supported under GADDS. The second special Job Name is $NULL. In this case, the frames are not output—they are thrown away.

/RUN=<s>..... (Run #) [0]

The Run Number of the series. This is not actually a number, but is rather taken as /RUNCHARS characters of ASCII text (where /RUNCHARS is defined in the CONFIGURE /EDIT input panel) to be used as the last /RUNCHARS characters of the output base filename (i.e., the last /RUNCHARS characters before the extension). Make sure that these values, and the frame naming parameters in CONFIGURE /EDIT are set the way you want before starting to scan, as described above.

/FRAMENO=<s> .. (Frame #) [000]

This is the starting frame number for the series defined by this line of the array. Make sure it conforms to the frame naming parameters currently set in CONFIGURE

/EDIT. Like the Run Number, this is actually taken as text rather than a numeric value. The text specified here will be used as the extension of the first output frame in the series, and will be incremented according to the frame naming parameters to form the extensions of subsequent frames.

/DISPLAY=<n>.....(Max Display Counts) [31]

0 = no display, otherwise # counts corresponding to white on the display. SAVE will optionally display the data being saved using this value as the upper display limit (see DISPLAY /NEW for more details). The default value is 16; the allowed range is from 0 to 10^6 counts.

/REAL TIME.....(Real-time Display (Y/N)) [Yes]

This qualifier, when present, displays data as it is being collected. The display does require additional processing time, and will limit the maximum rate at which counts can be accumulated. If the MAX DISPLAYED COUNTS qualifier is given a non-zero value, the frame will be automatically displayed at the end of each scan if real-time display is off. This latter display method has no effect on observed data rate. Unless your data rate is very low, it is better NOT to use real-time display in the course of a SCAN command, even though the default here is “Y.”

While real-time display is active, you can change the upper display limit using the plus key to increase or the minus key to decrease the current limit by a factor of two (the range is 7 to 524287). Modify the contrast using the left and right arrow keys. Modify the brightness using the up and down keys. Holding the control key down in combination with any arrow key results in a greater change of contrast or brightness.

5.37 Collect > Scan > CoupledScan • Conventional 2θ/θ coupled scan (Uses AD as a point detector)

Menu Command: Collect > Scan > Coupled-Scan

Accelerator: Ctrl+Shft+F7

User Level: 1

SLAM Syntax:

SCAN /COUPLED $1 $2 $3 /WIDTH=<n> /SCANTIME=<n> /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n> /NAME=<s> /RUN=<s> /ROTATE /X=<n> /Y=<n> /REAL TIME

Perform a conventional 2T/T coupled scan using a square portion of the area detector grid as a point detector. The omega axis is always driven at half the rate of the 2-theta axis.

Scan /Coupled performs a conventional 2T/T coupled scan using a square portion of the area detector grid as a point detector. The resulting scan data is displayed in 1D spectra, not 2D frames. The 1D spectra is saved as an additional range in a DIFFRAC-AT file suitable for input into other software packages such as PROFILE*plus* or EVA.

Data is collected from 2T start to 2T end. You may collect in negative 2T space and in negative 2T direction. The 1D spectrum is always stored in positive 2T direction. If both start and end 2T positions are in negative 2T space, the 1D spectrum is stored as positive 2T space.

The omega axis is always driven at half the rate of the 2-theta axis.

When invoked from the command line, SCAN /COUPLED can take the following arguments (where <n> represents a numeric value and & indicates continuation on the next line).

5.37.1 Arguments

Each argument is listed below by its command line name, followed by its input panel prompt in parentheses:

$1 ..... (2-Theta start) [5.0]

Enter the starting 2-Theta in degrees (“@”=current setting).

$2 ..... (2-Theta end) [90.0]

Enter the ending 2-Theta in degrees (“@”=current setting).

$3 ..... (Omega start) [2.5]

Enter the starting omega in degrees (“@”=current setting).

/WIDTH=<n> ..... (Step width) [0.1]

Enter degrees per step as a positive number.

/SCANTIME=<n> ..(Step time) [10.0]

Enter counting time in seconds for this frame.

/TITLE=<s> .....(Title) [Coupled scan]

Enter title for output frames (80 characters max).

/SAMPLE=<s> .....(Sample name) [Corundum]

n.y.i. Enter sample name, to be stored in frame header.

/NUMSAMPLE=<s>(Sample number) [0]

n.y.i. Enter sample number, to be stored in frame header.

/NAME=<s>.....(Job name) [CORUND]

Enter base name for frames.

/RUN=<s> .....(Run #) [0]

Enter data set # (base 10 or 36—see CONFIGURE form).

/ROTATE.....(Rotate sample Y/N) [N]

n.y.i. Y to perform sample rotation in phi, N otherwise.

/X=<n> .....(Active width) [2.0]

Enter active detector width about center in mm.

/Y=<n>..... (Active height) [2.0]

Enter active detector height about center in mm.

/REAL TIME ..... (Real-time Display?) [Yes]

Enter Y for real-time display, N otherwise.

5.38 Collect > Scan > ZonePhoto • Acquire a rotational photo along a zone (0KL, H0L, HK0)

Menu Command: Collect > Scan > Zone

Accelerator: Ctrl+Shft+F8

User Level: 1

SLAM Syntax: SCAN /ZONE $1 /WIDTH=<n> /SCANTIME=<n> /DISPLAY=<n>

Acquire > Zone acquires an omega-rotation picture centered on a crystallographic H0L, 0KL, or HK0 zone, according to the current orientation matrix. With a 3-circle goniometer, GADDS does not guarantee that all three zones will be accessible. Typically, you will have two possible omega settings at which to observe a zone. If more than one solution is accessible, GADDS will record the one which places omega farthest from the detector (at swing angle zero).

NOTE: Ensure that your collision limits are set correctly before using this command. GADDS uses them to determine if a solution is accessible. If the requested zone is not accessible, GADDS displays a message indicating so.

The frame is not automatically written to disk. Use Acquire > Save after collecting the still frame if you want to save the data to disk.

When invoked from the menu, or run from the command line without arguments, Acquire > Zone displays a dialog box where you can view/edit the arguments described below before performing the operation. Pressing the ENTER key or clicking the OK button starts the operation. Pressing ESC or the Cancel button stops the operation and returns you to the menu.

You can interrupt the operation by pressing CTRL+BREAK.

5.38.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Zone) [1]

Enter 1 to attempt collection of the 0KL zone, 2 for H0L, or 3 for HK0.

/WIDTH=<n> ..... (Frame Width) [-5.0]

Enter the frame width as defined under WIDTH in Section 3.4.

/SCANTIME=<n> . (Seconds/Frame) [30.0]

Enter the seconds per frame as defined under TIME in Section 3.4.

/DISPLAY=<n> ..... (Max Display Counts) [-1]

See Section 3.7 for an explanation of this argument. (See Acquire > Display for more details.)

5.39 Collect > Scan > Axial Image • Acquire a frame showing A, B, or C axial image

Menu Command: Collect > Scan > Axial

Accelerator: Ctrl+Shft+F8

User Level: 1

SLAM Syntax: SCAN /ZONE $1 /WIDTH=<n> /SCANTIME=<n> /DISPLAY=<n>

Acquire > Axial acquires an omega-rotation picture in which the crystal is rotated about the a, b, or c axis.

The frame is not automatically written to disk. Use Acquire > Save after collecting the still frame if you want to save the data to disk.

When invoked from the menu, or run from the command line without arguments, Acquire > Axial displays a dialog box where you can view/edit the arguments described below before performing the operation. Pressing the ENTER key or clicking the OK button starts the operation. Pressing ESC or the Cancel button stops the operation and returns you to the menu.

You can interrupt the operation by pressing CTRL+BREAK.

5.39.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Axis) [1]

Enter 1 to attempt collection of the a axis, 2 for b, or 3 for c.

/WIDTH=<n> ..... (Frame Width) [-0.5]

Enter the frame width as defined under WIDTH in Section 3.4.

/SCANTIME=<n> . (Seconds/Frame) [30.0]

Enter the seconds per frame as defined under TIME in Section 3.4.

/DISPLAY=<n> ..... (Max Display Counts) [-1]

See Section 3.7 for an explanation of this argument. (See Acquire > Display for more details.)

5.40 Collect > Scan > PickTargets • Manually drive and select target positions for MultiTarget list

Menu Command: Collect > Scan > PickTargets

Accelerator: Ctrl+Shft+F9

User Level: 1

SLAM Syntax: SCAN /SELECTTARGETS

SCAN /SELECTTARGETS manually select XYZ target position(s) and automatically enter the selected target into the SCAN /MULTITARGETS by appending the list.

When SELECTTARGETS is first entered, the user has the option of either clearing the target list or appending to the existing target list.

> Pre-clear the existing target list? Y/N

The video program should already be running in a separate window. SELECTTARGETS will turn the video to “live” and turn the laser ON. Manual speed ratios can be selected and the program enters manual mode. The user then drives to a position where data collection is requested, makes sure the laser is positioned within the video cross-hairs, then hits <Ctrl-G> to exit manual mode. The current sample position can be automatically entered into the target list.

> Do you want to enter this position in the targets list? Y/N
>
> Additional targets may be selected before exiting SELECTTARGETS
>
> Do you want to enter more positions in the targets list? Y/N

5.40.1 Arguments

None. Command executes immediately. This is an interactive command only.

5.41 Collect > Scan > GridTargets • Set up grid for MultiTarget list

Menu Command: Collect > Scan > GridTargets

Accelerator: Ctrl+Shft+F10

User Level: 1

SLAM Syntax:

SCAN /GRIDTARGETS /XBEG=<n> /XEND=<n> /XINC=<n> /YBEG=<n> /YEND=<n> /YINC=<n> /TRANSMISSION /APPEND

On systems equipped with an XYZ stage, it is possible to collect scans at multiple target locations. On flat samples such as wafers, one frequently wishes to take scans on target positions laid out on a rectangular grid. Instead of manually determining the Z axis position of each target on the grid, one can pre-determine the flat sample plane, then lay out the target locations using SCAN /GRIDTARGETS which will automatically calculated the correct Z axis value from the flat sample plane. See GONIOMETER /FLATSAMPLE.

NOTE: The list of targets is now optimized (sorted) for minimized drive between targets.

5.41.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

/XBEG=<n> ..... (X Begin) [-5.0]

/XEND=<n> ..... (X End) [5.0]

/XINC=<n> ..... (X Increment) [1.0]

Enter the starting, ending, and increment in mm. for the grid in the X direction. The X begin and end values may be equal. Also, X end may be less than X begin.

/YBEG=<n> ..... (Y Begin) [-5.0]

/YEND=<n> ..... (Y End) [5.0]

/YINC=<n> ..... (Y Incremen) [1.0]

Enter the starting, ending, and increment in mm. for the grid in the Y direction. The Y begin and end values may be equal. Also, Y end may be less than Y begin.

/TRANSMISSION . (Transmission mode X-Y Y-Z) [No]

Check for samples mount in transmission mode, where you wish to grid in Y & Z axes.

/APPEND..... (Append to existing target list) [No]

Check for append new grid list to end of existing list of targets. Unchecked will pre-clear the target list.

5.42 Collect > Scan > LineTargets • Set up line for MultiTarget list

Menu Command: Collect > Scan > LineTargets

Accelerator: None

User Level: 1

SLAM Syntax:

SCAN /LINETARGETS /XBEG=<n> /XEND=<n> /YBEG=<n> /YEND=<n> /INC=<n> /TRANSMISSION /APPEND

On systems equipped with an XYZ stage, it is possible to collect scans at multiple target locations. On flat samples, such as wafers, usually scans are taken on target positions laid out along a line. Instead of manually determining the Z-axis position of each target on the grid, one can predetermine the flat sample plane, then lay out the target locations using SCAN /LINETARGETS which will automatically calculate the correct Z-axis value from the flat sample plane. See GONIOMETER /FLATSAMPLE.

5.42.1 Arguments

Each argument is listed below by its command line name, followed by its dialog box prompt in parentheses:

/XBEG=<n>..... (X Begin) [-5.0]

/YBEG=<n>..... (Y Begin) [-5.0]

Enter the starting point in mm for the line.

/XEND=<n>..... (X End) [5.0]

/YEND=<n>..... (Y End) [5.0]

Enter the ending point in mm. for the line.

/INC=<n>..... (Y Incremen) [1.0]

Enter the increment in mm along the line.

/TRANSMISSION. (Transmission mode X-Y Y-Z) [No]

Check for samples mount in transmission mode, where you wish to grid in Y and Z axes.

/APPEND ..... (Append to existing target list) [No]

Check for append new grid list to end of existing list of targets. Unchecked will preclear the target list.

5.43 Collect > Scan > EditTargets • Edit parameters for MultiTarget scans

Menu Command: Collect > Scan > EditTargets

Accelerator: Ctrl+Shft+F11

User Level: 1

SLAM Syntax: SCAN /EDITTARGETS

Use this command to create, edit, or review a target list of sample positions that you wish to acquire in a single run fashion (where one series of contiguous frames are collected at each sample target position without intervention).

Because target positions are unique to particular samples and to a particular mounting of that sample, GADDS will not automatically load any previous target list. However, the user can easily save and load target lists from within Collect > Scan > EditTargets using the READ and WRITE options. For screen editing options and keys, see the section under keyboard conventions. Upon exiting GADDS, the current target list (if any) is saved in the file: targets.txt.

Upon entering a Collect > Scan > EditTargets command, GADDS displays a target list with current settings (a typical list follows).

Run#	Frame#	X	Y	Z
0	000	-1.0	-1.0	2.33
0	001	-1.5	-1.0	2.33
0	002	-1.0	-1.5	2.33
0	003	-1.5	-1.5	2.33

Each line in the array defines one target position. The scan series will be acquired in the order they appear in the array. When entering the individual target arguments, keep in mind the following special considerations:

- The RUN#, FRAME#, and #FRAMES must conform to the frame naming parameters. (See Edit > Configure > User settings command.)
- All generated filenames must be valid and should not create duplicate names (explained later in this section).
- The number of targets is limited to 2048.
- The number of runs (or lines) must not exceed the maximum number of runs allowed by RUNCHARS and RUNBASE (see Edit > Configure > User settings command). The default maximum number of runs is 36. The absolute maximum is 36*36.

With these considerations in mind, we recommend that you always configure the frame naming conventions as follows:

- For 36 or fewer runs, set the “Base of Run #” (in the Edit > Configure > User settings dialog) to base 36, which will prevent the run

number from wrapping from 9 to 0. The “Characters in Run #” should be 1. These are the default settings.

- For greater than 36 runs, you must set the “Characters in Run #” (in the Edit >Configure > User settings dialog) to 2 characters. The “Base of Run #” can be base 10, if you find it more convenient and you are collecting 100 or fewer targets.

Each line of the EDITTARGETS array contains the following items:

RUN#

This is the Run Number of the series. This is not actually a number, but is rather taken as RUNCHARS characters of ASCII text. Also, all characters must be valid characters to be used with filenames because the Run Number becomes part of the generated output filename. Basically, the Run Number is formatted and appended to the output base filename before the file extension. See Frame Naming Conventions, Edit > Configure > User settings command, and Collect > Scan > MultiTargets command for more details.

FRAME#

This is the starting frame number for the series. Like the Run Number, this is actually taken as text of length NUMCHARS rather than as a numeric value. The text specified here will be used as the extension of the first output frame in the series and will be incremented according to the frame naming parameters to form the extensions of subsequent frames. See Frame Naming Conventions, Edit > Configure > User settings command, and Collect > Scan > MultiTargets command for more details.

X

This is the sample X position in mm at which the goniometer will be positioned for this frame series. Entering “@” will be automatically replaced with current angle setting.

Y

This is the sample Y position in mm at which the goniometer will be positioned for this frame series. Entering “@” will be automatically replaced with current angle setting.

Z

This is the sample Z position in mm at which the goniometer will be positioned for this frame series. Entering “@” will be automatically replaced with current angle setting.

When you select this command (> EditTargets), GADDS displays a “scrollable” editing window listing all of the targets currently in the target array. You can add to, delete from, or reorganize the list as desired by using the appropriate screen-editing functions.

When you invoke the MultiTarget scan command (Collect > Scan > MultiTargets), each series will be acquired in the order they appear in the corresponding array. GADDS generates output filenames for each frame from the Job Name (in the Collect > Scan > MultiTargets dialog box). GADDS also generates the Run Number (given for the series in the array), the starting Frame# (given for the series in the array), the Frame# being collected, and the frame naming parameters (defined in the Edit > Configure > User settings input panel). The first and last generated filenames in each frame series must be valid. Also, the generated filenames between frame series should not overlap. Always check the bottom status line when you first start a new Collect > Scan > MultiTargets to ensure that filenames are being synthesized the way you want, to avoid duplication of filenames during data collection (which will overwrite the previous file).

The EditTargets command is an interactive command, meaning that you can invoke it from the command line, but it will not proceed without user intervention. And it has no built-in command-mode time-out as with other scrolling output windows. Additionally, the Collect > Scan > MultiTargets does not work well from script files, as you cannot define the run list in command mode. Thus, we recommend using the equivalent SCAN /SINGLERUN script commands instead.

5.43.1 Arguments

None. Command executes immediately. This is an interactive command only.

5.44 Collect > Scan > MultiTargets • Perform same scans on multiple targets on a single sample

Menu Command: Collect > Scan > MultiTargets

Accelerator: Ctrl+Shft+F12

User Level: 1

SLAM Syntax:

```
SCAN /MULTITARGETS $1
[/2THETA=<n> | /THETA1=<n>]
[/OMEGA=<n> | /THETA2=<n>] /PHI=<n>
/CHI=<n> /AXIS=<n> /WIDTH=<n>
/SCANTIME=<n> $2 /TITLE=<s>
/SAMPLE=<s> /NUMSAMPLE=<s>
/DISPLAY=<n> /REAL TIME /CLEAR
/STARTRUN=<n> /ENDRUN=<n>
/MODE=<n> /ROTATE /VIDEO
/OSCILLATE=<s> /AMPLITUDE=<n>
/AUTOZALIGN
```

This command allows you to collect multiple single scan series at different target positions on the same sample on systems equipped with an XYZ stage (or multiple samples attached to the XYZ stage). Normally, Collect > Scan > MultiTargets stores frames as an unwarped image, after applying the spatial correction table. It also applies the flood-field (intensity uniformity) corrections as the counts are received.

Before invoking Collect > Scan > MultiTargets, you must set the parameters that are unique from series to series. (See Section 5.43, Collect > Scan > EditTargets.) Then use Collect > Scan > MultiTargets to define those parameters that are the same for all the different scan series to be performed and to start the scans.

When you invoke the command from the menu, a dialog box appears where you can view/edit the arguments described below as follows:

- press ENTER or click the OK button to start scanning.
- press ESC or click the Cancel button to return to the menu.

You can interrupt a scan as follows:

- press ESC to stop after finishing collecting the current frame (soft abort).
- press CTRL+BREAK to interrupt the scan (hard abort or immediate abort).

To ensure that nothing scrapes the sample surface between drives, GADDS may perform a one mm back-drive, utilizing three separate drives. GADDS drives one mm down the Z-axis, then drives to the first target position minus one mm down, then drives up one mm. These extra drives are not performed when omega $\geq$ 10 degrees.

Unlike the MultiRuns command, a MultiTargets sequence interrupted by CTRL-BREAK or by a power failure can **NOT** be restarted where it left off with the Collect > Scan > Resume command.

RESUME works only with /MULTIRUN, not /MULTITARGETS. Instead, recollect starting at the scan series of the interrupted target position.

When you interrupt a scan with CTRL-BREAK, the goniometer returns to the starting scan angle of the current scan. This re-positioning is performed by backing up to the starting position minus one frame width (or +/- 0.5° maximum), then driving forward to the starting position. The same positioning technique is used when driving to the first scan in a new series. It makes the positioning extremely repeatable, but does require you to allow for an extra scan width at the beginning of the series when you're starting close to the goniometer collision limits.

SCAN /MULTITARTGETS checks for possible collision at the extremes of all scans before beginning the first run. If the first or last frame in a run is outside the currently set limits, the warning message

> PROBABLE COLLISION IN 1ST SCAN OF EDITTARGETS LINE <line #>
>
> or
>
> PROBABLE COLLISION IN LAST SCAN OF EDITTARGETS LINE <line #>

is displayed, where <line #> represents the number of the line (starting at 1) in the EDITRUNS array which produced the message. You can choose to continue with the scans or quit to re-edit the run list and try again.

The current configuration is saved in the current default configuration file (usually GADDS._NC) prior to starting the first scan. This also makes recovery easier in the event of a power failure, etc.

The filename of the first frame in each series in generated from the Job Name described below, the Run# and Frame# specified for the series in the EDITTARGETS array, and the frame naming parameters set in the CONFIGURE /EDIT input panel. Successive names are generated by incrementing the filename extension, again according to the naming parameters in the CONFIGURE /EDIT panel (see CONFIGURE /EDIT and the separate topic “FRAME NAMING CONVENTIONS” for more information). Note that with 256 lines in the EDITTARGETS array, it is possible to overflow a single-character run number even in base 36. It is recommended that run numbers for the output frame files be set up as follows:

1. Use base 36 (0–9,A–Z) for run numbers to prevent them from wrapping from 9 to 0. Set this in the CONFIGURE /EDIT panel item called “Base of Run #.”
2. If you have more than 36 runs in the array, you MUST set the number of characters in the run number to at least 2. Note that for DOS-compatible filenames, this reduces the number of possible characters in the data set name (Job ID in the SCAN panel) to 6 (8 characters for data set + run number). Set

this in the CONFIGURE /EDIT panel item called “Characters in Run #.” In this case, it should be OK to use base-10 run numbers if you find them more convenient.

5.44.1 Arguments

Each argument is listed below by its command line name, followed by its input panel prompt in parentheses. These arguments are the same as the similar singlerun type scans and are, thus, explained once in Section 5.30. See that section for explanations.

$1 .....(# Frames) [1]
/2THETA=<n> .....(2-Theta) [0.00]
(or /THETA1=<n>..(Theta-1) [0.00])
/OMEGA=<n> .....(Omega) [0.00]
(or /THETA2=<n>..(Theta-2) [0.00])
/PHI=<n>.....(Phi) [0.00]
/CHI=<n> .....(Chi) [0.00]
/AXIS=<n> .....(Scan Axis #) [2]
/WIDTH=<n>.....(Frame Widith) [-0.25]
/SCANTIME=<n> ..(Seconds / Frame) [1:00]

See Section 5.30.

$2 .....(Job Name) [NEWFRAM]

See /NAME=<s> argument under Section 5.30.

/TITLE=<s> .....(Title) [New frame]
/SAMPLE=<s> .....(Sample Name) [Corundum]
/NUMSAMPLE=<s>(Sample Number) [0]
/DISPLAY=<n>.....(Max Display Counts) [31]
/REAL TIME ..... (Real-time Display?) [Yes]
/CLEAR ..... (Pre-Clear?) [Yes]

See Section 5.30.

/STARTRUN=<n> . (Sequence # of Starting Run) [1]

You can collect just a specified range of the scan series set up in the EDITRUNS array by using /STARTRUN and /ENDRUN. /STARTRUN specifies the first line number (NOT the RUN#) in the EDITRUNS array for which data collection is to be performed. The lines are numbered 1–50. The default is 1 and valid range is 1 to 50.

/ENDRUN=<n>..... (Sequence # of Ending Run) [9999]

You can collect just a specified range of the scan series set up in the EDITRUNS array by using /STARTRUN and /ENDRUN. /ENDRUN specifies the line number (NOT the RUN#) in the EDITRUNS array after which data collection is to be terminated. The lines are numbered 1–50. The default is 9999 (works the same as 50) and valid range is 1 to 32767.

/MODE=<n> ..... (Mode (Scan/Oscillate/Step)) [Scan]
/ROTATE..... (Rotate Sample?) [No]
/VIDEO ..... (Capture Video Image?) [no]

/OSCILLATE=<s>..(Sample Osc) [None]
/AMPLITUDE=<n> (Amplitude) [0.0]

See Section 5.30.

/AUTOZALIGN .....(Auto Z Align) [No]

See Section 5.30.

NOTE: On failure, the algorithm proceeds to the next target and continues collecting data.

5.45 Collect > Scan > Master • Place frame buffer into single detector or dual master mode

Menu Command: Collect > Scan > Master

Accelerator: None

User Level: 3

SLAM Syntax:

SCAN /MASTER $1 /SEND_CONFIG

SCAN /MASTER is used to select single or dual detector operation mode and to optionally update the SLAVE configuration menu.

NOTE: Invoking SCAN /MASTER on a frame buffer connected to a GGCS (not a SLAVE frame buffer) may place the GGCS in an inoperable mode. The most recent release of the GGCS software fixes this problem.

The MASTER frame buffer can function in two modes. The default, single detector mode mimics the standard single detector system—the SLAVE detector becomes dead weight on the goniometer. Flood fields and fudicial plate images are collected in single detector mode. Alternately, the MASTER frame buffer may be placed in dual detector mode. Here, the MASTER may send the SLAVE specific instructions: begin collecting data, stop collecting, save image, etc., as well as control the GGCS; how-

ever, the user will only notice a few changes to the Scan menus.

For single run data collections on dual detectors, three new options appear in the input panel for Scan /Singlerun. They are:

SNAME .....(Slave Job name) [NEWFRA2]

Enter base name for frames.

SRUN.....(Slave Run #) [0]

Enter data set # (base 10 or 36; see CONFIGURE form).

SFRAMENO.....(Slave Frame #) [000]

Enter starting frame # (base 10 or 36; see CONFIGURE form).

For multirun data collections on dual detectors, only the job name is additional.

SNAME .....(Slave Job name) [NEWFRA2]

Enter base name for frames. Should be different from the Master's job name.

Before starting data collection, the Master will update the Slave with new values for: title, sample, sample number, display counts, real time, pre-clear, xengen output, oscillate, and name. Before each frame series, the Master will update the Slave with new values for: # of frames, time, set, and frame no. Finally, while collecting individual frames, the Master communicates to the Slave when to prepare for next frame, queue the drive request, collect frame, and save frame or retry collecting the same frame.

The user must ensure that the frame naming conventions for both the Master and Slave will produce unique filenames. This becomes crucial whenever both the Master and Slave collect frames directly to the same host computer directory. Also, while the Master will prompt to overwrite the first frame, the Slave will always overwrite any existing frame files.

NOTE: This command is not available on theta-theta systems.

5.45.1 Arguments

Each argument is listed below by its command line name, followed by its input panel prompt in parentheses.

$1 ..... (Num. of Detectors) [1]

Enter number of detectors to control (not physical!).

/SEND_CONFIG .. (Send Config?) [No]

Check to update configuration on Slave frame buffer.

5.46 Collect > Scan > Slave • Place frame buffer into slave mode for dual detector system

Menu Command: Collect > Scan > Slave

Accelerator: None

User Level: 3

SLAM Syntax: SCAN /SLAVE

SCAN /SLAVE is used to place the frame buffer in “slave” mode. That is, a second frame buffer will take over all goniometer operations (see SCAN /MASTER). The MASTER frame buffer is attached through COM2:, while the GGCS is attached to COM1:. Before entering SLAVE mode, one should collect a flood field and fudicial plate image as well as verify that the CONFIGURE /EDIT menu is correct (distance, angle offset, frame naming conventions, detector center, etc.).

NOTE: Before running GADDS on the Master frame buffer, the frame buffer, which is attached to the GGCS, MUST BE IN SLAVE MODE.

When invoked with the SLAVE option from the SCAN submenu, the current bias and flood field settings are check, then the user is prompted for confirmation.

Enter SLAVE mode: are you sure?

Once in SLAVE mode, all menus disappear and “Frame buffer in SLAVE mode...” is printed in the message window. The SLAVE keyboard is dead with the exception of the interrupt keys: <Ctrl-C>, <Ctrl-F>, <Ctrl-G>, and <Ctrl-Break>. The SLAVE frame processor accepts goniometer commands from the MASTER frame buffer and passes these through to the GGCS. When GGCS status reports are received, these are passed through to the MASTER frame buffer. Thus, in the default SLAVE mode, the SLAVE frame buffer is simply a pass through device; the MASTER frame buffer doesn't know or care if it's there. This enables the MASTER frame buffer to collect flood fields and fudicial plate images or to operate in single detector mode.

Alternately, the MASTER frame buffer may be placed in dual detector mode. Here, the MASTER may send the SLAVE specific instructions: begin collecting data, stop collecting, save image, etc., as well as control the GGCS; however, the user will only notice a few changes to the Scan menus (see Scan /Master command).

Only minimal information will be displayed on the Slave, such as the drive, shutter and attenuator status, the frame being collected, and any repeat frame attempts. By default, the message “Frame Buffer in SLAVE mode...” is displayed. Errors during data acquisition or frame saves will terminate the Slave process and typically create a controller timeout error on the Master frame buffer.

Before exiting slave mode, terminate Gadds on the master frame buffer, then on the slave frame buffer, exit slave mode by typing <Ctrl-Break>. If you leave slave mode first, the master frame buffer will lose communication with the GGCS and become confused.

NOTE: This command is not available on theta-theta systems.

5.46.1 Arguments

None. Command executes immediately after confirmation.

5.47 Collect > Add • Accumulate an area detector frame (Still frame)

Menu Command: Collect > Add

Accelerator: Ctrl+Shft+A

User Level: 1

SLAM Syntax:

ADD $1 /CLEAR /PATTERN
/COUNTS=<n> /DISPLAY=<n>
/REAL TIME /RESET=<n> /SHUTTER
/ATTENUATOR

Collect > Add allows you to collect a single “still” frame of data at a fixed goniometer position (use any of the Collect > Scan commands to collect multiple data frames). The Collect > Goniometer > Manual command also lets you acquire a still frame while operating the goniometer with the manual control box. (See Collect > Goniometer > Manual for details.) Data are Data are continuously acquired until a specified amount of time has elapsed or a specified number of counts is reached, whichever occurs first.

You can optionally display the accumulated frame after it has been acquired, or update the display immediately as each count is recorded (referred to as “real-time display”). If you elect one of the display options, ADD also updates the current frame status information displayed at the upper right of the screen.

The frame is not automatically written to disk. Use File > Save after collecting the still frame if you want to save the data to disk.

When invoked from the menu, or run from the command line without arguments, Add displays a dialog box where you can view/edit the arguments described below before performing the operation/function. Pressing the ENTER key or clicking the OK button starts the operation. Pressing ESC or the Cancel button stops the operation and returns you to the menu. You can interrupt the operation by pressing CTRL+BREAK.

5.47.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Max Seconds) [30.0]

This is the maximum count time (in seconds). The default value is 30; the range is from 1 to 65,535 seconds. Times can be entered in decimal seconds or in HH:MM:SS.SS (hours, minutes and seconds) format. Data collection ends when the specified time has elapsed, or when the maximum count limit (see MAX COUNTS below) has been reached.

/CLEAR .....(Pre-Clear?) [Yes]

This qualifier, when set, clears memory before the new data frame is collected. If it is not set, the new data are added to the image already in the frame accumulation memory (for example, an image left over from a previous ADD, LOAD, or SCAN command).

/PATTERN ..... (Test Pattern Y/N) [No]

This qualifier, when present, draws a test grid into the frame accumulation memory prior to collecting data. The test grid is used for factory alignment, and consists of grid lines on a 64-pixel spacing; two circles, one with a 270-pixel radius and one with a 280-pixel radius; and two crosses rotated to 45 degrees, one linear cross, and one passed through the current flood field correction.

/COUNTS ..... (Max Counts) [10,000,000]

This qualifier sets an upper limit on how many counts may occur before data collection is terminated. When the specified number is reached the system ends the data collection, saving the data frame. The default value is 10,000,000 counts, with a range from 0 to 2,147,483,647 (i.e., (2^{31})-1) counts. Data collection will also be terminated if MAX SECONDS is reached before MAX COUNTS.

/DISPLAY=<n> ..... (Max Displayed Counts) [7]

0 = no display, otherwise # counts corresponding to white on the display. The initial

default is 7; the allowed range is from 1 to 10^6.

/REAL TIME .....(Real-time Display?) [Yes]

This qualifier, when present, displays data as it is being collected. The display does require additional processing time, and will limit the maximum rate at which counts can be accumulated. If the MAX DISPLAYED COUNTS qualifier is given a non-zero value, the frame will be automatically displayed at the end of the ADD if real-time display is off. This latter display method has no effect on observed data rate.

If you're not sure whether real-time display will affect the observed data rate significantly at your current incident count rate, check the late counts in the frame header of a representative frame with the FRAME_INFO command. If the late counts are more than a few percent of the total counts, your data collection will be more efficient if real-time display is turned off. In general, you should be able to use real-time display for set-up and sample evaluation, but you should disable it during collection of frame series which will be used as input to data reduction (see the similar SCAN command display options).

While real-time display is active, you can change the upper display limit using the plus key to increase or the minus key to decrease the current limit by a factor of two. (The range is 7 to 524287). Modify the contrast using the left and right arrow keys. Modify the brightness using the up and down keys. Hold down the control key and an arrow to increase the change of contrast or brightness.

/RESET=<n> ..... (Reset Interval) [0]

This qualifier specifies the number of seconds before repetitive auto-clear of frame memory (0 = do not clear). The default value is 0; the range is from 1 to 65,535 seconds. This parameter is useful in conjunction with real-time display if you're looking for a change in intensity over time. For instance, if you're driving the goniometer manually to look for or maximize the intensity of a reflection, it helps to clear the screen frequently, for example every 1 second by setting the reset interval to 1.

/SHUTTER ..... (Open & Close Shutter) [No]

If present on the command line or checked “Y” in the dialog box, this qualifier causes the shutter to open at the start of Collect > Add, and to close at the end. Otherwise, the shutter stays in its current state for the duration of the exposure.

/ATTENUATOR.....(Insert Attenuator) [No]

If present on the command line or checked "Y" in the dialog box, this qualifier causes the shutter to open with the attenuator inserted at the start of Collect > Add, and to close at the end. Otherwise, the shutter stays in its current state for the duration of the exposure.

5.48 Collect > Shutter • Open/close X-ray beam shutter

Menu Command: Collect > Goniometer > Shutter or Collect > Shutter

Accelerator: Ctrl+Shift+S

User Level: 1

SLAM Syntax:

GONIOMETER /SHUTTER
or SHUTTER

See Section 5.20 Collect > Goniometer > Shutter.

6. Process Routines

6.1 Process > Flood > New • Acquire data to generate new flood-field correction

Menu Command: Process > Flood > New

Accelerator: none

User Level: 3

SLAM Syntax:

FLOOD /NEW $1 /COUNTS=<n> /DISPLAY=<n> /REALTIME /FILE=<s> /XMIN=<n> /YMIN=<n> /MAG=<n> /SHUTTER

This selection is used to collect a single frame of data for use in flood field calibration, followed by automatic computation and installation of a new flood-field correction based on that data. The purpose of this calibration is to produce a smooth detector data image from a uniform, spherically radiating point source, such as the Fe^{55} source supplied with the system. The correction works by slightly altering the POSITIONS of counted photons according to a "rubber-sheet" stretching/shrinking in regions along the X and Y detector axes, in order to make the Fe^{55} image more uniform. It does not alter the recorded number of photons.

FLOOD /NEW requires you to enter the approximate source to detector distance. This distance should be the same as the sample to detector distance (since in this case, the source is at the sample position). Make sure to remove all obstructions to the detector face (such as the beam stop). Note that the source distance is measured in cm from the flat front of the detector (where the fiducial plate mounts). Usually, you should create a new flood-field correction prior to data collection on each sample, before the brass fiducial-plate image is taken.

The best procedure for acquiring new flood-field data is to accumulate 10,000,000 counts. This procedure accounts for variation in activity of different Fe^{55} sources and the decrease in intensity of an Fe^{55} source as it ages (the half-life is about 2.5 years). Typically, it will take about half an hour to accumulate 10M counts. In order to set up the acquisition of a new flood field in this manner, set the MAX SECONDS argument described below to a large value, for example, $1.0x10^4$ seconds, and set MAX COUNTS to $1.0x10^7$ counts.

WHEN YOU TAKE A FE^{55} FLOOD-FIELD IMAGE, BE SURE THAT THE DETECTOR BIAS IS SET CORRECTLY FOR FE^{55}. Also be sure to reset the bias back to the correct level for your x-ray generator (e.g., for Cu radiation) when finished with flood-field and fiducial-plate data collection.

After running FLOOD /NEW, it is a good idea to take a 120 second frame to verify that you have a good flood-field correction. The image should look more uniform than a “raw” image taken with no flood-field correction. Remember that appearance of any residual lines results only from a bias in the POSITIONING of those events, not from any error in the number of counted photons. The SPATIAL (fiducial-plate) calibration will reduce or eliminate this residual positional error. If lines are present, they may have a second-order effect on integrated intensities due to resulting variation of spot shapes across the detector, but they are not a problem unless they are prominent.

FLOOD /NEW computes the flood-field table from an X-projection and Y-projection of the Fe^{55} image. These projection arrays are by convention stored in a plottable ASCII file ending in a ._pj extension, in the current frame directory specified in the CONFIGURE /EDIT panel. The flood-field correction itself is stored similarly, except with a ._fl extension. The name of the current flood-field correction is shown on the display in the current status area at the bottom right of the screen. FLOOD /NEW updates this name when a new correction is acquired. When you exit FLOOD /NEW after successful completion, the new correction automatically goes into effect.

The /XMIN=<n>, /YMIN=<n> and /MAG=<n> arguments described below allow you to create a flood-field table that results in 512x512 or 1024x1024 output data frames that correspond to a specific area of the detector rather than to its entire area. For this calculation, the full detector is considered to be an array of 16376 x 16376 “bins.” Its origin is by default coincident with the output frame origin, and its bins are by default summed in 32 x 32 blocks to form a normal 512 x 512 output frame. These arguments allow you to choose the detector bin at which the output frame origin is placed, and to use a re-binning factor less than 32 to effectively magnify a smaller detector region to cover the whole 512 x 512 output frame. For example, /MAG=2

results in re-binning by 16:1 instead of 32:1. In general, this feature is useful only for special (e.g., non-crystallographic) applications, and these settings should be left at their defaults.

In the case of a foil, illumination by the electrical x-ray source causes fluorescence, creating a secondary point-source where the incident beam strikes the foil. 1-mil Fe foil is a good choice for a Cu source. Because the foil not only fluoresces, but also scatters and diffracts the incident beam, you need to swing the detector far enough in 2-theta to 1) avoid any beam-stop shadow or scatter and 2) eliminate any diffraction rings strong enough to affect the calibration. For Fe/Cu calibrations, -50 to -60 degrees appears to work well at a 15 cm distance with the 9 cm diameter detector. When illuminating the foil, use a collimator barrel from which all pinholes have been removed. This not only increases the intensity, but also substantially smooths any diffraction rings which you can't otherwise avoid. In order to evenly illuminate the detector, it is very important that the plane of the foil be parallel to the detector face. If your image does not appear uniform it is probably because either the foil is not centered at the instrument center (the foil plane must contain the 2-theta rotation axis) or the plane of the foil is not parallel to the detector face. Prior to performing the calibration take an exposure with ADD to make sure that you're getting uniform illumination. The predominant low-frequency feature in the image should be a reasonably symmetric radial falloff.

When the setup looks good, make sure the detector distance and beam center are correctly set in the CONFIGURE /EDIT input panel, then take a good 10,000,000 count flood-field image (with the shutter control option set to “Y”).

When invoked with the NEW option from the FLOOD submenu or when run from the command line without arguments, FLOOD /NEW displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins collection of flood-field data with subsequent automatic computation and installation of a new flood-field correction; the ESC key or right mouse button returns you to the FLOOD submenu. You can interrupt a flood-field data collection in progress with the CTRL-BREAK key combination; however, the current flood-field correction at that point is undefined—either re-collect new data or restore the correction to a known state with the FLOOD /LOAD or FLOOD /LINEAR command.

6.1.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Max Seconds) [15:00]

This is the maximum count time (in seconds). The default value is 900; the range is from 1 to 65,535 seconds. Times can be entered in decimal seconds or in HH:MM:SS.SS (hours, minutes and seconds) format. Data collection ends when the specified time has elapsed, or when the maximum count limit (see MAX COUNTS below) has been reached.

/COUNTS=<n>.....(Max Counts) [10,000,000]

This qualifier sets an upper limit on how many counts may occur before data collection is terminated. When the specified number is reached the system ends the data collection, saving the data frame. The default value is 10,000,000 counts, with a range from 0 to 10^{37} counts. Data collection will also be terminated if MAX SECONDS is reached before MAX COUNTS.

/DISPLAY=<n>.....(Max Displayed Counts) [100]

0 = no display, otherwise # counts corresponding to white on the display. The initial default is 100; the allowed range is from 1 to 10^{6}.

/REALTIME..... (Realtime Display (Y/N)) [Y]

This qualifier, when present, displays data as it is being collected. The display does require additional processing time, and will limit the maximum rate at which counts can be accumulated. If the MAX DISPLAYED COUNTS qualifier is given a non-zero value, the frame will be automatically displayed at the end of the frame collection if realtime display is off. This latter display method has no effect on observed data rate. Since the data rate in Fe^{55} source frames is not very high, use of /REALTIME with FLOOD /NEW will rarely cause any loss in counting efficiency, and you can keep this set to “Y.”

While real-time display is active, change the upper display limit using the plus key to increase or the minus key to decrease the current limit by a factor of two. (The range is 7 to 524287). Modify the contrast using the left and right arrow keys. Modify the brightness using the up and down keys. Hold down the control key and an arrow key to increase the change of contrast or brightness.

/FILE= .....(Output Filename) [normal._fl]

Enter the filename for the output correction data. By default, output files are created with a ._fl extension in the frame directory specified in the CONFIGURE /EDIT input panel. More specifically, the filename you enter here is merged with the default filespec Frame_root:*._fl, where Frame_root refers to the directory in the CONFIGURE / EDIT panel. See CONFIGURE /EDIT for details on how filenames are merged. The intermediate X and Y projection arrays are stored similarly, but with a ._pj extension.

In menumode, the filename is defaulted to the standard naming convention of "SIZE_DDD._FL", where "SIZE" is replaced by "0512" or "1024" and "DDD" is replaced by the detector distance in cm.

/XMIN=<n>.....(Lower X of Corrected Frame) [0]

Enter the X detector bin number to use as left side of corrected frame. The default value is 0; the range is from 0 to 16365.

/YMIN=<n>.....(Lower Y of Corrected Frame) [0]

Enter the Y detector bin number to use as bottom of corrected frame. The default value is 0; the range is from 0 to 16365.

/MAG=<n>..... (Magnification of Corrected Frame) [1]

Enter the magnification factor of the correction table. The default value is 1; the range is from 1 to 32.

/SHUTTER ..... (Open & Close Shutter Y/N) [N]

This qualifier, if present on the command line or given as "Y" in the input panel, causes the shutter to open at the start of each exposure, and to close at the end. Otherwise, the shutter stays in its current state for the duration of the command. It is used for the Fe foil method of generating a point source. Keep the shutter closed for Fe^{55} sources.

6.2 Process > Flood > Load • Install a disk-resident flood-field correction table

Menu Command: Process > Flood > Load

Accelerator: none

User Level: 2

SLAM Syntax: FLOOD /LOAD $1

This command is used to read and install a flood field calibration file that was previously created with FLOOD /NEW or FLOOD /REPROCESS. These commands compute a flood-field table from an X-projection and Y-projection of an Fe^{55} image. By convention, each flood-field correction is stored in a plottable ASCII file ending in a ._FL extension, in the current frame directory specified in the CONFIGURE /EDIT panel. Although you can thus keep several different flood-field corrections available at any time, re-using old flood-field corrections is not really very useful, since your results will be better if you run FLOOD /NEW prior to data collection on each new sample.

The name of the current flood-field correction is shown on the display in the current status area at the bottom right of the screen. FLOOD /LOAD updates this name when the correction is changed.

When invoked with the LOAD option from the FLOOD submenu or when run from the command line without arguments, FLOOD /LOAD displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins reading in the specified correction; the ESC key or right mouse button returns you to the FLOOD submenu.

6.2.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Filename) [normal._fl]

Name of the flood-field correction to read. This filename is merged with the current frame directory specified in the CONFIGURE /EDIT panel before the program attempts to access the file. See CONFIGURE /EDIT for a description of how this is done. If you leave this field blank or specify a wildcard filename pattern in the FLOOD /LOAD input panel, the program will display a list of filenames from which you can select the desired correction (see DISPLAY /NEW for a more complete description of filename selection). The default filespec for filename selection is Frame_root:*._FL, where Frame_root is the frame directory specified in the CONFIGURE /EDIT panel.

The special filename of “$DEFAULT” is replaced with the standard naming convention of “SIZE_DDD._FL”, where “SIZE” is

replaced by “0512” or “1024” and “DDD” is replaced by the detector distance in cm.

6.3 Process > Flood > Reprocess • Generate a new table from previous projection data (on disk)

Menu Command: Process > Flood > Reprocess

Accelerator: none

User Level: 3

SLAM Syntax: FLOOD /REPROCESS $1 $2 /XMIN=<n> /YMIN=<n> /MAG=<n>

This command is used to reprocess an existing flood field file projection file to use it with different X, Y or magnification settings.

The /XMIN=<n>, /YMIN=<n> and /MAG=<n> arguments described below allow you to create a flood-field table that results in 512x512 or 1024x1024 output data frames that correspond to a specific area of the detector rather than to its entire area. For this calculation, the full detector is considered to be an array of 16376 x 16376 “bins.” Its origin is by default coincident with the output frame origin, and its bins are by default summed in 32 x 32 blocks to form a normal 512 x 512 output frame. These arguments allow you to choose the detector bin at which the output frame origin is placed, and to use a re-binning factor less than 32 to effectively magnify a smaller detector region to cover the whole 512 x 512 output frame. For example, /MAG=2 results in re-binning by 16:1 instead of 32:1. In general, this feature is useful only for special

(e.g., non-crystallographic) applications, and these settings should be left at their defaults.

When invoked with the REPROCESS option from the FLOOD submenu or when run from the command line without arguments, FLOOD /REPROCESS displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins computation installation of the new flood-field correction; the ESC key or right mouse button returns you to the FLOOD submenu.

6.3.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input Projection Filename) [normal._fl]

Enter the filename for input projection data (._PJ). The default file is NORMAL._PJ. By convention, these files reside in the frame directory specified in the CONFIGURE /EDIT input panel. The filename you specify here is merged with the default specification Frame_root:*._pj before the program attempts to access the file. See CONFIGURE /EDIT for details on how this merging is performed. If you leave this item blank, or specify a “wildcard” filename pattern, pressing the ENTER key or the left mouse button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or the left mouse button. You will be returned to the input panel with the selected filename filled in. If you leave this item blank, it is the same as entering a *.* wildcard pattern (which is then merged as described above).

$2 ..... (Output Correction Filename) [zoom._fl]

Enter the filename for the output correction data. The default file is ZOOM._FL. convention, these files reside in the frame directory specified in the CONFIGURE /EDIT input panel. The filename you specify here is merged with the default specification Frame_root:*._fl before the program attempts to access the file. See CONFIGURE /EDIT for details on how this merging is performed.

/XMIN=<n> ..... (Lower X of Corrected Frame) [1024]

Enter the X detector bin number to use as left side of corrected frame. The default value is 0; the range is from 0 to 4095.

/YMIN=<n> ..... (Lower Y of Corrected Frame) [1024]

Enter the Y detector bin number to use as bottom of corrected frame. The default value is 0; the range is from 0 to 4095.

/MAG=<n>.....(Magnification of Corrected Frame) [2]

Enter the magnification factor of the correction table. The default value is 1; the range is from 1 to 8.

6.4 Process > Flood > Linear • Reset to linear table (i.e., no correction)

Menu Command: Process > Flood > Linear

Accelerator: none

User Level: 2

SLAM Syntax: FLOOD /LINEAR

Selecting FLOOD /LINEAR with the LINEAR option from the FLOOD submenu or from the command line specifies that no flood field calibration file will be used in subsequent data acquisition (linear scaling of event positions). The name of the current flood-field correction is shown on the display in the current status area at the bottom right of the screen. FLOOD /LINEAR updates this name to “LINEAR.” Since you will in general obtain better data if a flood-field correction is in effect, the ADD, SPATIAL /NEW and SCAN commands will issue a warning if you start data collection with a linear flood-field correction.

FLOOD /LINEAR runs immediately without prompting for additional input.

6.4.1 Arguments

None. Command executes immediately.

6.5 Process > Bad Pixels > Process • Process flood image to determine bad pixels

Menu Command: Process > Bad Pixels > Process

Accelerator: none

User Level: 3

SLAM Syntax: BADPIXELS /PROCESS $1 $2 $3 $4 $5 $6 $7 /LOCAL

Used by Bruker manufacturing and service engineers to evaluate detector for aberrations in pixel sensitivity.

6.5.1 Evaluation Region

Used to determine the area of the frame to evaluate for bad pixels. Radius from detector center (not beam center) should be around 260 for 512 frames or 520 for 1024 frames. A circle will be drawn at this radius, so you can visual see if you're off. Border pixels determine how many rows around the border of the frame should be ignored. 0=ingore only the overflow row (1st and last).

The algorithm will average the total pixels at each radius from the detector center (excluding border pixels) up to and including the requested radius, then apply a three-point smoothing function. This produces a function of the expected intensity versus distance from detector center. Alternately, one can use a local average calculated using a box (15x15 for 512 frames, 31x31 for 1024 frames), where the center 3x3 box is excluded from the calculations.

6.5.2 Bad Pixel Criteria

The user enters the weakness criteria in percentage at the center of the detector and the weakness criteria at the entered radius to evaluate. The program assumes the weakness criteria function is linear with respect to radius from center. Here a pixel at the center must be within 85% of the average intensity to be considered good. A pixel near the edge only needs to be within 75% to be considered good. At a radius of 130, the criterion is 80%.

Hot pixels are treated similarly, with the tightest restriction being for the center and the least restrictive requirement at the edge.

6.5.3 Rejection Criteria

After all bad pixels are determined, the program displays the evaluation radius, the border, and all bad pixels as an overlay on top of the flood field image. Next, a table is displayed consisting of the bad pixels with comments and clusters identified. Comments include:

- >Weaker< 5% weaker than criteria
- >Hotter< 5% hotter than criteria
- >>>DEAD<<< Below 10% of expected
- >>>BURNT<<< Above 900% of expected

Currently, we add up the total adjacent bad pixels around each bad pixel (number of bad neighbor pixels). If this number is greater than or equal to the entered cluster size, then the pixel is identified as “Cluster.” This will not identify long single pixel lines of bad pixels.

6.5.4 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Radius) [260 | 520 | 1040]

Radius, in pixels, from center pixel (not beam center) which defines evaluation region.

$2 .....(Border) [0]

Border, in pixels, to exclude from evaluation region. 0 means to exclude only the overflow rows (first and last rows/columns).

$3 .....(Weak) [75%]

$4 .....(Weak) [85%]

Percentage of average pixel below which pixel is considered weak. Lower criteria is used for edge (at radius) and higher criteria is used for center. Assume linear function with respect to radius.

$5 ..... (Hot) [115%]

$6 ..... (Hot) [125%]

Percentage of average pixel above which pixel is considered hot. Lower criteria is used for center and higher criteria is used for edge (at radius). Assume linear function with respect to radius.

$7 ..... (Cluster) [3]

Number of adjacent neighbor pixels to be considered a cluster (excludes bad pixel in question). Clusters of questionable pixels at or above this size are flagged. Range is 0 to 8.

/LOCAL ..... (Local average) [Yes]

Check to calculate average pixel within a box of 15x15 for 512 frames, 31x31 for 1024 frames, or 63x63 for 2048 frames. The center 3x3 pixels are skipped as are the overflow rows. Uncheck to use average pixel as a function of radius from center.

6.6 Process > Spatial > New • Acquire data and generate a new spatial correction

Menu Command: Process > Spatial > New

Accelerator: none

User Level: 3

SLAM Syntax:

SPATIAL /NEW $1 /COUNTS=<n> /DISPLAY=<n> /REALTIME /FILE=<s> /XENGEN /THRESHOLD=<n> /SHUTTER

This routine is used to collect a brass fiducial plate image at a specific detector distance and automatically compute and install a spatial correction for data subsequently collected at that distance. This will be necessary when you collect a new flood field, whenever experimental parameters change (e.g., the detector distance is moved) or whenever the instrument has been modified (e.g., the goniometer has been realigned, etc.).

Prior to running SPATIAL /NEW, make sure the correct value for the current sample-to-detector distance is entered in the CONFIGURE /EDIT panel (see CONFIGURE /EDIT for more information).

The correction is computed from a frame acquired with the brass fiducial plate fastened to the front of the detector face, and with a reasonably uniformly radiating point source positioned at the center of the goniometer. The supplied Fe^{55} source is good for this purpose. You should acquire and compute a new spatial correction from such a frame before starting data collection on each new sample, but AFTER acquiring and computing a new flood-field correction (see the description of the FLOOD command). The sample-to-detector distance for this frame must be exactly the same as it will be for the frames collected from the sample crystal. Usually a fiducial plate frame with a time cutoff of about 30 minutes or a count cutoff of about 100,000 counts is adequate (a rule-of-thumb which works well is to use the same collection time as for the flood-field data plus 5 minutes, but no less than 15 minutes).

It is essential that the brass plate be properly fastened to the area detector face (see figure in manual). The flat side of the brass plate rests against the detector face; the side with the counter-sunk holes faces the sample. Insert and tighten ALL the fastening screws to eliminate any small warpage in the fiducial plate.

Either remove the beam stop or make sure that the detector is swung out far enough that the beam stop will cast no shadow when you acquire the brass-plate image. Make sure that the Fe^{55} source is properly centered in the goniometer, and directly faces the area detector.

The name of the spatial correction currently in effect is displayed in the current status area at the lower right of the screen. This correction is

used by the CURSOR commands when they output HKL values and “unwarped” X,Y coordinates, and by all the REFL_ARRAY commands, which extract spots from a series of frames, index the diffraction pattern, and compute a least-squares crystal orientation matrix.

SPATIAL /NEW writes four output files, all created in the current frame directory set in CONFIGURE /EDIT. The first is written in a frame file format. The other three output files are all ASCII files in PLOTSO format, which can be displayed with the GRAPH /FILE command.

._br File containing the brass-plate frame, suitable for input to data reduction programs, such as XENGEN (be sure it is written in the correct format).

._ix Contains the indexed fiducial spot positions. It can be used to restore a previously computed spatial correction when it is read in with the SPATIAL /LOAD command.

._if Shows the spatial correction table used to transform pixel X,Y coordinates FROM raw to corrected values;

._it Shows the table which transforms corrected coordinates TO raw coordinates.

Both the ._if and ._it plot files are strictly informational—the program doesn't require them (since the information in them is automatically re-generated from the ._ix file by FRAMBO when SPATIAL /LOAD is used), and you can delete them if desired.

When invoked with the NEW option from the SPATIAL submenu or when run from the command line without arguments, SPATIAL /NEW displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins collecting the fiducial plate image; the ESC key or right mouse button returns you to the SPATIAL submenu. You can interrupt acquisition in progress by pressing the CTRL-BREAK keyboard combination; however, at that point the current spatial correction is undefined.

Before taking data, SPATIAL /NEW displays the current CONFIGURE /EDIT distance and direct beam center on the bottom status line, and asks you to confirm that they are correct before proceeding. If these values don't correspond to your current experimental setup, run CONFIGURE /EDIT and correct them before acquiring the brass-plate data. These values are stored in the output frame header and are used in subsequent processing, for example, in the spatial correction. If you don't supply the correct values, you may not be able to auto-index your frames (without a lot of extra effort).

Since collected data are of higher quality when a flood-field correction is made, the message

WARNING: NO FLOOD-FIELD CORRECTION. CONTINUE?

is displayed on the bottom status line in the case where SPATIAL /NEW is run with no current active flood-field correction.

When acquisition of the fiducial-plate image begins, the progress message

COLLECTING SPATIAL CALIBRATION DATA...

is displayed on the bottom status line.

After the fiducial-plate image has been acquired, SPATIAL /NEW automatically processes it to extract positions of the spots and, based on the known positions of the corresponding holes in the fiducial plate, computes a new spatial correction. In the course of processing the data, it must index the rows and columns (curved, due to the pincushion distortion) of fiducial spots in order to match each spot with a hole of known position on the fiducial plate. When the indexing is complete, a graphic map of the fiducial spot positions extracted from the frame is drawn. This graph is actually a GRAPH /FILE of the plottable ASCII ._ix spatial calibration file. Dashed lines are drawn along the rows and columns of the indexed pattern. If a line jumps from one row or column to another, the holes have been mis-indexed, and the spatial calibration will not be valid.

If this happens, use the CONTRAST command to check the quality of the fiducial plate frame. If the frame looks OK, you can try re-processing it with SPATIAL /PROCESS with a different I/sigma level for thresholding spots from the image. Another possibility is to acquire a fiducial-plate image for a longer period of time. Usually, mis-indexing occurs because the I/sigma threshold is set too low, causing the program to interpret background as a spot. The default threshold of 4 works well on brass-plate images which contain 80,000 to 100,000 total counts. If your image contains more counts, you will probably have to raise the threshold accordingly; for example, if the image contains 1,000,000 counts (i.e., about 10 times the nominal number) increase the threshold by a factor of about sqrt(10)—12 would be a good value in this case.

6.6.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Max Seconds) [15:00]

This is the maximum count time (in seconds). The default value is 900; the range is from 1 to 65,535 seconds. Times can be entered in decimal seconds or in HH:MM:SS.SS (hours, minutes and seconds) format. Data collection ends when the specified time has elapsed, or when the maximum count limit (see MAX COUNTS below) has been reached.

Usually a fiducial plate frame with a time cutoff of about 30 min or a count cutoff of about 100,000 counts is adequate (a rule-of-thumb which works well is to use the same collection time as for the flood-field data plus 5 minutes, but no less than 15 minutes).

/COUNT=<n>.....(Max Counts) [150,000]

This qualifier sets an upper limit on how many counts may occur before data collection is terminated. When the specified number is reached the system ends the data collection, saving the data frame. The default value is 150,000 counts, with a range from 0 to 10^{37} counts. Data collection will also be terminated if MAX SECONDS is reached before MAX COUNTS.

/DISPLAY=<n>.....(Max Displayed Counts) [100]

0 = no display, otherwise # counts corresponding to white on the display. The initial default is 100; the allowed range is from 1 to 10^{6}.

/REALTIME .....(/Realtime) [Yes]

This qualifier, when present, displays data as it is being collected. The display does require additional processing time, and will limit the maximum rate at which counts can be accumulated. If the MAX DISPLAYED COUNTS qualifier is given a non-zero value, the frame will be automatically displayed at the end of the frame collection if realtime display is off. This latter display method has no effect on observed data rate. Since the data rate in Fe^{55} source frames is not very high, use of /REALTIME with SPATIAL / NEW will rarely cause any loss in counting efficiency, and you can keep this set to “Y”.

/FILE=<s>..... (Output Filename) [brass]

Enter the base filename for the output frame and correction data. By default, all four output files (._br, ._ix, ._if, and ._it, as described above) in the frame directory specified in the CONFIGURE /EDIT input panel. More specifically, the filename you enter here is merged with the default filespec Frame_root:*._br, ._ix, etc. where Frame_root refers to the directory in the CONFIGURE /EDIT panel. See CONFIGURE /EDIT for details on how filenames are merged. The default name is “brass.”

In menumode, the filename is defaulted to the standard naming convention of “SIZE_DDD._BR,” where “SIZE” is replaced by “0512” or “1024” and “DDD” is replaced by the detector distance in cm.

If you supply a filename extension here, it is overridden with the extensions ._br, ._ix, ._it, and ._if as appropriate.

If you leave this item blank, or specify a “wildcard” filename pattern, pressing the ENTER key or the left mouse button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or the left mouse button. You will be returned to the input panel with the selected filename filled in. If you leave this item blank, it is the same as entering a *._ix wildcard pattern. Both filenames and patterns entered here are merged with the CONFIGURE /EDIT frame directory, as described above.

/XENGEN.....(Xengen Output Format (Y/N)) [No]

In the input panel, enter “Y” to write the output ._br frame in XENGEN format (more correctly, in the old PCS computer format), “N” otherwise. The default selection is “N” (Bruker format). While the Bruker format will be used increasingly in later releases, you need to be sure that your data reduction package will support it before using it. If you're not sure whether your data reduction package will read Bruker format, it is probably safer to specify Y here.

/THRESHOLD=<n>(Threshold) [8.0]

When extracting fiducial spots from the brass-plate image, the I/sigma(I) (i.e., intensity divided by its standard deviation) of each spot is computed based on counting statistics. Spots with an I/sigma(I) less than the value specified here are considered to be background fluctuations and are ignored. The default value of 8 should be satisfactory for brass-plate images with 80,000 to 100,000 total counts (see the discussion above). Valid range is 0.1 to 9999.

/SHUTTER ..... (Open & Close Shutter (Y/N)) [No]

This qualifier, if present on the command line or given as “Y” in the input panel, causes the shutter to open at the start of each exposure, and to close at the end. Otherwise, the shutter stays in its current state for the duration of the command. It is used for the Fe foil method of generating a point source. Keep the shutter closed for Fe^{55} sources.

6.7 Process > Spatial > Load • Install a disk-resident spatial correction

Menu Command: Process > Spatial > Load

Accelerator: none

User Level: 2

SLAM Syntax: SPATIAL /LOAD $1

This command is used to read and install a spatial correction that was previously created with SPATIAL /NEW or SPATIAL /PROCESS. These commands compute a spatial correction from an Fe^{55} image taken with the brass fiducial plate fastened to the front of the area detector. By convention, each spatial correction is stored in a plottable ASCII file ending in a ._IX extension, in the current frame directory specified in the CONFIGURE /EDIT panel. Although you can thus keep several different spatial corrections available at any time, re-using old spatial corrections is really not very useful, since your results will be better if you run SPATIAL /NEW prior to data collection on each new sample. However, if you're analyzing frames on a different computer from that on which the spatial correction was determined, you can transfer the spatial correction by moving the ._IX file over the network (if necessary) and loading it with SPATIAL /LOAD.

Don't confuse SPATIAL /LOAD with the LOAD command on the master menu, which reads a detector frame instead of an ASCII spatial correction file.

The name of the current spatial correction is shown on the display in the current status area at the bottom right of the screen. SPATIAL /LOAD updates this name when the correction is changed.

When invoked with the LOAD option from the SPATIAL submenu or when run from the command line without arguments, SPATIAL /LOAD displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins reading in the specified correction; the ESC key or right mouse button returns you to the SPATIAL submenu.

During the loading process SPATIAL /LOAD displays the progress messages:

Reading table ...

Building correction tables ...

Some computation is necessary since the ._IX file contains just the fiducial spot positions, not the correction tables themselves. Loading and computation of the correction tables should be completed in a few seconds.

6.7.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Filename) [brass._ix]

Name of the spatial correction to read. This filename is merged with the current frame directory specified in the CONFIGURE /EDIT panel before the program attempts to access the file. See CONFIGURE /EDIT for a description of how this is done. If you leave this field blank or specify a wildcard filename pattern in the SPATIAL /LOAD input panel, the program will display a list of filenames from which you can select the desired correction (see DISPLAY /NEW for a more complete description of filename selection). The default filespec for filename selection is Frame_root:*._IX, where Frame_root is the frame directory specified in the CONFIGURE /EDIT panel.

The special filename of “$DEFAULT” is replaced with the standard naming convention of “SIZE_DDD._IX,” where “SIZE” is replaced by “0512” or “1024” and “DDD” is replaced by the detector distance in cm.

6.8 Process > Spatial > Linear • Revert to linear table (i.e., no correction)

Menu Command: Process > Spatial > Linear

Accelerator: none

User Level: 2

SLAM Syntax: SPATIAL /LINEAR

Selecting SPATIAL /LINEAR with the LINEAR option from the SPATIAL submenu or from the command line specifies that no spatial correction will be used in subsequent data acquisition (linear scaling of frame X,Y coordinates). The name of the current spatial correction is shown on the display in the current status area at the bottom right of the screen. SPATIAL /LINEAR updates this name to “LINEAR.” Since you will in general not be able to determine HKL indices and crystal orientation if no spatial correction is in effect, the REFL_ARRAY /INDEX and / LEASTSQ will issue a warning if you run them with a linear spatial correction.

SPATIAL /LINEAR runs immediately without prompting for additional input.

6.8.1 Arguments

None. Command executes immediately.

6.9 Process > Spatial > Process • Compute correction from current LOADed brass plate frame

Menu Command: Process > Spatial > PROCESS

Accelerator: none

User Level: 3

SLAM Syntax: SPATIAL /PROCESS $1 /THRESHOLD=<n>

SPATIAL /PROCESS can be used to compute and install a spatial correction given a fiducial plate image collected with a previous SPATIAL /NEW or ADD command. The fiducial plate image must reside in the 32-bit frame accumulation memory prior to running this command. It must, therefore, be left from an earlier SPATIAL / NEW, ADD or SCAN (with no intervening commands which overwrite accumulation memory having been issued—see the SAVE command description for a list of these commands), or must be read in with a LOAD command (not DISPLAY, and not SPATIAL /LOAD).

When invoked from the master menu or from the command line without arguments, SPATIAL / PROCESS displays an input panel where you can view/edit the items described below prior to computing the spatial correction. If you press the ENTER key or left mouse button when in this input panel, the computation begins. The ESC key or right mouse button returns you from the input panel to SPATIAL submenu. When computation has started, SPATIAL /PROCESS displays the progress message on the bottom status line:

BUILDING CORRECTION TABLES...

Computations should be complete within a few seconds. During this process, SPATIAL /PROCESS automatically extracts positions of the fiducial spots from the input frame and, based on the known positions of the corresponding holes in the fiducial plate, computes a new spatial correction. In the course of processing the data, it must index the rows and columns (curved, due to the pincushion distortion) of fiducial spots in order to match each spot with a hole of known position on the fiducial plate. When the indexing is complete, a graphic map of the fiducial spot positions extracted from the frame is drawn. This graph is actually a GRAPH /FILE of the plottable ASCII ._ix spatial calibration file (see below). Dashed lines are drawn along the rows and columns of the indexed pattern. If a line jumps from one row or column to another, the holes have been mis-indexed, and the spatial calibration will not be valid.

If this happens, use the CONTRAST command to check the quality of the fiducial plate frame. If the frame looks OK, you can try re-processing it with SPATIAL /PROCESS with a different I/ sigma level for thresholding spots from the image. Another possibility is to acquire a fiducial-plate image for a longer period of time. Usu-

ally, mis-indexing occurs because the I/sigma threshold is set too low, causing the program to interpret background as a spot. The default threshold of 4 works well on brass-plate images which contain 80,000 to 100,000 total counts. If your image contains more counts, you will probably have to raise the threshold accordingly; for example, if the image contains 1,000,000 counts (i.e., about 10 times the nominal number) increase the threshold by a factor of about sqrt(10)—12 would be a good value in this case.

The name of the spatial correction is updated in the current status area at the lower right of the screen. This correction is used by the CURSOR commands when they output HKL values and “unwarped” X,Y coordinates, and by all the REFL_ARRAY commands, which extract spots from a series of frames, index the diffraction pattern, and compute a least-squares crystal orientation matrix.

SPATIAL /PROCESS writes three output files. All three files are ASCII files in PLOTSO format, which can be displayed with the GRAPH /FILE command:

._ix Contains the indexed fiducial spot positions; can be used to restore a previously computed spatial correction when it is read in with the SPATIAL /LOAD command.

._if Shows the spatial correction table used to transform pixel X,Y coordinates FROM raw to corrected values;

._it Shows the table which transforms corrected coordinates TO raw coordinates.

Both the ._if and ._it plot files are strictly informational—the program doesn't require them (since the information in them is automatically re-generated from the ._ix file by FRAMBO when SPATIAL /LOAD is used), and you can delete them if desired.

All three of the output files are by default created in the current frame directory set in the CONFIGURE /EDIT panel.

6.9.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Output Filename) [brass]

Enter the base filename for the output correction data. By default, all three output files (._ix, ._if, and ._it, as described above) in the frame directory specified in the CONFIGURE /EDIT input panel. More specifically, the filename you enter here is merged with the default filespec Frame_root:*._ix, ._if, etc. where Frame_root refers to the directory in the CONFIGURE /EDIT panel. See CONFIGURE /EDIT for details on how

filenames are merged. The default name is “brass.”

If you supply a filename extension here, it is overridden with the extensions ._ix, ._it, and ._if as appropriate.

If you leave this item blank, or specify a “wildcard” filename pattern, pressing the ENTER key or the left mouse button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or the left mouse button. You will be returned to the input panel with the selected filename filled in. If you leave this item blank, it is the same as entering a *._ix wildcard pattern. Both filenames and patterns entered here are merged with the CONFIGURE /EDIT frame directory, as described above.

/THRESHOLD=<n>(# Sigmas Spot Threshold) [8.0]

When extracting fiducial spots from the brass-plate image, the I/sigma(I) (i.e., intensity divided by its standard deviation) of each spot is computed based on counting statistics. Spots with an I/sigma(I) less than the value specified here are considered to be background fluctuations and are ignored. The default value of 8 should be satisfactory for brass-plate images with 80,000 to 100,000 total counts (see the discussion above). Valid range is 0.1 to 9999.

6.10 Process > Spatial > Unwarp • Apply spatial correction and write unwarped output frame(s)

Menu Command: Process > Spatial > Unwarp

Accelerator: Ctrl+U

User Level: 1

SLAM Syntax:

SPATIAL /UNWARP $1 $2 $3
/DISPLAY=<n> /NOBEAMCENTER

SPATIAL /UWWARP writes an output data frame generated by spatially remapping the specified input frame to correct the inherent geometrical pincushion distortion, based on the currently active spatial correction. Unwarping is important for frames which are to be processed by GADDS or other programs which need spatially corrected input. The data reduction programs for crystallographic data perform the spatial correction internally, and do not require unwarped frames. Users of FRAMBO and SADIE would use SPATIAL /UNWARP only in special cases.

Each pixel of the corrected output frame is generated by splitting the counts of each raw pixel into its corresponding unwarped pixel bins. First the exact unwarped pixel location (real value) is computed from the raw pixel location (integer value). Next the weighting fractions (real values) are computed for the four surrounding unwarped pixel locations (integer values). Using these weighting fractions, the raw pixel's counts are divided into the four surrounding unwarped pixel bins, so the sum of bins equals the original raw pixel counts. Therefore, each count is preserved during the unwarping process, although some counts are spatially corrected off the frame image dimensions, so the total counts in the frame will decrease slightly.

An unwarped frame image is equivalent to a perfect flat detector. Pixels are perfect squares across this flat detector. There is no spatial distortion or pin cushioning effects. There is no variation of intensity sensitivity between pixels. A perfectly radiating point source will not produce a flat intensity image, but rather a slight decay of intensity from the detector center to the edges. Geometric effects cause pixels at the edges to represent a smaller solid angular region than the pixels at the detector center. Software processing will handle these geometric variations of frame pixels during integration into raw spectrum.

NOTE: The isotope source is not a true point source, but rather a Lambert radiator where the intensity will drop as the cosine of the incidence angle.

6.10.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input Frame Filename) [frame1.000]

Name of first file to be unwarped. Default is frame1.000. If you leave this item blank, or specify a “wildcard” filename pattern, pressing the ENTER key or the left mouse button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or the left mouse button. You will be returned to the input panel with the selected filename filled in. If you leave this item blank, it is the same as entering a *.* wildcard pattern. Both filenames and patterns entered here are merged with the CONFIGURE /EDIT frame directory, as described above.

$2 .....(# of Frames to Process) [1]

Number of frames in the series to unwarp.

$3 .....(Output Frame Filename) [frame1u.000]

Name of unwarped frame file that will be created. The default is frame1.unw. If no output extension is specified, a .unw extension is used. If you leave this item blank, or specify a “wildcard” filename pattern, pressing the ENTER key or the left mouse button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or the left mouse button. You will be returned to the input panel with the selected filename filled in. If you leave this item blank, it is the same as entering a *.* wildcard pattern. Both filenames and patterns entered here are merged with the CONFIGURE /EDIT frame directory, as described above.

/NONORMALIZATION(Suppress I Normalization (Y/N)?) [no]

In command line mode, enter “nonormalization” if you want the system to bypass intensity normalization (described above). In the input panel specify “Y” at the prompt to bypass intensity normalization (the default “N” causes the system to normalize intensities).

/DISPLAY=<n> ..... (Max Display Counts) [16]

Enter 0 if you do not want the correction frame displayed; any other number selects display and is used to set the white level of the display.

/XENGEN.....(Xengen output format (Y/N)?) [no]

In the input panel, enter “Y” to write the output frame in XENGEN format (more correctly, in the old PCS computer format), “N” otherwise. The default selection is “N” (Bruker format). If you're going to use these frames as input to GADDS, use “N” here.

/NOBEAMCENTER(Suppress Unwarping Beam Ctr (Y/N)) [yes]

Normally, SPATIAL /UNWARP overwrites the X,Y beam center coordinates stored in the output frame header with the spatially corrected values. /NOBEAMCENTER suppresses the update of the beam center in the output header. In GADDS, where the beam center may already be unwarped, /NOBEAMCENTER is usually required, while in FRAMBO where the beam center is always stored in warped coordinates, this option is left off. The default in the input panel is “Y.”

6.11 Process > Corrections > LPA

Menu Command: Process > Corrections > LPA

Accelerator: none

User Level: 2

SLAM Syntax:

CORRECTIONS /LPA $1 $2 $3
/MONOCHROMATOR=<n> /AIRMU=<n>
/NOREVERSE

Calculate and apply Lorentz, polarization, air and faceplate absorption corrections, then apply the “reverse” corrections for Lorentz and polarization to obtain intensities equivalent to a conventional powder diffractometer with a monochromator and scintillation counter.

6.11.1 Lorentz

For a completely random sample the forward and reverse Lorentz corrections are identical and effectively cancel each other out.

6.11.2 Polarization

The forward polarization correction:

$$corr = I^* \frac{1+\cos^2 2\alpha}{\cos 2\beta + \sin 2\beta \cos^2 2\alpha + \left[\sin 2\beta + \cos 2\beta \cos^2 2\alpha\right]\cos^2 2\theta}$$

The reverse polarization correction:

$$corr = I^* \left[1+\cos^2 2\alpha \ \cos^2 2\theta\right] / 2$$

where:

2α = two-theta of monochromator

2θ = two-theta of Bragg reflection

2β = angle of reflection vector from horizontal plane

6.11.3 Air and Faceplate Absorption

Be absorption calculations account for path length differences due to geometry. Photons at the center of the detector travel through a shorter Be path than a photon at the edge of the detector.

Nominal AIRMU is 0.00021 per pixel; (about .01 per cm) assuming 8.0KV (Cu K(alpha)), 80:20 N2:O2, 20°C, 760mm Hg, 47.5 pixels/cm. At detector distance of 12 cm, difference in correction across face is < 1%, so AIRMU need not be very precise.

For speed considerations, we will only calculate the LPA correction every 16 (or 32 for 1K frames) pixels along the detector. Intermediate pixel corrections may be determined using linear extrapolation.

6.11.4 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input Filename) [$FRAME]

Enter filename for first input frame in series to process.

$2 .....(# of Frames to Process) [1]

Enter # consecutive frames to process.

$3 .....(Output Filename) [$NULL]

Enter filename for first output corrected frame.

/MONOCHROMATOR=<n>(Mono. 2T) [26.6]

Enter monochromator 2-theta (0 if filter).

/AIRMU=<n> .....(Air Mu in Cm-1) [0.01]

Enter air absorption coefficient.

/NOREVERSE .....(Suppress Reverse Corr. Y/N) [No]

Enter Y to suppress reverse polarization correction.

6.12 Process > Corrections > Fiber

Menu Command: Process > Corrections > Fiber

Accelerator: none

User Level: 2

SLAM Syntax:

CORRECTIONS /FIBER $1 $2 $3
/X=<n> /Y=<n> /Z=<n>
/NSTEPS=<n> /MU=<n> /RADIUS=<n>

Calculates an absorption correction table based on a long fiber. It is assumed that the fiber along its axis is longer than the diameter of the incident beam in all orientations. In the directions perpendicular to the fiber axis, the fiber is smaller than the diameter of the incident beam.

The sample vector is expressed in goniometer head coordinates where when the goniometer angles are all zero:

+X = direction of incident beam (away from tube)

+Y = normal to X & Z and forms right-handed coordinate system

+Z = vertical direction (up)

For speed considerations, we will only calculate the absorption correction every 16 (or 32 for 1K frames) pixels along the detector. Intermediate pixel corrections may be determined using linear extrapolation.

Divide the cross section of the fiber into little boxes of volume dV.

Let: p = path length to box

q = path length of diffracted beam

a = incident beam angle to normal

b = diffracted beam angle to normal

μ = absorption coefficient

Then the absorption formula is given by:

$$A = \sum ae^{-\mu(ap_i + bq_i)dV_i}$$

6.12.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Input File) [$FRAME]

Enter filename for first input frame in series to process.

$2 ..... (# Frames to Process) [1]

Enter # consecutive frames to process.

$3 ..... (Output File) [$NULL]

Enter filename for first output corrected frame.

X=<n> .....(Sample vector X) [1]

Y=<n> .....(Sample vector Y) [0]

Z=<n> .....(Sample vector Z) [0]

Input the coordinates (in the goniometer head coordinate system) of the vector which is along the fiber axis. If the fiber axis points vertically, the coordinates are 0,0,1.

NSTEPS=<n> .....(Num integration steps) [10]

For the numerical integration algorithm input the number of integration steps along the radius. The more integration steps the greater the accuracy, but the longer the time for calculation. A value of 10 seems to give sufficient accuracy.

MU=<n> .....(Sample mu cm-1) [3.0]

Enter sample mu in cm-1.

RADIUS=<n> .....(Radius cm) [0.03]

Enter sample radius in cm.

6.13 Process > Corrections > Plate

Menu Command: Process > Corrections > Plate

Accelerator: none

User Level: 2

SLAM Syntax:

CORRECTIONS /PLATE $1 $2 $3
/X=<n> /Y=<n> /Z=<n> /MU=<n>
/THICKNESS=<n>

Calculates an absorption correction table based on a flat plate of infinite dimensions and a given thickness. Thus, the flat plate is larger than the incident beam in all directions for all orientations.

The sample vector is expressed in goniometer head coordinates where when the goniometer angles are all zero:

+X = direction of incident beam (away from tube)

+Y = normal to X and Z and forms right-handed coordinate system

+Z = vertical direction (up)

For speed considerations, we will only calculate the absorption correction every 16 (or 32 for 1K frames) pixels along the detector. Intermediate pixel corrections may be determined using linear extrapolation.

Both transmission and reflection cases are handled:

t = thickness of plate

a = incident beam angle to normal

b = diffracted beam angle to normal

μ = absorption coefficient

$$x = \frac{1}{\cos a} - \frac{1}{\cos b}$$

Reflection absorption formula is given by:

$$A = \frac{1 - e^{-\mu t x}}{\mu x \cos a}$$

Transmission absorption formula is given by:

$$A = \frac{e^{-\mu t / \cos b} - e^{-\mu t / \cos a}}{\mu x \cos a}$$

6.13.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$FRAME]

Enter filename for first input frame in series to process.

$2 .....(# Frames to Process) [1]

Enter # consecutive frames to process.

$3 .....(Output File) [$NULL]

Enter filename for first output corrected frame.

X=<n> .....(Sample vector X) [1]

Y=<n> .....(Sample vector Y) [0]

Z=<n> .....(Sample vector Z) [0]

Input the coordinates (in the goniometer head coordinate system) of the vector which is normal to the face of the sample and points away from the incident beam side of the sample. If the x-ray beam is along the normal to the sample face the vector coordinates are equal to 1,0,0.

MU=<n> .....(Sample mu cm-1) [3.0]

Enter sample mu in cm-1.

THICKNESS=<n> .(Thickness cm) [0.03]

Enter sample thickness in cm.

6.14 Process > Smooth > Average • Smooth image with 3x3 boxcar average filter

Menu Command: Process > Smooth > Average

Accelerator: none

User Level: 1

SLAM Syntax: SMOOTH /AVERAGE

Two filters are provided to smooth frame images: average will compute the average pixel value, while median determines the median pixel value. Both filters utilize a 3x3 pixel box and ignore any pixel outside the active pixel map (see MASK).

6.14.1 Arguments

None. Command executes immediately.

6.15 Process > Smooth > Median • Smooth image with 3x3 median filter

Menu Command: Process > Smooth > Median

Accelerator: none

User Level: 1

SLAM Syntax: SMOOTH /MEDIAN

Two filters are provided to smooth frame images: average will compute the average pixel value, while median determines the median pixel value. Both filters utilize a 3x3 pixel box and ignore any pixel outside the active pixel map (see MASK).

6.15.1 Arguments

None. Command executes immediately.

6.16 Process > Smooth > Convolve • Smooth image by convolving with average neighborhood

Menu Command: Process > Smooth > Convolve

Accelerator: none

User Level: 1

SLAM Syntax: SMOOTH /CONVOLVE $1

The average neighborhood filter will smooth the frame image using the average pixel value of a user-defined pixel box. This filter will ignore the active pixel map (see MASK).

6.16.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Width in pixels) [2]

Enter width in pixels of neighborhood to convolve.

6.17 Process > Calibrate • Calibrate detector distance, angle and center using a known standard

Menu Command: Process > Calibrate

Accelerator: none

User Level: 1

SLAM Syntax:

CALIBRATE $1 /MININT=<n>
/DISTANCE=<n> $2 /ANGLE=<n> $3
/X=<n> /Y=<n> $4 /AUTO /NOERASE
/DELAY=<n>

Precise detector position cannot be determined by visual methods, but require taking a frame of a known standard and comparing the measured Debye-Scherrer rings with the calculated lines based on various detector positional parameters. Detector distance, swing angle, and beam center are determined permitting accurate 2-theta and chi values from other routines, such as INTEGRATE.

The calibration process requires a data frame(s) using a known standard sample. Typically corundum, quartz, or silicon is used but in practice any material exhibiting high stability and extremely sharp diffraction lines can be used. Also uses GADDS$SYSTEM:profile.pro for definition of the lineshape function.

In interactive mode, the standard d/I file is superimposed over the collected data frame.

The user can move the detector position or the detector beam position using either the cursor keys or the trackball. On a fully calibrated frame, the calculated Debye-Sherrer lines will precisely center over the lines in the data frame.

Toggling between the calibration of the detector distance and the swing angle and the calibration of the detector center is performed by pressing the “C” key. As an aid during interactive calibration the detector distance, swing angle, and center are continuously displayed and updated on the screen.

To align the detector center, move the calibration lines until a calculated and a measured Debye-ring exhibit the same center. This is most easily accomplished with an on-axis data frame; if the data frame is off-axis, it can still be done by examining the offset at the extreme top and bottom of the display.

To align the detector distance, use the cursor keys to expand or contract the calibration lines. To align the swing angle, use the cursor keys to shift left or right the calibration lines. When correctly calibrated, all calculated Debye-rings will be precisely centered over the corresponding lines in the data frame.

Upon exiting CALIBRATE, the detector parameter offsets are stored in the frame header. General GADDS users cannot change the calibration and must inform their administrator if the calibration is off. If the user is an administrator, this message appears: “Update configura-

tion with new distance and beam center?" Answer yes to update the current configuration with the new distance and beam center. All future frames collected will have the calibrated values in their frame headers. Thus, CALIBRATE should be performed before any data frames are collected in order that the proper experimental values are written into the frame header.

If the detector distance was changed, the SPATIAL /UNWARP file will be wrong. You will need to reload the brass image, set the correct detector distance, and reprocess the spatial correction tables. Secondly, the beam center stored in the configuration setup is already unwarped, so during any SPATIAL /UNWARP command, set the /NOBEAMCENTER switch to "Y."

6.17.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Standard filename / PDF2 number) [corundum.std]

The input standard calibration file contains a list of d-spacing's and intensities for a given standard. GADDS is supplied with files for alumina, corundum, quartz, and silicon. Other standards can be added with a text editor. By default the directory GADDS$SYSDATA: (or SAXI$SYSTEM:) is used unless otherwise specified. If available, the JCPDS PDF2 CD-ROM may be read for any standard -- simply enter a valid PDF number separated by " ", "," or "-".

/MININT=<n>..... (Minimum relative intensity) [5]

When reading the standard file, all lines below this threshold will be ignored and thus not displayed.

/DISTANCE=<n> .. (Sample to detector distance (cm)) [from frame header]

The default is read from the frame header. This distance is measured from the sample to the front of the detector face and is read off the scale below the detector.

$2 ..... (Delta distance) [0.05]

Enter the interactive sensitivity for calibrating the detector distance in cm.

/ANGLE=<n>..... (Detector swing angle) [from frame header]

Default from frame header. Detector swing angle in degrees.

$3 ..... (Delta angle) [0.00]

Enter the interactive sensitivity for calibrating the detector angle in degrees.

/X=<n> .....(Detector X-center) [from frame header]

Default from frame header. Detector X-center in pixels. The origin is taken as lower left corner of frame.

/X=<n> .....(Detector Y-center) [from frame header]

Default from frame header. Detector Y-center in pixels.

$4 .....(Delta XY) [0.5]

Enter the interactive sensitivity for calibrating the detector center in pixels. Range 0.1 to 10.

/AUTO .....(Auto mode Y/N) [No]

Enter “Y” to perform an automatic least squares fit of the calibration standard line(s), prior to allowing user manipulation of the detector parameters.

/DELAY=<n> .....() [0.0]

Delay before exiting routine—useful in demo loops only.

/NOERASE .....() [No]

Prevents erasing the calibration lines when exiting routine.

7. Analyze Routines

7.1 Analyze > Cursors > Box • Display statistics of pixels in rectangular region

Menu Command: Analyze > Cursors > Box

Accelerator: F5

User Level: 1

SLAM Syntax: CURSORS /BOX $1 $2 $3 $4 /DELAY=<n> /NOERASE

When invoked from the menu or when run from the command line without arguments, Analyze > Cursor > Box starts running directly (that is, there are no dialog items to be filled in). A rectangular cursor (from 2x2 to 1024x1024 pixels in size) appears in the detector frame area and can be dragged or resized by the mouse or keyboard arrow keys. Several quantities (described below) related to the currently displayed frame at the cursor position are displayed in real time at the right of the image. Pressing ENTER or releasing the left mouse button exits, returning you to the menu. Pressing ESC or clicking the right mouse button while dragging with the left button pressed toggles between position-change mode and size-change mode. The center of the box remains fixed while the size changes as the mouse is dragged.

When moving or sizing the box with the arrow keys, you can press CTRL along with an arrow key to move in increments ten times larger than for the unmodified arrow key.

Analyze > Cursor > Box can also be used to clear or fill the area inside a box to a specified value, allowing you to edit the image with basic functions. When you press BACKSPACE (or DELETE on the extended, middle keypad), GADDS displays a dialog box where you can enter a value to set all pixels inside the box cursor. The default value is equal to the current

background estimate based on pixel values around the box perimeter. Pressing ESC or clicking the Cancel button exits without changing pixel values. After editing the image, you can use the SAVE command to write the image in edited form. This function can be performed only interactively (that is, there is no way to clear the area in a box with command-line commands).

By providing arguments on the command line, you can direct GADDS to compute the box calculations once at one specified position, after which control returns immediately to the command line.

The line weight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

Analyze > Cursor > Box can display HKL indices corresponding to the centroid position based on the current orientation matrix (that is, the one refined in the last ReflArray > LeastSquares command). These values will be correct for frames acquired in Bruker-format frames in general. They will probably NOT be correct for XENGEN–1.3-format frames, because those frames do not contain the required setting angle information.

If logging is turned on (see the File > LogFile command for more information), the quantities computed for the final position of the cursor prior to exiting the command are written to the output logfile. If scripting is enabled (see File > ScriptFile), a non-interactive CURSOR command corresponding to the final cursor position is written to the output script file.

The SLAM command arguments are:

$1

The X-coordinate of the lower left of the box in pixels. The range is from 0 to framesize-1; default value is 256.

$2

The Y-coordinate of the lower left of the box in pixels. The range is from 0 to framesize-1; default value is 256.

$3

The width of the box in pixels. The range is from 0 to framesize-1; default is 32.

$4

The height of the box in pixels. The range is from 0 to framesize-1; default is 32.

/DELAY=<n>

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain

on screen long enough for the user to discern its position.

/NOERASE:

Suppresses erasure of the cursor on exit. Since the cursors are drawn by “toggling” the sense of the screen pixels, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The Analyze > Clear command is another way to erase cursors left over from /NOERASE options.

The following output statistics are displayed on screen in real time, and are also written to the log file if applicable.

XY-PIXEL:

X- and Y-center of box in pixels (range from 0 to framesize-1), with the origin (X=0,Y=0) at the lower left of the screen.

WIDTH,HT:

Width and height of the box, in pixels.

TOTALCTS:

Sum of the pixel values in rectangular box.

MAXIMUM:

Largest pixel value in the box.

MEAN:

The average of the pixels values contained in the box.

I:

Integrated intensity (minus background). The background is computed as the average of the points on the perimeter of the box, excluding all points which are more than 3 standard deviations above the mean.

SIGMA(I):

Standard deviation of integrated intensity, I.

I/SIGMA(I):

Integrated intensity divided by its standard deviation.

BACKGND:

Average of points on perimeter of box, excluding those points which are more than 3 standard deviations above the mean.

XCNTROID:

Raw X-coordinate of centroid of intensity, in pixels.

YCNTROID:

Raw Y-coordinate of centroid of intensity, in pixels.

HKL:

If an orientation matrix is in effect, the HKL indices corresponding to the intensity centroid are also output.

XUNWARPED:

If a spatial correction is in use, this provides spatially corrected X-coordinate of centroid of intensity, otherwise this value will be identical to the raw coordinate.

YUNWARPED:

If a spatial correction is in use, this provides spatially corrected raw Y-coordinate of centroid of intensity, otherwise this value will be identical to the raw coordinate.

7.2 Analyze > Cursors > Circle • Display position and size of circular cursor

Menu Command: Analyze > Cursors > Circle

Accelerator: F6

User Level: 1

SLAM Syntax: CURSORS /CIRCLE $1 $2 $3 /DELAY=<n> /NOERASE

When invoked from the menu or when run from the command line without arguments, Analyze > Cursor > Circle starts running directly; that is, there are no dialog items to be filled in. A circular cursor with a small crosshair at its center appears in the detector frame area, and can be dragged or resized under control of the mouse and/or keyboard arrow keys. Several quantities (described below) related to the currently displayed frame at the cursor position are displayed in real time at the right of the image. Pressing ENTER or releasing the left mouse button exits, returning you to the menu. Pressing ESC or clicking the right mouse button while dragging with the left button pressed toggles between position-change mode and size-change mode where the center of the circle remains fixed while the size changes as the mouse is dragged.

When moving or sizing the circle with the arrow keys, you can press CTRL along with an arrow key to move in increments ten times larger than for the unmodified arrow key.

When used in this interactive manner, the command also provides the option to drive the spindle axis (phi) to a position where the zero-layer diffraction circle represented by the circular cursor would be at its closest approach to the direct beam center. Pressing the D key drives the phi axis to the new position (as indicated in the prompt on the bottom status line).

By providing arguments on the command line, you can direct the cursor computations to be performed once at a single specified position, after which control returns immediately to the command line.

The line weight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

If logging is turned on (see the File > LogFile command for more information), the quantities computed for the final position of the cursor prior to exiting the command are written to the output logfile. If scripting is enabled (see File > ScriptFile), a non-interactive CURSOR command cor-

responding to the final cursor position is written to the output script file.

The SLAM command arguments are:

$1

X-coordinate of the circle center in pixels. The range is from 0 to framesize-1; default value is 256.

$2

Y-coordinate of the circle center in pixels. The range is from 0 to framesize-1; default value is 256.

$3

Radius of the circle in pixels. The range is from 0 to framesize/2 -1; the default value is 64.

/DELAY=<n>

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on screen long enough for the user to discern its position.

/NOERASE

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The Analyze > Clear command is another way to erase cursors left over from /NOERASE options.

The following output statistics are displayed on screen in real time and written to the logfile, if applicable (for non-pole figure frames).

COUNTS:

Value of pixel at circle center.

XY-PIXEL:

X- and Y-coordinate of circle center (range from 0 to framesize-1), with origin (X=0, Y=0) being located at lower left of screen.

R-PIXELS:

Radius of circle in pixels.

DEGREES:

Radius of circle in degrees 2-theta.

ANGSTRMS:

Radius of circle, Angstroms.

The following output statistics are related to single-crystal alignment based on the position of a circle of reflections arising from a zero-level layer.

LAYER(A):

Spacing of planes normal to the beam axis in the case where the crystal is aligned, so that the diffracted layer circles are centered on the direct beam.

SPINDLE:

Change required to phi axis position (in degrees) to move the diffracted layer circle to the beam center

PARA-ARC:

Change required to goniometer head arc which is parallel to the detector plane at 2-theta,omega,phi = (0,0,0), in order to move the diffracted layer circle to the beam center.

PERP-ARC:

Change required to goniometer head arc which is perpendicular to the detector plane at 2-theta,omega, phi = (0,0,0), in order to move the diffracted layer circle to the beam center.

Pole figures are handled slightly differently. On these frames, the following output statistics are displayed on-screen in real time, and are also written to the logfile if applicable.

XY-Pixel:

Coordinates of current pixel (range from 0 to {framesize-1}), with origin (0,0) being located at lower left of screen.

R-Pixels:

Radius in pixels.

TotalCts:

Sum of counts on/inside circular box.

Maximum:

Maximum pixel intensity in circular box.

Mean:

Average counts in circular box.

I:

Integrated intensity (minus background). The background is computed as the average of the points on the perimeter of the box, excluding all points which are more than three standard deviations above the mean.

sigma(I):

Standard deviation of integrated intensity.

I/SimgaI:

Integrated intensity divided by its standard deviation.

Backgnd:

Average of points on perimeter of box, excluding those points which are more than three standard deviations above the mean.

XCntroid:

Raw X-coordinate of centroid of intensity.

YCntroid:

Raw Y-coordinate of centroid of intensity.

ACntroid:

Alpha angle of centroid of intensity.

BCntroid:

Beta angle of centroid of intensity.

7.3 Analyze > Cursors > Pixel • Show pixel positions and values in displayed frame

Menu Command: Analyze > Cursors > Pixel

Accelerator: F7

User Level: 1

SLAM Syntax: CURSORS /PIXEL $1 $2 /DELAY=<n> /NOERASE /DUMP

When invoked from the menu, or run from the command line without arguments, Analyze > Cursor > Pixel starts directly (that is, it requires no additional input). A full-window crosshair cursor appears in the detector frame area and can be dragged under control of the mouse and/or keyboard arrow keys. Several quantities (described below), related to the currently displayed frame at the cursor position, are displayed in real time to the right of the image. Pressing ENTER or releasing the left mouse button exits, returning you to the menu. Pressing ESC or clicking the right mouse button while dragging with the left button pressed displays a pixel map of the numeric values in memory for a 17- x 17-pixel grid centered on the pixel under the crosshair. In this display, a box appears around the value for the pixel currently underneath the cursor. Pressing any mouse or keyboard key returns to display of the data frame and the interactive crosshair cursor.

When dragging the cursor with the arrow keys, you can press CTRL along with an arrow key to move in increments ten times larger than for the unmodified arrow key.

By providing arguments on the command line, you can direct the cursor computations to be performed once at a single specified position, after which control returns immediately to the command line.

The line weight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

Analyze > Cursor > Pixel can display HKL indices corresponding to the cursor position based on the current orientation matrix (that is, the one refined in the last Crystal > LS command). These values will be correct for frames acquired with GADDS and for Bruker-format frames in general. They will probably NOT be correct for XENGEN–1.3-format multi-wire detector frames acquired data collection software earlier than FRAMBO V2, since those frames do not contain the required setting angle information.

If logging is turned on (see the File > LogFile command for more information), the quantities

computed for the final position of the cursor prior to exiting the command are written to the output logfile, as are the values in each 17x17 numeric pixel dump. If scripting is enabled (see File > ScriptFile), a non-interactive CURSOR command corresponding to the final cursor position is written to the output script file.

The SLAM command arguments are:

$1

X-coordinate in pixels of the crosshair center. The range is from 0 to framesize-1; default value is 256.

$2

Y-coordinate in pixels of the crosshair center. The range is from 0 to framesize-1; default value is 256.

/DELAY=<n>

Specifies a time interval to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on screen long enough for the user to discern its position.

/NOERASE

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The Analyze > Clear command is another way to erase cursors left over from /NOERASE options.

/DUMP

Displays a 17x17 numeric pixel dump at the specified position. If a keyboard or mouse event doesn't occur within the time-out value set in the Edit > Config dialog, the display times out and control is returned to the command line. If logging is enabled, a copy of the pixel dump is also written to the logfile.

The following output statistics are displayed on screen in real time and are also written to the logfile if applicable (for non-pole figures).

XY-PIXEL:

X- and Y-coordinates of current pixel (range from 0 to framesize-1), with origin (0,0) being located at lower left of screen.

COUNTS:

Counts at current pixel.

XUNWARPED:

If a spatial correction is in use, provides spatially corrected X-coordinate of current pixel, otherwise this value will be identical to the raw coordinate.

YUNWARPED:

If a spatial correction is in use, provides spatially corrected Y-coordinate, otherwise this value will be identical to the raw coordinate.

DX:

Signed pixel X-distance from frame center.

DY:

Signed pixel Y-distance from frame center.

2-THETA:

2-Theta value at current pixel.

ANGSTRMS:

Resolution in Angstroms at current pixel.

HKL:

If an orientation matrix is in effect, the HKL indices corresponding to the current pixel are also output.

Pole images are handled slightly differently. On these frames, the following output statistics are displayed on-screen in real time and are also written to the logfile if applicable.

XY-PIXEL:

X- and Y-coordinates of current pixel (range from 0 to framesize-1), with origin (0,0) being located at lower left of screen.

COUNTS:

Counts at current pixel.

DX:

Signed pixel X-distance from frame center.

DY:

Signed pixel Y-distance from frame center.

Alpha:

Alpha angle at current pixel.

Beta:

Beta angle at current pixel.

Chi:

Chi angle at current pixel (90-alpha).

Phi:

Phi angle at current pixel (same as beta).

7.4 Analyze > Cursors > Vector • Measure distances on displayed frame

Menu Command: Analyze > Cursors > Vector

Accelerator: F8

User Level: 1

SLAM Syntax: CURSORS/VECTOR $1 $2 $3 $4 /DELAY=<n> /NOERASE

When invoked from the menu or when run from the command line without arguments, Analyze > Cursor > Vector starts running directly (that is, there are no dialog items to be filled in). A rubber-band vector cursor appears in the detector frame area and can be dragged or resized by the mouse or keyboard arrow keys. Several quantities (described below) related to the currently displayed frame at the cursor position are displayed in real time at the right of the image. Pressing ENTER or releasing the left mouse button exits, returning you to the menu. Pressing ESC or clicking the right mouse button while dragging with the left button pressed toggles between position-change mode and size-change mode. The vector origin remains anchored while the vector endpoint moves as the mouse is dragged.

When moving or sizing the cursor with the arrow keys, you can press CTRL along with an arrow key to move in increments ten times larger than for the unmodified arrow key.

By providing arguments on the command line, you can direct GADDS to compute the calculations once at one specified position, after which control returns immediately to the command line.

The line weight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

If logging is turned on (see the File > LogFile command for more information), the quantities computed for the final position of the cursor prior to exiting the command are written to the output logfile. If scripting is enabled (see File > ScriptFile), a non-interactive CURSOR command corresponding to the final cursor position is written to the output script file.

The SLAM command arguments are:

$1

The X-coordinate of the lower left of the vector in pixels. The range is from 0 to framesize-1; default value is 256.

$2

The Y-coordinate of the lower left of the vector in pixels. The range is from 0 to framesize-1; default value is 256.

$3

The X-length of the vector pixels. The range is from 0 to framesize-1; default value is 32.

$4

The Y-length of the vector in pixels. The range is from 0 to framesize-1; default value is 1.

/DELAY=<n>

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on screen long enough for the user to discern its position.

/NOERASE

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by "toggling" the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The Analyze > Clear command also provides a way to erase cursors left over from /NOERASE options.

The following output statistics are displayed on screen in real time and are also written to the logfile if applicable (for non-pole figure frames).

ORIGCNTS:

Counts of pixel at vector origin.

ENDPCNTS:

Counts of pixel at vector endpoint.

X-ORIGIN:

X-coordinate of origin in pixels.

Y-ORIGIN:

Y-coordinate of origin in pixels.

X-ENDPT:

X-coordinate of endpoint in pixels.

Y-ENDPT:

Y-coordinate of endpoint in pixels.

X-MIDPT:

X-coordinate of midpoint in pixels.

Y-MIDPT:

Y-coordinate of midpoint in pixels.

D-PIXEL:

Length of vector in pixels.

D-~DEG:

Length of vector in degrees 2-theta.

D-~ANGST:

Length of vector in Angstroms.

CHI:

Angle of the vector in degrees clockwise from -χ. This chi convention is the same as that used on a 4-circle diffractometer (that is, if the vector origin is at the beam center and the endpoint is on a reflection taken at omega=0, chi is the angle to which you would drive the goniometer to place the reflection in the equatorial plane on the positive 2-theta side).

Pole image frames are handled slightly differently. On these frames, the following output statistics are displayed on-screen in real time and are also written to the logfile if applicable.

ORIGCNTS:

Counts of pixel at vector origin.

ENDPCNTS:

Counts of pixel at vector endpoint.

X-ORIGIN:

X-coordinate of origin in pixels.

Y-ORIGIN:

Y-coordinate of origin in pixels.

X-ENDPT:

X-coordinate of endpoint in pixels.

Y-ENDPT:

Y-coordinate of endpoint in pixels.

A-Origin:

Alpha angle at origin in degrees.

A-Endpt:

Alpha angle at end point in degrees.

B-Origin:

Beta angle at origin in degrees.

B-Endpt:

Beta angle at end point in degrees.

Angle:

Angle between two poles in degrees.

7.5 Analyze > Cursors > Conic • Display constant two-theta conic lines

Menu Command: Analyze > Cursors > Conic

Accelerator: F9

User Level: 1

SLAM Syntax: CURSORS /CONIC $1 $2 /DELAY=<n> /NOERASE

When invoked with the CONIC option from the CURSORS submenu or when run from the command line without arguments, CURSORS /CONIC starts running directly (that is, there are no items to be filled in on an input panel). A full-window conic cursor appears in the detector frame area, and can be moved under control of the mouse and/or keyboard arrow keys. Pressing the ENTER key or left mouse button exits, returning you to the CURSORS submenu.

The lineweight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

By providing arguments on the command line, you can direct the CURSORS /CONIC computations to be performed once at a single specified position, after which control returns immediately to the command line.

If logging is turned on (see the LOGFILE command for more information), the quantities computed for the final position of the cursor, prior to exiting the command, are written to the output logfile. If scripting is enabled (again, see LOGFILE), a non-interactive CURSORS command corresponding to the final cursor position is written to the output script file.

The SLAM command arguments are:

$1

X-coordinate in pixels of the crosshair center. The range is from 0 to {framesize-1}; default value is 256.

$2

Y-coordinate in pixels of the crosshair center. The range is from 0 to {framesize-1}; default value is 256.

/DELAY=<n>

Specifies a time interval to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on-screen long enough for the user to discern its position.

/NOERASE

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The CLEAR command also provides a way to erase cursors left over from /NOERASE options.

The following output statistics are displayed on-screen in real time and are also written to the logfile if applicable.

Counts:

Counts at current pixel.

XY-Pixel:

X- and Y-coordinate of current pixel (range from 0 to {framesize-1}), with origin (X=0, Y=0) being located at lower left of screen.

2-Theta:

2-Theta value of Debye-Scherrer ring at current pixel.

Angstrms:

Angstroms of Debye-Scherrer ring at current pixel.

Lambda:

Wavelength used to calculate statistics.

Chi:

Chi value of Debye-Scherrer ring at current pixel.

7.6 Analyze > Cursors > Rbox • Display statistics of pixels in rotated rectangular region

Menu Command: Analyze > Cursors > Rbox

Accelerator: F10

User Level: 1

SLAM Syntax: CURSORS /RBOX $1 $2 $3 $4 /DELAY=<n> /NOERASE

When invoked with the RBOX option from the CURSORS submenu or when run from the command line without arguments, CURSORS /RBOX starts running directly (that is, there are no items to be filled in on an input panel). A rectangular cursor from 2x2 to 128x128 pixels in size appears in the detector frame area, and can be moved or re-sized under control of the mouse and/or keyboard arrow keys. Pressing the ENTER key or left mouse button exits, returning you to the CURSORS submenu. Pressing the ESC key or the right mouse button toggles between position-change mode and size-change mode where the lower left corner of the box remains anchored while the upper left corner moves under mouse control.

Analyze > Cursor > RBox can also be used to clear or fill the area inside a box to a specified value, allowing you to edit the image with basic functions. When you press BACKSPACE (or DELETE on the extended, middle keypad), GADDS displays a dialog box where you can enter a value to set all pixels inside the box cursor. The default value is equal to the current background estimate based on pixel values around the box perimeter. Pressing ESC or clicking the Cancel button exits without changing pixel values. After editing the image, you can use the SAVE command to write the image in edited form. This function can be performed only interactively (that is, there is no way to clear the area in a box with command-line commands).

The lineweight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

By providing arguments on the command line, you can direct the CURSORS /RBOX computations to be performed once at a single specified position, after which control returns immediately to the command line.

If logging is turned on (see the LOGFILE command for more information), the quantities computed, for the final position of the cursor prior to exiting the command, are written to the output logfile. If scripting is enabled (again, see LOGFILE), a non-interactive CURSORS command corresponding to the final cursor position is written to the output script file.

The SLAM command arguments are:

$1

The X-coordinate of the center of the box in pixels. The range is from 0 to {framesize-1}; default value is 256.

$2

The Y-coordinate of the center of the box in pixels. The range is from 0 to {framesize-1}; default value is 256.

$3

The width of the box in pixels. The range is from 0 to 128; default value is 32.

$4

The height of the box in pixels. The range is from 0 to 128; default value is 32.

/DELAY=<n>

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on-screen long enough for the user to discern its position.

/NOERASE

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The CLEAR command also provides a way to erase cursors left over from /NOERASE options.

The following output statistics are displayed on-screen in real time and are also written to the logfile, if applicable.

X-Center:

X-center of box in pixels (range from 0 to {framesize-1}), with origin (X=0) being located at lower left of screen.

Y-Center:

Y-center of box in pixels (range from 0 to {framesize-1}), with origin (Y=0) being located at lower left of screen.

Width:

Width of box in pixels.

Height:

Height of box in pixels.

TotalCts:

Sum of counts in rectangular box.

I:

Integrated intensity (minus background). The background is computed as the average of the points on the perimeter of the box, excluding all points which are more than three standard deviations above the mean.

Sigma(I):

Standard deviation of integrated intensity.

I/SigmaI:

Integrated intensity divided by its standard deviation.

Backgnd:

Average of points on perimeter of box, excluding those points which are more than three standard deviations above the mean.

XCntroid:

Raw X-coordinate of centroid of intensity.

YCntroid:

Raw Y-coordinate of centroid of intensity.

Maximum:

Maximum pixel intensity in box.

Mean:

Average counts in box.

HKL:

If an orientation matrix is in effect, the HKL indices corresponding to the current intensity centroid are also outputted.

XUnwarped:

If a spatial correction is in use, provides spatially corrected X-coordinate of centroid of intensity, otherwise this value will be identical to the raw coordinate.

YUnwarped:

If a spatial correction is in use, provides spatially corrected raw Y-coordinate of centroid of intensity, otherwise this value will be identical to the raw coordinate.

7.7 Analyze > Graph > File • Plot points from ASCII disk file

Menu Command: Analyze > Graph > File

Accelerator: Ctrl+G

User Level: 1

SLAM Syntax: GRAPH /FILE $1 /QUADRANT=<n> /PRECLEAR /NOCLEAR

This command plots X-Y graphs from disk-resident data. The input data file must be in PLOTSO format (as described in Appendix D). Examples of PLOTSO-format files generated by GADDS are ._pj flood-field projection intermediate data files, ._fl flood-field corrections, ._ix spatial correction files, ._if raw-to-corrected spatial maps, and ._it corrected-to-raw spatial maps.

When invoked from the menu, or run from the command line without arguments, Analyze > Graph > File displays a dialog box where you can view/edit the arguments described below. Pressing ENTER or clicking the OK button starts graphing the specified file. Pressing ESC or the Cancel button returns you to the menu.

See PLOTSO file format, Section 13.7, for more details.

7.7.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Plot Data Filename) [plotso.dat]

This parameter specifies the ASCII data file to graph. This filename is merged with the current data directory specified in the Project > New/Edit/Copy dialog before the program attempts to access the file. If you leave this field blank or enter a wildcard filename pattern in the Analyze > Graph > File dialog, the program will display a list of filenames from which you can select the desired data file.

/QUADRANT=<n> (Quadrant) [0]

This argument specifies whether you want the graph to appear covering the entire frame display area (enter “0”), or just one of the four quadrants (enter 1 through 4 as appropriate). The default value is 0 (full frame window). Quadrants are 0 = full window, 1 = lower left, 2 = lower right, 3 = upper left, and 4 = upper right.

/PRECLEAR..... (Pre-Clear (Y/N) ?) [No]

This argument specifies whether or not the screen area (full or quadrant, depending on the value of /QUADRANT above) will be cleared before the plot is drawn. In menu

mode, check this item to clear the memory, or leave it unchecked if you want to superimpose the graph on the data frame currently displayed in that quadrant.

/NOCLEAR.....(No-Clear (Y/N) ?) [No]

This parameter is specified to suppress clearing any previously displayed graph. It is useful in script mode to add labels to graphs before printing.

7.8 Analyze > Graph > Vector • Plot profile along vector in displayed frame

Menu Command: Analyze > Graph > Vector

Accelerator: Ctrl+V

User Level: 1

SLAM Syntax: GRAPH /VECTOR $1 $2 $3 $4 /QUADRANT=<n> /DELAY=<n> /NOERASE

When you want to plot an arbitrary one-pixel slice through the data use the GRAPH /VECTOR sub-command. This routine is similar to CURSOR /VECTOR in that you use the cursor to identify the beginning and ending points of a rubber-band vector. When you've specified the path of interest in this manner, GRAPH /VECTOR then plots the intensities of all pixels located along that path as an X-Y graph of intensity (counts) versus position along the line (in pixels).

When invoked with the VECTOR option from the GRAPH submenu or when run from the command line without arguments, GRAPH /VECTOR displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins interactive path-of-interest selection with a vector cursor. The ESC key or right mouse button returns you from the input panel to the GRAPH submenu.

When you're selecting a path-of-interest, a rubber-band like vector cursor appears in the detector frame area, and can be moved or re-sized under control of the mouse and/or keyboard arrow keys. Pressing the ENTER key or left mouse button plots the graph of pixel value versus distance along the vector, then exits, returning you to the GRAPH submenu. Pressing the ESC key or right mouse button toggles between position-change mode and size-change mode where the vector origin remains anchored while the vector endpoint moves under mouse control. If you want to exit without computing and drawing the graph, use CTRL-BREAK.

The lineweight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

By providing arguments on the command line, you can direct the GRAPH /VECTOR computations and graphing to be performed once at a single specified position, after which control returns immediately to the command line.

If logging is turned on (see the LOGFILE command for more information), the quantities computed, for the final position of the cursor prior to exiting the command, are written to the output

logfile. If scripting is enabled (again, see LOGFILE), a non-interactive GRAPH /VECTOR command corresponding to the final cursor position is written to the output script file.

7.8.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(X-Origin) [256]

The X-coordinate of the lower left of the box defining the region-of-interest in pixels. The range is from 0 to {framesize-1}; default value is 256.

$2 .....(Y-Origin) [256]

The Y-coordinate of the lower left of the box defining the region-of-interest in pixels. The range is from 0 to {framesize-1}; default value is 256.

$3 .....(X-Length) [32]

The X-length of the vector pixels. The range is from 0 to {framesize-1}; default value is 32.

$4 .....(Y-Length) [0]

The Y-length of the vector in pixels. The range is from 0 to {framesize-1}; default value is 1.

/QUADRANT=<n> (Quadrant) [0]

This parameter specifies whether you want the graph to appear covering the entire data frame (enter “0”), or just one of the four quadrants (enter 1 through 4 as appropriate). The default value is 0 (full frame window). Quadrants are 0 = full window, 1 = lower left, 2 = lower right, 3 = upper left, and 4 = upper right.

/DELAY=<n>..... () [0.0]—available in command mode only

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on-screen long enough for the user to discern its position.

/NOERASE..... () [No]—available in command mode only

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The CLEAR command also provides a way to erase cursors left over from /NOERASE options.

The following output statistics are displayed on-screen in real time, and are also written to the logfile if applicable.

OrigCnts:

Counts of pixel at vector origin.

EndpCnts:

Counts of pixel at vector endpoint.

X-Origin:

X-coordinate of origin in pixels.

Y-Origin:

Y-coordinate of origin in pixels.

X-Endpt:

X-coordinate of endpoint in pixels.

Y-Endpt:

Y-coordinate of endpoint in pixels.

X-Midpt:

X-coordinate of midpoint in pixels.

Y-Midpt:

Y-coordinate of midpoint in pixels.

D-Pixel:

Length of vector in pixels.

D-~Deg:

Length of vector in degrees 2-theta.

D-~Angst:

Length of vector in Angstroms.

Chi:

Angle of the vector in degrees clockwise from -X. This chi convention is the same as that used on a 4-circle diffractometer (i.e., if the vector origin is at the beam center and the endpoint is on a reflection taken at omega=0, chi is the angle to which you would drive the goniometer to place the reflection in the equatorial plane on the positive 2-theta side).

7.9 Analyze > Graph > Rocking • Plot rocking curve profile through frames

Menu Command: Analyze > Graph > Rocking

Accelerator: Ctrl+R

User Level: 1

SLAM Syntax:

GRAPH /ROCKING $1 $2 $3 $4
/QUADRANT=<n>
/FRAME_HALFWIDTH=<n>
/DELAY=<n> /NOERASE

GRAPH/ROCKING draws a graph in the frame window (or a specified quadrant) called a “rocking curve.” This graph shows integrated intensity in a specified rectangular area as a function of scan angle, and requires that you have a contiguous series of frames available for input.

Before running GRAPH /ROCKING, a set of data frames must be collected with fixed step size in any angle. Use the DISPLAY or LOAD command to display the central frame about which you want the rocking curve to be computed. Then, invoke GRAPH /ROCKING, where a rectangular cursor like the one in CURSORS /BOX is used to select a region within the data frame. From this, the program calculates the background-subtracted intensity for that region in each frame and displays the results in a plot of intensity versus scan angle. Background-subtracted intensity is determined in the same way as for CURSORS /BOX. The background is computed as the average of the points on the perimeter of the box, excluding those points which are more than 3 standard deviations above the mean. You have to be careful to choose the correct box size, since in some cases the X,Y centroid of the x-ray reflection may change as a function of scan angle.

While the program attempts to graph the intensity as a function of scan angle, if the scan angle is not available in the frame headers, or if the frame headers all contain the same value for the scan angle, the intensity is graphed as a function of frame number.

When invoked with the ROCKING option from the GRAPH submenu or when run from the command line without arguments, GRAPH /ROCKING displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins interactive region-of-interest selection with a box cursor. The ESC key or right mouse button returns you from the input panel to the GRAPH submenu.

When you're selecting a region-of-interest, a rectangular cursor from 2x2 to 128x128 pixels in size appears in the detector frame area, and can be moved or re-sized under control of the mouse and/or keyboard arrow keys. The arrow keys are very useful for precise, 1-pixel adjustments. Pressing the ENTER key or left mouse

button computes the intensity versus scan angle curve and draws it on the screen. Pressing the ESC key or right mouse button toggles between position-change mode and size-change mode where the lower left corner of the box remains anchored while the upper left corner moves under mouse control. If you want to exit without computing and drawing the graph, use CTRL-BREAK. Depending on the number of frames specified with the FRAME HALFWIDTH argument (see below) the rocking curve can take several seconds to compute.

The lineweight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

By providing arguments on the command line, you can direct the GRAPH /ROCKING computations and graphing to be performed once at a single specified position, after which control returns immediately to the command line.

If logging is turned on (see the LOGFILE command for more information), the quantities computed, for the final position of the cursor prior to exiting the command, are written to the output logfile. If scripting is enabled (again, see LOGFILE), a non-interactive GRAPH /ROCKING command corresponding to the final cursor position is written to the output script file.

7.9.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (X-Origin) [256]

The X-coordinate of the lower left of the box defining the region-of-interest in pixels. The range is from 0 to {framesize-1}; default value is 256.

$2 ..... (Y-Origin) [256]

The Y-coordinate of the lower left of the box defining the region-of-interest in pixels. The range is from 0 to {framesize-1}; default value is 256.

$3 ..... (Width) [16]

The width of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 16.

$4 ..... (Height) [16]

The height of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 16.

/QUADRANT=<n> (Quadrant) [0]

This parameter specifies whether you want the graph to appear covering the entire data frame (enter “0”), or just one of the four

quadrants (enter 1 through 4 as appropriate). The default value is 0 (full frame window). Quadrants are 0 = full window, 1 = lower left, 2 = lower right, 3 = upper left, and 4 = upper right.

/FRAME_HALFWIDTH=<n>(Frame Halfwidth) [5]

Enter the number of frames ON EACH SIDE of the currently displayed frame to be included in the rocking curve. Make sure that you don't exceed the number of frames actually available for processing in either direction.

/DELAY=<n> .....() [0.0]—available in command mode only

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on-screen long enough for the user to discern its position.

/NOERASE .....() [No]—available in command mode only

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The CLEAR command also provides a way to erase cursors left over from /NOERASE options.

The following output statistics are displayed on-screen, and are also written to the logfile if applicable.

X-Center:

X-center of box in pixels (range from 0 to {framesize-1}), with origin (X=0) being located at lower left of screen.

Y-Center:

Y-center of box in pixels (range from 0 to {framesize-1}), with origin (Y=0) being located at lower left of screen.

Width:

Width of box in pixels.

Height:

Height of box in pixels.

TotalCts:

Sum of counts in rectangular box in the central frame

I:

Integrated intensity (minus background) in the central frame. The background is computed as the average of the points on the perimeter of the box, excluding all points which are more than three standard deviations above the mean.

Sigma(I):

Standard deviation of integrated intensity in the central frame. This value is not displayed if an orientation matrix is available. Instead, the HKL's area displayed.

I/SigmaI:

Integrated intensity divided by its standard deviation in the central frame. This value is not displayed if an orientation matrix is available. Instead, the HKL's area displayed.

I (3D):

3D integrated intensity for the spot. This is the sum of the 2D background-subtracted intensity on each of the component frames.

I3D/Sig:

The 3D integrated intensity divided by its standard deviation

XCntroid:

The X-centroid, in pixels, of the 3D integrated intensity

YCntroid:

The Y-centroid, in pixels, of the 3D integrated intensity

ZCntroid:

The Z-centroid, of the 3D integrated intensity. This is the centroid in the direction through the frames, and is expressed in degrees, or in frame number if the scan angle wasn't available in the component frame headers. That is, the units are the same as those indicated for the X-axis on the resulting graph.

HKL:

If an orientation matrix is in effect, the HKL indices corresponding to the 3D intensity centroid are also output.

7.10 Analyze > Graph > Poster • Interactively annotate displayed graph or frame

Menu Command: Analyze > Graph > Poster

Accelerator: None

User Level: 1

SLAM Syntax: GRAPH /POSTER

Analyze > Annotate has several subcommands to produce hard-copy plots and pictures suitable for poster presentation and publishing. When you choose this command from the menu, the program displays a right-cascading submenu containing these subcommands. When you invoke GRAPH /POSTER from the command line, no qualifiers are allowed, a submenu of dialog buttons will appear and the program will wait until you've made a selection. GRAPH /POSTER will execute only in interactive mode.

The subcommands are summarized in the following table:

Menu	SLAM	Description
New	/NEW	Start a new list of annotations
Edit	/EDIT	Edit current annotations
Clear	/CLEAR	Clear annotations within rectangular region
Save	/SAVE	Save annotations to PLOTSO file
Text	/TEXT	Position text on screen
Label	/LABEL	Label spots/peaks using d, I, hkl, TH, 2T, etc
Arrow	/DRAW / ARROW	Draws an arrow pointer
Box	/DRAW / BOX	Draws a rectangular box
Circle	/DRAW / CIRCLE	Draws an ellipse
Dot	/DRAW / DOT	Draws a single dot
Line	/DRAW / LINE	Draws a straight line
Style	/DRAW / STYLE	Switches between solid and dashed line styles

Each subcommand is described below.

Menu Command: Analyze > Annotate > New

SLAM Syntax: GRAPH /POSTER /NEW

This command clears the annotation list in preparation for starting a new series of annotations. Subsequent annotation commands are appended to the annotation list, which can then be saved with the Analyze > Annotate > Save subcommand. A saved annotation list can later be redisplayed with the Analyze > Graph > File command.

Menu Command: Analyze > Annotate > Edit

SLAM Syntax: GRAPH /POSTER /EDIT

All poster annotations are stored in a PLOTSO file format. These commands can be edited with a simple screen editor. After

exiting the /EDIT command, the graphics plane is erased and the poster annotations are redrawn.

NOTE: This will erase all graphs displayed prior to invoking the Analyze > Annotate command.

Menu Command: Analyze > Annotate > Clear

SLAM Syntax: GRAPH /POSTER /CLEAR

This command will clear a rectangular region. When selected, a cross hair cursor is visible. Position the crosshairs at a corner of the box to be erased. Anchor the corner by pressing ENTER or the left mouse button. (The cross hairs will disappear and be replaced with a rectangular box with one corner being the anchored point just selected and the other corner at the current cursor position). Press ENTER or the left mouse button to position the second box corner. The box is erased, and a crosshair cursor appears for positioning the next box. Pressing ESC or the right mouse button will return you to the menu.

Menu Command: Analyze > Annotate > Save

SLAM Syntax: GRAPH /POSTER /SAVE

This command will save all poster annotations in a PLOTSO file on disk. It can later be loaded with the Analyze > Graph > File command.

Menu Command: Analyze > Annotate > Text

SLAM Syntax: GRAPH /POSTER /TEXT

Text can be positioned and sized interactively using GRAPH /POSTER /TEXT. When selected, the user must first enter the text string to be displayed. All trailing spaces are removed from the text string, but leading spaces are retained. A box cursor will appear reflecting the size of the text string. Position the box cursor, then press ENTER or the left mouse button. The box will disappear, the text will be drawn, and the user will be prompted to enter the next text string to drawn. Pressing ESC or the right mouse button will return you to the draw menu. Pressing <F1> or the center mouse button will toggle the size mode. Moving the cursor left (or right) will increase (or decrease) the size of the text string in the x direction. Up and down cursor movement will change the height of the text. Press ENTER or the left mouse button to anchor the text size.

Menu Command: Analyze > Annotate > Label

SLAM Syntax: GRAPH /POSTER /LABEL

Spots or peaks can be labeled interactively with this command. When selected, a dialog box will appear. Choose what type of data to retrieve (either theta's, 2-theta's, d's, I's, or hkl's); and choose where to retrieve that data from (either the frame, raw trace, or peaks table). And choose what marker char-

acter to use to highlight the data. A crosshairs cursor will appear and the selected label will appear within the message window. Pressing ENTER or the left mouse button will draw the marker at the current cursor position and automatically send the user into the /TEXT option to edit, position, and size the label to be drawn (see Analyze > Annotate > Text). Pressing ESC or the right mouse button will return you to the menu without drawing the label.

Menu Command: Analyze > Annotate > Arrow

SLAM Syntax: GRAPH /POSTER /DRAW /ARROW

This command will draw an arrow. When selected, a cross hair cursor is visible. Position the crosshairs at the point of the arrow to be drawn, press ENTER or the left mouse button. The crosshairs will disappear and be replaced with an arrow with the point anchored at the selected position and the tail at the current cursor position. Position the tail of the arrow, press ENTER or the left mouse button. The arrow is drawn, and a crosshair cursor appears for positioning the next arrow. Pressing ESC or the right mouse button will return you to the menu.

Menu Command: Analyze > Annotate > Box

SLAM Syntax: GRAPH /POSTER /DRAW /BOX

This command will draw a rectangular box. When selected, a crosshair cursor is visible. Position the crosshairs at a corner of the box to be drawn. Anchor the corner by pressing ENTER or the left mouse button. The crosshairs will disappear and be replaced with a rectangular box with one corner being the anchored point just selected and the other corner at the current cursor position. Position the second box corner, press ENTER or the left mouse button. The box is drawn, and a crosshair cursor appears for positioning the next box. Pressing ESC or the right mouse button will return you to the menu.

Menu Command: Analyze > Annotate > Circle

SLAM Syntax: GRAPH /POSTER /DRAW /CIRCLE

This command will draw an ellipse. When selected, a crosshair cursor is visible. Position the crosshairs at the center of the ellipse and press ENTER or the left mouse button to anchor this spot. The crosshairs will disappear and be replaced with an ellipse drawn with the center anchored and the width and height selected from the cursor. Move the mouse until the width and height are correct, press ENTER or the left mouse button. The ellipse is drawn, and a

crosshair cursor appears for positioning the ellipse center. Pressing ESC or the right mouse button will return you to the menu.

Menu Command: Analyze > Annotate > Dot

SLAM Syntax: GRAPH /POSTER /DRAW /DOT

This command will draw a single dot. When selected, a crosshair cursor is visible. Position the crosshairs at the position to draw the dot and press ENTER or the left mouse button. A dot is drawn and the crosshairs will remain for positioning the next dot. Pressing ESC or the right mouse button will return you to the menu.

Menu Command: Analyze > Annotate > Line

SLAM Syntax: GRAPH /POSTER /DRAW /LINE

This command will draw a line segment between two points. When selected, a crosshair cursor is visible. Position the crosshairs at the start of the line segment and anchor the line segment by pressing ENTER or the left mouse button. The crosshairs will disappear and be replaced with a line segment between the anchored point and the current cursor position. Position the line segment end point and press ENTER or the left mouse button. The line segment is drawn, and a crosshair cursor appears for positioning the next line. Pressing ESC or the right mouse button will return you to the menu.

Menu Command: Analyze > Annotate > Style

SLAM Syntax: GRAPH /POSTER /DRAW /STYLE

This command will toggle between drawing objects with a solid line style to drawing the objects with a dashed line style. The current style is displayed in the DRAW submenu title bar when using the SLAM command line.

7.11 Analyze > Graph > HKL • Plot HKL curve profile through frames

Menu Command: Analyze > Graph > HKL

Accelerator: None

User Level: 2

SLAM Syntax: GRAPH /HKL $1 /QUADRANT=<n> $2 $3 /DELAY=<n> /NOERASE

GRAPH/HKL draws a graph in the frame window (or a specified quadrant) called an “hkl curve.” This graph shows integrated intensity in a specified rectangular area as a function of hkl position, and requires that you have a contiguous series of frames collected using SCAN /HKL, available for input.

7.11.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(1st frame) [hkl01.000]

The name of the first frame in the HKL scan series.

/QUADRANT=<n>.(Quadrant) [0]

This parameter specifies whether you want the graph to appear covering the entire data frame (enter “0”), or just one of the four quadrants (enter 1 through 4 as appropriate). The default value is 0 (full frame window). Quadrants are 0 = full window, 1 = lower left, 2 = lower right, 3 = upper left, and 4 = upper right.

$2 ..... (Width) [32]

The width of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 32.

$3 ..... (Height) [32]

The height of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 32.

/DELAY=<n>..... () [0.0]—available in command mode only

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on-screen long enough for the user to discern its position.

/NOERASE..... () [No]—available in command mode only

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The CLEAR command also provides a way to erase cursors left over from /NOERASE options.

7.12 Analyze > Graph > Psi • Plot Psi curve profile through frames

Menu Command: Analyze > Graph > Psi

Accelerator: None

User Level: 2

SLAM Syntax: GRAPH /PSI $1 /QUADRANT=<n> $2 $3 /DELAY=<n> /NOERASE

GRAPH/PSI draws a graph in the frame window (or a specified quadrant) called an “psi curve.” This graph shows integrated intensity in a specified rectangular area as a function of psi angle, and requires that you have a contiguous series of frames collected using SCAN /PSI, available for input.

7.12.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(1st frame) [psi01.000]

The name of the first frame in the PSI scan series.

/QUADRANT=<n>.(Quadrant) [0]

This parameter specifies whether you want the graph to appear covering the entire data frame (enter “0”), or just one of the four quadrants (enter 1 through 4 as appropriate). The default value is 0 (full frame window). Quadrants are 0 = full window, 1 = lower left, 2 = lower right, 3 = upper left, and 4 = upper right.

$2 ..... (Width) [32]

The width of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 32.

$3 ..... (Height) [32]

The height of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 32.

/DELAY=<n>..... () [0.0]—available in command mode only

Specifies a time interval in seconds to wait before erasing the cursor and returning control to the program. This is for use in scripts, where it is desirable for the cursor to remain on-screen long enough for the user to discern its position.

/NOERASE..... () [No]—available in command mode only

Suppresses erasure of the cursor on exit. Note that the cursors are drawn by “toggling” the sense of the screen pixels; thus, you can erase a cursor left from a /NOERASE by reissuing the command with the same parameters. The CLEAR command also provides a way to erase cursors left over from /NOERASE options.

7.13 Analyze > Graph > Write • Write generated curve to file

Menu Command: Analyze > Graph > Write

Accelerator: None

User Level: 1

SLAM Syntax:

INTEGRATE /WRITE $1 /FILENAME=<s> /FORMAT=<s> /APPEND /SCALE=<n>

See Peaks > Integrate > Write command.

7.14 Analyze > Percent Crystal > External • Amorphous region external from Bragg peak

Menu Command: Analyze > Percent Crystal > External

Accelerator: None

User Level: 1

SLAM Syntax: PER_CRYSTAL /EXTERNAL $1 $2 $3 $4 $5 $6 $7 $8 /COMPTON

PER_CRYSTAL provides a quick method to estimate a percent crystallinity using frame data. Frames must have air scatter (and sample holder scattering) effects subtracted out to obtain meaningful results.

Calculates percent crystallinity within an user-defined region. The user must specify both an amorphous only region and a crystalline plus amorphous region. These regions should not overlap. Pixels are summed in both regions.

With the separation of amorphous and crystalline contributions, the percent crystallinity calculation is simply,

$$\%C = 100\% \frac{\sum I_C - \sum I_A}{\sum I_C}$$

where:

%C=percent crystallinity

I_c=intensity in crystalline region

I_a=intensity in amorphous region

7.14.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Two-Theta Begin for Amorphous Reg) [10]

$2 ..... (Two-Theta End for Amorphous Reg) [20]

$3 ..... (Chi Begin for Amorphous Region) [0]

$4 ..... (Chi End for Amorphous Region) [30]
Defines conic region for amorphous region.

$5 ..... (Two-Theta Begin for Crystalline Reg) [10]

$6 ..... (Two-Theta End for Crystalline Region) [20]

$7 ..... (Chi Begin for Crystalline Region) [60]

$8 ..... (Chi End for Crystalline Region) [90]
Defines conic region for crystalline region.

/COMPTON.....(Compton Scattering Y/N) [No]
Enter “Y” to subtract the Compton scattering effect from the amorphous result. The Compton scattering must be previously calculated using PER_CRYSTAL /COMPTON.

7.15 Analyze > Percent Crystal > Internal • Amorphous region surrounds Bragg peak

Menu Command: Analyze > Percent Crystal > Internal

Accelerator: None

User Level: 1

SLAM Syntax: PER_CRYSTAL /INTERNAL $1 $2 $3 $4 $5 $6 $7 $8 /LINEAR /COMPTON

PER_CRYSTAL provides a quick method to estimate a percent crystallinity using frame data. Frames must have air scatter (and sample holder scattering) effects subtracted out to obtain meaningful results.

Calculates percent crystallinity within a user-defined region. The user must specify both an amorphous region and an internal crystalline region. Pixels along the 2-theta boundaries of the crystalline region are integrated to obtain a left and right background value. The amorphous contribution under the crystalline region is assumed to be a linear function in 2-theta and constant in chi.

An alternate, non-linear background function is available. All pixels selected within the amorphous only region are used to solve for a 2nd order polynomial using a least-squares technique:

$bkg = a_0 + a_1 * x + a_2 * y + a_3 * x^2 + a_4 * x * y + a_5 * y^2$

With the separation of amorphous and crystalline contributions, the percent crystallinity calculation is simply,

$$\%C = 100\% \frac{\sum_{C}(I_O - I_B)}{\sum_{A+C} I_O}$$

where:

%C=percent crystallinity

I_O=observed intensity

I_C=calculated background

C= over crystalline region

A+C=over amorphous and crystalline region

7.15.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Two-Theta Begin for Amorphous Reg) [0]

$2 ..... (Two-Theta End for Amorphous Reg) [30]

$3 ..... (Chi Begin for Amorphous Region) [0]

$4 ..... (Chi End for Amorphous Region) [360]
Defines conic region for amorphous region.

$5 ..... (Two-Theta Begin for Crystalline Region) [5]

$6 ..... (Two-Theta End for Crystalline Region) [25]

$7 ..... (Chi Begin for Crystalline Region) [5]

$8 ..... (Chi End for Crystalline Region) [355]
Defines conic region for crystalline region.

/LINEAR .....(Linear Algorithm Y/N?) [Yes]

Use to specify either a linear amorphous function underneath the crystalline peak, or a polynomial function.

/COMPTON.....(Compton Scattering Y/N) [No]

Enter “Y” to subtract the Compton scattering effect from the amorphous result. The Compton scattering must be previously calculated using PER_CRYSTAL /COMPTON.

7.16 Analyze > Percent Crystal > Compton • Define the incoherent scattering due to the Compton effect

Menu Command: Analyze > Percent Crystal > Compton

Accelerator: None

User Level: 1

SLAM Syntax: PER_CRYSTAL /COMPTON $1 / SCALE=<n> /XSCALE=<n>

Calculates and displays the Compton scattering curve. Uses table in file: GADDS$SYSDATA:compton.tbl.

7.16.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Empirical Formula) [Al+3 2 O-2 3]

Enter empirical formula with valence states of ions.

/SCALE=<n> .....(Scale) [1.0]

Enter scaling factor multiplier.

/XSCALE=<n> .....(X Scale) [0]

Enter X scale: 0=(sin theta)/lambda, 1=theta, 2=2theta.

7.17 Analyze > Percent Crystal > Full • Calculate and use an amorphous background frame

Menu Command: Analyze > Percent Crystal > Full

Accelerator: None

User Level: 1

SLAM Syntax: PER_CRYSTAL /FULL $1 /DISPLAY=<n> $2 /RADIUS=<n> /HEIGHT=<n>

PER_CRYSTAL provides a quick method to estimate a percent crystallinity using frame data. Frames must have air scatter (and sample holder scattering) effects subtracted out to obtain meaningful results.

Calculates the percent crystallinity by extracting an amorphous background frame. With the separation of amorphous and crystalline contributions, the percent crystallinity calculation is simply,

$$\%C = 100\% \frac{\sum (I_O - I_B)}{\sum I_O}$$

where:

%C=percent crystallinity

I_O=observed intensity

I_B=intensity background frame

In the case of polymers, where part of the structure is unstructured and part of it is crystalline in nature, there are two contributors to the diffraction pattern: a lower-level broadly distributed intensity which is the result of amorphous scattering, and the stronger peeks which are the result of structure element of the polymer.

A method for background estimation that has proven effective in other domains is based on morphological processing. Morphological image processing is based on two operations: dilation and erosion. The parameters of the operations are defined by a matrix of kernel values, called the operator's “structure element” (SE). The dilation of an image F by a structuring element S, denoted as D = F ⊕ S, is defined as

$$d(x, y) = \max_{i,j}[f(x - i, y - j) + s(i, j)]$$

where d ∈ D, f ∈ F, and s ∈ S. Conversely, the erosion of an image F by a structuring element S, denoted as E = F _ S, is defined as

$$e(x, y) = \min_{i,j}[f(x + i, y + j) - s(i, j)]$$

where f and s are as before and e ∈ E.

The background of a diffraction pattern can be estimated with a composite morphological operation, called “opening.” The morphological opening operation (denoted as M = F o S) is defined as

$$m(x, y) = (F \varnothing S) \oplus S$$

where m $\in$ M and the same SE is used in both the erosion and the dilation.

Opening can be interpreted physically as taking an object whose top surface is described by the SE, pressing it up against the underside of the intensity surface of the image and moving it about, as shown in Figure 7.1. The result of the opening is found by tracing the highest point reached by the object at each pixel in the image. If the object is a sphere, then the algorithm has been called the “rolling ball algorithm.” As long as the ball is large enough, it can not enter the positive excursions that correspond to the peaks; however, it can track a slowly varying background very well.

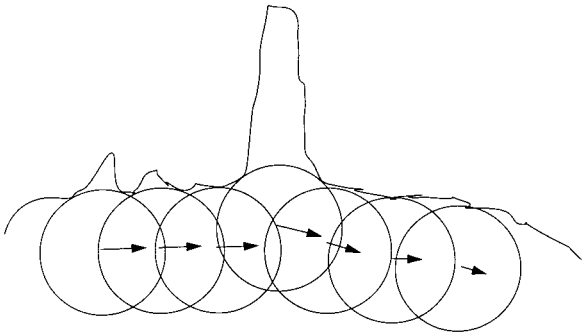


Figure 7.1 - A metaphor for the rolling ball algorithm

Unfortunately, the background estimate produced by the rolling ball filter is not robust in the presence of noise. As shown in Figure 7.2, noise spike “gouges” jutting sharply into the background will force the ball sharply downward, producing erroneous background estimation (i.e. the ball will follow the noise spike, not the true background). By applying a noise reduction technique to remove these negative excursions before the rolling ball operation, the background estimation becomes much more robust with respect to noise (see SMOOTH).

The 3D shape of the rolling ball is a half-ellipsoid where both axes in the XY plane are identical and the negative intensity direction is irrelevant, thus producing a half-dome shape.

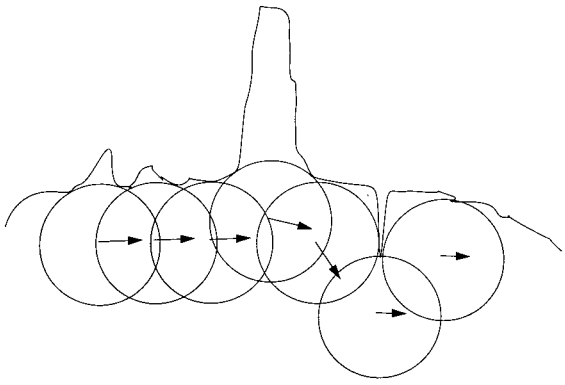


Figure 7.2 - Depiction of why rolling ball filter is sensitive to noise

7.17.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input frame) [$FRAME]

Enter name of input frame or $frame.

/DISPLAY=<n> .....(Max display counts) [16]

Enter # counts corresponding to white.

$2 .....(Bkgd frame) [$NULL]

Enter name of output background frame or $null.

/RADIUS=<n> .....(Radius) [25]

Enter the radius of the rolling ball in pixels. This determines the size in the XY plane for the rolling ball. Range is 1 to 50. You should determine the half-width (in pixels) of the broadest feature in your frame images and use a value greater than that half-width. Remember that the broadest feature may consist of overlapping peaks; use the half-width of background to background of these overlapping peaks feature.

/HEIGHT=<n> .....(HEIGHT) [2]

Enter the height of the rolling ball in pixels. This determines the shape or flatness of the rolling ball in the intensity direction. Range is 0 to 20. A rule of thumb is height < radius / 2. Use lower numbers to reduce the effects of upward creep, where the ball can fit inside the peaks, and produce background frames with some crystallinity intensity not removed.

7.18 Analyze > Pole Figure > Scheme • Determine data collection scheme for pole figure

Menu Command: Analyze > Pole Figure > Scheme

Accelerator: None

User Level: 1

SLAM Syntax:

```
POLE_FIG /SCHEME $1
/DISTANCE=<n> /2THETA1=<n>
/OMEGA1=<n> /PHI1=<n> /CHI1=<n>
/AXIS1=<n> /WIDTH1=<n> /NUM1=<n>
/THETA11=<n> /THETA21=<n>
/2THETA2=<n> /OMEGA2=<n>
/PHI2=<n> /CHI2=<n> /AXIS2=<n>
/WIDTH2=<n> /NUM2=<n>
/THETA12=<n>
/THETA22=<n>/2THETA3=<n>
/OMEGA3=<n> /PHI3=<n> /CHI3=<n>
/AXIS3=<n> /WIDTH3=<n> /NUM3=<n>
/THETA13=<n>
/THETA23=<n>/2THETA4=<n>
/OMEGA4=<n> /PHI4=<n> /CHI4=<n>
/AXIS4=<n> /WIDTH4=<n> /NUM4=<n>
/THETA14=<n> /THETA24=<n>
/DIRECTION=<s> /MAPPING=<s>
/REFLECTION /X=<n> /Y=<n> /Z=<n>
```

Pole figure frames are stereographic projections of the pole density sphere where each pixel of the pole figure frame represents the pole density of crystallites possessing a particular orientation. Pole maps of this kind are the preferred method for describing a material's texture.

The radius of the pole figure is called alpha and the azimuthal angle is called beta. These angles are related to the sample orientation by:

alpha—angle between reflecting plane and normal to the reference plane in the sample.

beta—angle between the reference direction and the normal to the diffractometer direction.

Consider a polycrystalline-textured specimen at a fixed orientation within an x-ray beam. The diffracted rays from a particular hkl plane form a cone, where the azimuthal intensity variation is related to the orientation of the sample about the incident x-ray beam. The intersection of this diffraction cone and an area detector form a circle of intensity data that maps to a great circle on the pole sphere. By varying the sample orientation to the incident beam, this circle of data can map to other regions of the pole sphere. Thus by measuring the distribution of diffracted rays at various sample positions, the relative pole density at every point along the pole figure may be obtained.

7.18.1 Scheme

The complexity of the pole figure and the required precision will determine the number of frames that are necessary to collect. Further complications arise whenever the area detector is off-axis and only intersects a portion of the diffracted cone. To aid the diffractionist, the data collection scheme can be determined using the SCHEME command. After inputting the goniometer settings, the scan angle, step, and number of frames, along with the 2-theta of the desired pole, the SCHEME option will display where the simulated data will map on the pole figure projection. Complete coverage of the pole sphere can be assured, along with the reduction of duplicate data for shorter data collection times.

For complete coverage, omega must be half of the frame 2-theta angle. Otherwise a hole will be in the center of the pole image.

In script mode, always use /2THETA1=<> through /2THETA4=<>, where runs not used should have blank values.

7.18.2 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Pole 2T) [10.]

2-theta of desired hkl pole. While the pole 2T can be different than the detector 2T, it must intersect the detector face.

/DISTANCE=<n>…(Distance) [7.0]

Detector distance in cm.

/NUM=<n>..... (# Frames) [36]

Number of frames to collect at these settings.

/2THETA=<n>..... (2Theta) [0.0]

/THETA1=<n>..... (Theta-1) [0.0]

Initial 2-theta goniometer setting. On θ-θ systems, this is the θ1 tube axis.

/OMEGA=<n>..... (Omega) [0.0]

/THETA2=<n>..... (Theta-2) [0.0]

Initial omega goniometer setting. On θ-θ systems, this is the θ2 detector axis.

/PHI=<n> ..... (Phi) [0.0]

Initial phi goniometer setting.

/CHI=<n> ..... (Chi) [0.0]

Initial chi goniometer setting.

/AXIS=<n>..... (Scan Axis #) [3]

Goniometer axis for scanning: 2=OM, 3=PH, 4=CH.

/WIDTH=<n> ..... (Frame Width) [5.0]

Step size of scan axis between frames.

/CLEAR .....(Pre-Clear Y/N) [Yes]

Y will clear both the screen display and any output file or SCAN /MULTIRUN menu requests. N will draw additional pole data onto previous SCHEME results and also append to any output file or the SCAN /MULTIRUN list.

/DIRECTION=<S> (Projection Direction) [1]

Enter projection direction of sphere: 1=X (beam), 2=Y, 3=Z (Up).

/MAPPING=<s> ....(Mapping) [Stereo]

Enter Stereo or Polar.

/REFLECTION .....(Reflection only? Y/N) [No]

Enter “Y” for reflection only mode. All points from transmission through the sample are tossed out. Requires sample vector to be entered.

/X=<n> .....(Sample vector X) [0]

Enter sample vector in X direction on goniometer head.

/Y=<n> .....(Sample vector Y) [0]

Enter sample vector in Y direction on goniometer head.

/Z=<n> .....(Sample vector Z) [1]

Enter sample vector in Z direction on goniometer head.

7.19 Analyze > Pole Figure > Process • Process frames into pole figure image

Menu Command: Analyze > Pole Figure > Process

Accelerator: None

User Level: 1

SLAM Syntax:

POLE_FIG /PROCESS $1 $2 $3 $4 $5 /POLE=<n> /MAPPING=<s> /BACKGROUND $6 $7 $8 $9 /FIBERGEOM /ABSORPTION=<s> /X=<n> /Y=<n> /Z=<n> /MU=<n> /RADIUS=<n> /NSTEPS=<n> /REFLECTION

Pole figure frames are stereographic projections of the pole density sphere where each pixel of the pole figure frame represents the pole density of crystallites possessing a particular orientation. Pole maps of this kind are the preferred method for describing a material's texture.

The radius of the pole figure is called alpha and the azimuthal angle is called beta. These angles are related to the sample orientation by:

alpha—angle between reflecting plane and normal to the reference plane in the sample.

beta—angle between the reference direction and the normal to the diffractometer direction.

Consider a polycrystalline-textured specimen at a fixed orientation within an x-ray beam. The diffracted rays from a particular hkl plane form a cone, where the azimuthal intensity variation is related to the orientation of the sample about the incident x-ray beam. The intersection of this diffraction cone and an area detector form a circle of intensity data that maps to a great circle on the pole sphere. By varying the sample orientation to the incident beam, this circle of data can map to other regions of the pole sphere. Thus by measuring the distribution of diffracted rays at various sample positions, the relative pole density at every point along the pole figure may be obtained.

7.19.1 Process

GADDS provides a quick processing of a series of frames to obtain pole figures at a specific two-theta. For each frame in the series, a 2-theta integration is performed using the normalized-bin method with the resulting chi trace mapped to a appropriate pixel locations on a pole figure frame. Where multiple chi intensities map to the same pixel on the pole image, the average intensity is used. Likewise, if multiple intensities from different data frames map to the same pixel on the pole image, the average of the possibly averaged intensities is used.

The background correction is made by integrating background intensity values in the immediate vicinity of the Bragg angle. Two background values are determined, their angles being below

and above the Bragg angle, with the final background determined by linear extrapolation between the low and high background values. It is important that the background intensity values are determined at a two-theta value that avoids any Bragg peak intensity in all frames of the series.

For a particular Bragg angle, the background intensity is determined by integrating a low and high background region in two-theta. Each resulting background trace (in chi) is smoothed using a three-point average. The background below the Bragg peak is determined by linear interpolation between the low and high background values.

If the background obtained for a certain value of sample inclination is higher than the measured intensity in the pole figure, its subtraction would lead to a negative intensity in the pole figure. This would be physically meaningless because there cannot be negative probability in the pole figure. The background correction will simply replace any negative values with zero and display a warning message with the maximum negative value that was encountered. Usually significant errors of this sort occur by the misplacement of the two-theta values for integrating the background regions.

$$I_{low}(\chi) = \int_{2\theta\ low\ beg}^{2\theta\ low\ end} I(\chi, 2\theta)\ d2\theta \qquad I_{high}(\chi) = \int_{2\theta\ high\ beg}^{2\theta\ high\ end} I(\chi, 2\theta)\ d2\theta$$

$$I_b(\chi) = \frac{I_{low}(\chi) * (2\theta_{high} - 2\theta_{bragg}) + I_{high}(\chi) * (2\theta_{bragg} - 2\theta_{low})}{(2\theta_{high} - 2\theta_{low})}$$

$$I_{corr}(\chi, a) = I_{mess}(\chi, a) - I_b(\chi)$$

7.19.2 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(2theta start) [24.5]

Two-theta start of Bragg peak region.

$2 .....(2theta end) [26.5]

Two-theta end of Bragg peak region.

$3 .....(Chi start) [0.0]

Chi start of Bragg peak region.

$4 .....(Chi end) [360.0]

Chi end of Bragg peak region.

$5 .....(Output file) [pole_fig.dat]

Output file name for pole figure which is stored as a psuedo frame image.

/POLE=<n> .....(Projection direction) [1]

The processed pole figure may have it's normal direction along 1=X (beam), 2=Y, or 3=Z (up). The correct value depends on the orientation of the sample.

/MAPPING=<s> ....(Mapping) [STEREO]

Enter STEREO or POLAR. Usually STEREO.

/BACKGROUND... (Remove background Y/N) [Yes]

Present to perform background correction. Background is calculated for each frame.

$6 ..... (Low bkg begin) [24.0]

$7 ..... (Low bkg end) [24.2]

Two-theta start and end of low background region.

$8 ..... (High bkg begin) [26.8]

$9 ..... (High bkg end) [27.0]

Two-theta start and end of high background region.

/FIBERGEOM..... (One fiber frame Y/N) [No]

Enter “Y” to extract a pole figure from a single frame using fiber geometry. Basically, the phi direction is indeterminate for fibers, thus the single frame will be used at various phi positions—every two degrees.

/ABSORPTION=<s>(Absorption model) [None]

Enter absorption model as “None,” “Fiber,” or “Plate.”

/X=<n> .....(Sample vector X) [0]

/Y=<n> .....(Sample vector Y) [0]

/Z=<n> .....(Sample vector Z) [1]

Enter sample vector in X,Y,Z direction on goniometer head.

/MU=<n> .....(Sample mu cm-1) [131.22]

Enter sample mu in cm-1.

/RADIUS=<n> .....(Radius/Thickness cm) [0.05]

Enter sample radius (for fibers) or thickness (for plates) in cm.

/NSTEPS=<n> .....(Num integration steps) [10]

Enter number of steps.

/REFLECTION .....(Reflection only? Y/N) [No]

Enter “Y” for reflection only mode. All points from transmission through the sample are tossed out.

7.20 Analyze > Pole Figure > Interpolate • Interpolate a processed pole figure image

Menu Command: Analyze > Pole Figure > Interpolate

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /INTERPOLATE $1 /DISPLAY=<n> /WIDTH=<n> $2

Pole figures are displayed using a bitmapped image with each pixel location representing an alpha and beta sample orientation. Mapped pixels have intensities of the pole density plus one, while unmapped pixels possess the value of zero. For better visualization of the pole figure image, it is useful to interpolate a value for all the unmapped pixels.

7.20.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$FRAME]

Input filename for pole figure or $frame.

/DISPLAY=<n>.....(Max Display Counts) [-2]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -2; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image look brighter; larger values make look darker.

/WIDTH=<n> ..... (Width) [2]

Half-width of interpolation box in pixels.

$2 ..... (Outputfile) [$NULL]

Output filename to store interpolated pole figure image or $null.

7.21 Analyze > Pole Figure > Tilt • Tilt pole figure about a new polar origin

Menu Command: Analyze > Pole Figure > Tilt

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /TILT $1 /DISPLAY=<n> /X=<n> /Y=<n> $2

Frequently, the diffractionist would like to visualize the pole sphere from a different viewing angle or orientation. Or perhaps the pole figure needs to be positioned with particular sample directions. For these reasons, the TILT and ROTATE options have been provided. The TILT option allows a new position on the sphere to be positioned at the origin of the projection, while the ROTATE option performs rotation of the image about the origin. INVERT flips the image from top to bottom.

7.21.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$FRAME]

Input filename for pole figure or $frame.

/DISPLAY=<n>.....(Max Display Counts) [-2]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -2; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image look brighter; larger values make look darker.

/X=<n>..... (X Origin) [0]

x offset of new origin.

/Y=<n>..... (Y Origin) [0]

y offset of new origin.

$2 ..... (Output File) [$NULL]

Output filename to store tilted pole figure image or $null.

7.22 Analyze > Pole Figure > Rotate • Rotate pole figure about beta (azimuthal) angle

Menu Command: Analyze > Pole Figure > Rotate

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /ROTATE $1 /DISPLAY=<n> $2

Frequently, the diffractionist would like to visualize the pole sphere from a different viewing angle or orientation, or perhaps the pole figure needs to be positioned with particular sample directions. For these reasons, the TILT and ROTATE options have been provided. The TILT option allows a new position on the sphere to be positioned at the origin of the projection, while the ROTATE option performs rotation of the image about the origin. INVERT flips the image from top to bottom.

7.22.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$FRAME]

Input filename for pole figure or $frame.

/DISPLAY=<n> ..... (Max Display Counts) [-2]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -2; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image look brighter; larger values make look darker.

/ANGLE=<n>..... (CCW Angle) [0.0]

Angle of rotation about the origin (center).

$2 ..... (Output File) [$NULL]

Output filename to store rotated pole figure image or $null.

7.23 Analyze > Pole Figure > Symmetrize • Symmetrize pole figure using various Laue symmetries

Menu Command: Analyze > Pole Figure > Symmetrize

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /SYMMETRIZE $1 /DISPLAY=<n> $2 /LAUE=<s>

All pole spheres possess Laue symmetry (e.g., orthorhombic materials exhibit mmm symmetry), therefore one needs to collect only an octant or quadrant of the pole sphere to generate the entire sphere. Conversely, one can use the symmetry feature as a smoothing function.

SYMMETRIZE supports Laue symmetries for triclinics (i), monoclinics (2/m), orthorhombics (mmm), and tetragonals (4/m, 4/mmm). Laue symmetries for trigonals, hexagonals, and cubics are not supported at this time; however one can use 2/m or mmm for hexagonals and mmm for cubics.

7.23.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$FRAME]

Input filename for pole figure or $frame.

/DISPLAY=<n> ..... (Max Display Counts) [-2]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -2; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image look brighter; larger values make look darker.

$2 ..... (Output File) [$NULL]

Output filename to store symmetrized pole figure image or $null.

/LAUE=<s> ..... (Laue Symmetry) [2/m]

Enter Laue symmetry as “i,” “2/m,” “mmm,” “4/m,” “4/mmm.” Currently other Laue symmetries are not supported, but some may be approximated by using a lower inherent symmetry. For instance, hexagonals “6/m” inherently possess “2/m” symmetry and “6/mmm” possess “mmm” symmetry, while cubics “m3” or “m3m” possess “mmm” symmetry.

7.24 Analyze > Pole Figure > Invert • Invert pole figure about x-axis

Menu Command: Analyze > Pole Figure > Invert

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /INVERT $1 /DISPLAY=<n> $2

Frequently, the diffractionist would like to visualize the pole sphere from a different viewing angle or orientation, or perhaps the pole figure needs to be positioned with particular sample directions. For these reasons, the TILT and ROTATE options have been provided. The TILT option allows a new position on the sphere to be positioned at the origin of the projection, while the ROTATE option performs rotation of the image about the origin. INVERT flips the image from top to bottom.

7.24.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$frame]

input filename for pole figure or $frame.

/DISPLAY=<n>.....(Max Display Counts) [-2]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -2; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image look brighter; larger values make look darker.

$2 ..... (Output File) [$null]

Output filename to store inverted pole figure image or $null.

7.25 Analyze > Pole Figure > Texture-AT • Create Texture-AT file from pole figure frame (binary)

Menu Command: Analyze > Pole Figure > TextureAT

Accelerator: None

User Level: 1

SLAM Syntax:

POLE_FIG /TEXTUREAT $1 /TITLE=<n> /HKL=<n> /APPEND /ALPHAINC=<n> /BETAINC=<n> /REFLECTION

Besides the storing of bitmapped images, the pole figure may be exported in either TEXTURE-AT file format or popLA file format for ODF calculations or other processing with those or other software packages. See appendices for the format of these data files. A 3 x 3 pixel region is averaged before writing to a TEXTURE-AT file.

ODF-AT performs an ODF using harmonic methods which represents the ODF as a weighted sum of spherical harmonic functions chosen so as to possess the symmetry of both the specimen and the crystal system. Unfortunately, the spherical harmonic expansion can lead to non-physical results, because the best fit ODF may exhibit regions in which the values are negative, which is nonsense for a probability density function. Such problems particularly arise in cases where the ODF is sharply peaked, thus the harmonic method is more suited to ODFs which are not sharply peaked.

7.25.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Texture-AT File) [texture]

Output filename for TEXTURE-AT data file. Extension defaults to either *.trw (transmission) or *.rrw (reflection).

/TITLE=<n> ..... (Title) [$title]

Title for data file.

/HKL=<n> ..... (HKL) [100]

hkl of this pole.

/APPEND ..... (Append Y/N?) [No]

Y to add this pole figure to an existing TEXTURE-AT file, N to deleted any existing file and create a new TEXTURE-AT file. For ODF calculations, two or three poles must be collected in the same TEXTURE-AT data file.

/ALPHAINC=<n> .. (Declination Inc.) [1.0]

Step size of alpha, declination angle.

/BETAINC=<n>..... (Azimuthal Inc.) [1.0]

Step size of beta, azimuthal angle.

/REFLECTION .....(Reflection mode Yes/No) [No]

Present to produce TEXTURE-AT file in reflection mode format.

7.26 Analyze > Pole Figure > popLA • Create popLA data file from pole figure frame (ASCII)

Menu Command: Analyze > Pole Figure > PopLA

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /POPLA $1 /TITLE=<n> /HKL=<n> /APPEND

Besides the storing of bitmapped images, the pole figure may be exported in either TEXTURE-AT file format or popLA file format for ODF calculations or other processing with those or other software packages. See appendices for the format of these data files.

popLA performs an ODF using vector methods. The orientation space is divided up into a number of “cells” within which the ODF is assigned a constant value. A simple initial value of each cell is determined from the experimental data. The resultant pole figures from such an ODF are compared with the observed pole figures and adjustments are made to improve the match. This process is repeated until no further improvement is observed. Vector methods are best suited to ODFs that contain a few sharp features.

7.26.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Popla File) [popla.epf]

Enter output popLA file name (*.epf).

/TITLE=<n>.....(Title) [$TITLE]

Enter pole figure title (or “$TITLE” for frame title).

/HKL=<n>.....(HKL) [100]

Enter hkl indices, i.e. 111 (or “hkl” if unknown).

/APPEND .....(Append Y/N?) [No]

Append to existing output file [no => overwrites].

7.27 Analyze > Pole Figure > Orientate • Calculate Hermans and White-Spruiell orientation indices

Menu Command: Analyze > Pole Figure > Orientate

Accelerator: None

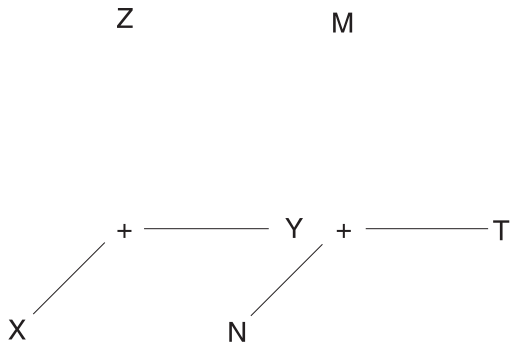
User Level: 1

SLAM Syntax: POLE_FIG /ORIENT $1 /DISPLAY=<n> $2 /APPEND /FILM /HKL=<s>

A widely used analytical representation of unit cells in a specimen is based on the second-order moment of a specific unit cell direction (hkl) with respect to a specific direction in the specimen (M). These second moment functions are used to define an orientation index for a one-dimensional structure (fiber) and an index for a two-dimensional structure (film). These indices are directly related to certain physical properties such as birefringence.

Calculation of orientation indices requires evaluation of the angle between a specific crystallographic direction and a processing direction.

Both the sample and the pole projection must be defined as below:



NOTE: The crystallographic axes must be orthogonal. We have only implemented the algorithm for orthorhombic symmetry (and thus tetragonals and cubics).

For materials oriented uniaxially about a single processing direction (such as would be the case for spun fibers), one usually calculates Hermans orientation indices for each crystallographic axis with respect to that processing axis. Herman's orientation indices are defined by:

$$F(X,x)=\frac{3\langle\cos^2 a\rangle-1}{2}$$

where:

X = processing direction, i.e. MD, TD, N

x = crystallographic direction

a = angle between above

<...> = averaged over entire pole figure

Table 7.1 – Some limiting cases of orientation and their second moments and orientation indices

Orientation	Angle c,z	$\langle\cos^2 c,z\rangle$	Fc,z
Chain axis is parallel to the fiber axis	0	1	+1.0
Chain axis perpendicular to the fiber axis	90	0	-0.5
Chain axis oriented a random	random	1/3	0.0
Equal bimodal orientation of chains	0 or 90	1/3	0.0

Typically, Herman's indices are plotted on a Stein triangle. The three apexes of the triangle correspond to the crystallographic axis (a, b, c) being parallel to the z-axis of the sample. The edges of the triangle represent the orientation of a crystallographic axis being perpendicular to the z-axis. A condition of no orientation is the origin.

White-Spruiell orientation indices are useful on polymer films, where orientations occur with some degree of biaxial character. White-Spruiell orientation indices are usually displayed on an isosceles triangle. The three apexes of the triangle correspond to perfect orientation along a particular direction, whereas the center of the triangle corresponds to isotropic orientation.

$S(MD,x) = 2\langle\cos^2 a\rangle MD,x + \langle\cos^2 a\rangle TD,x - 1$

$S(TD,x) = 2\langle\cos^2 a\rangle TD,x + \langle\cos^2 a\rangle MD,x - 1$

7.27.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Pole Figure File) [$FRAME]

Enter pole figure file name (or $FRAME for current frame).

/DISPLAY ..... (Max Display Counts) [15]

Enter # counts corresponding to white.

$2 ..... (Increment) [1.0]

Enter delta angle in degrees for summations.

/APPEND ..... (Append Y/N) [No]

Enter “Y” to append results to previous triangle plot.

/FILM ..... (Film Y/N) [No]

Enter “Y” for 2D structures such as films, “N” for 1D structures such as fibers.

/HKL=<s> ..... (HKL) [001]

Enter hkl of pole figure used for labelling purposes. If unknown, enter “hkl.”

7.28 Analyze > Pole Figure > Stein • Plot Stein triangle using calculated Hermans indices

Menu Command: Analyze > Pole Figure > Stein

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /STEIN $1 $2 /APPEND

Typically, Herman's indices are plotted on a Stein triangle. The three apexes of the triangle correspond to the crystallographic axis (a, b, c) being parallel to the z-axis of the sample. The edges of the triangle represent the orientation of a crystallographic axis being perpendicular to the z-axis. A condition of no orientation is the origin.

In certain cases the reflection from the hkl plane will be too week in intensity to give useful data. In such cases, one must interpolate the desired second-moment from second-moments of two or more other hkl poles for which data is obtainable. For our orthogonal case, the expression of second-moments for orthogonal relationships:

$\langle\cos^2 a,z\rangle + \langle\cos^2 b,z\rangle + \langle\cos^2 c,z\rangle = 1$ eq. 1

From which it follows:

$Fa,z + Fb,z + Fc,z = 0$ eq. 2

Second-moment for an hk0 pole can be interpolated using:

$\langle\cos^2 hk0,z\rangle = e^2 \langle\cos^2 a,z\rangle + f^2 \langle\cos^2 b,z\rangle$

eq. 3

where e and f are the direction cosines between the a- and b-axes with the hk0 plane.

Stein triangles are plotted using Fa,z and Fc,z Herman's indices. These are directly calculated from h00 and 00l poles. Alternately, one can obtain these two values from h00 and 0k0 poles or 0k0 and 00l poles and applying equation 2. Otherwise, it gets more complicated. One needs the crystal lattice and at least three poles, such as 110, 210, and 001. By applying equation 3, one can derive the Herman's indices.

For more details and for other non-orthogonal crystal systems, the reader is referred to:

Wilchinsky, Z. W., “Recent Developments in the Measurement of Orientation in Polymers by X-ray Diffraction,” Advances in X-ray Analysis, 6, 231-241, 1962.

Alexander, L. E., X-ray Diffraction Methods in Polymer Science, Wiley-Interscience, 1969, section 4.4.

7.28.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(F(a,z)) [0.0]

Enter fa,z: typically F(MD,h00) from /ORIENTATE command.

$2 .....(F(c,z)) [0.0]

Enter fc,z: typically F(MD,00l) from /ORIENTATE command.

/APPEND .....(Append Y/N) [No]

Enter “Y” to append results to previous triangle plot.

7.29 Analyze > Pole Figure > Normalize • Normalize pole image, so random = 100 counts

Menu Command: Analyze > Pole Figure > Normalize

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /NORMALIZE $1 /DISPLAY=<n> /NVAL=<n> $2

Normalize the pole image to either the average intensity of a random sample or psuedo-normalize to the average intensity of the collect pole image. In the normalized pole image, an intensity of 100 represents the random intensity.

7.29.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$frame]

Input filename for pole figure or $frame.

/NVAL=<n>.....(Norm Value) [0]

Normalization value or 0=pseudo normalize using the average intensity value of the displayed pole image.

/DISPLAY=<n>.....(Max Display Counts) [255]

Intensity to map as white.

$2 ..... (Output File) [$null]

Output filename to store interpolated pole figure image or $null.

7.30 Analyze > Pole Figure > Contours • Draw contour plot of pole figure

Menu Command: Analyze > Pole Figure > Contours

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /CONTOURS $1 /INTERVAL=<n>

Pole figures can be displayed in three methods:

1. As frame images were each pixel is displayed by a color indicating it's intensity.
2. As a contour plot were lines of equal intensity are drawn at given intervals.
3. As a 3D surface plot where intensity is represented by height.

7.30.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Input File) [$FRAME]

Enter the input pole figure filename (or $FRAME).

/INTERVAL=<n>....(Contour Interval) [16]

Enter the contour interval.

7.31 Analyze > Pole Figure > Surface • Draw 2D surface plot of pole figure

Menu Command: Analyze > Pole Figure > Surface

Accelerator: None

User Level: 1

SLAM Syntax:

POLE_FIG /SURFACE $1 /ROTATION=<n> /ELEVATION=<n> /COARSENESS=<n> /LOGSCALE

Pole figures can be displayed in three methods:

1. As frame images were each pixel is displayed by a color indicating it's intensity.
2. As a contour plot were lines of equal intensity are drawn at given intervals.
3. As a 3D surface plot where intensity is represented by height.

The surface algorithm is very susceptible to noise. If the frame was not smoothed, then a Process > Smooth > Convolve command is automatically suggested (see Section 6.16), however, in command mode, only a warning is displayed “Frame type is not SMOOTHED.”

7.31.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Input File) [$FRAME]

Enter the input pole figure filename (or $FRAME).

/ROTATION=<n> .. (Rotation) [0]

Enter the rotation angle.

/ELEVATION =<n> (Elevation) [30]

Enter the elevation angle for viewing 3D plot.

/COARSENESS=<n>(Coarseness) [5]

Enter the coarseness for drawing the surface plot.

/LOGSCALE..... (Logscale) [No]

Check to display using a logrithmic intensity scale.

7.32 Analyze > Pole Figure > Fiber • Take a “cut” through pole figure and display I versus tilt angle

Menu Command: Analyze > Pole Figure > Fiber

Accelerator: None

User Level: 1

SLAM Syntax: POLE_FIG /FIBERPLOT $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n>

Use this command to display a slice through the pole figure as an intensity-versus-alpha angle plot.

7.32.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Tilt Start) [0.0]

Enter starting tilt angle in degrees.

$2 .....(Tilt End) [90.0]

Enter ending tilt angle in degrees.

$3 .....(Beta) [0.0]

Enter beta of conic region in degrees.

$4 .....(Height) [0]

Enter height of conic region. Range 0 to 5 degrees.

/NORMAL=<>..... (Normalize Intensity) [1]

Normalize intensities. 0=sum, 1=avg.

/STEPSIZE=<n>... (Step Size) [0.5]

Enter step size for tilt angle axis in degrees.

7.33 Analyze > Stress > Conventional • Process frame images into data file for STRESS^{plus} package

Menu Command: Analyze > Stress > Conventional

Accelerator: None

User Level: 1

SLAM Syntax:

STRESS /CONVENTIONAL $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n> /2THETA=<n> $5 /FILENAME=<s>

DIFFRAC^{plus}STRESS is Windows NT-based software designed for residual stress calculations. This document describes the use of DIFFRAC^{plus}STRESS to analyze residual stress data collected with a General Area Detector Diffraction System (GADDS).

7.33.1 Hardware Requirement for Stress Measurements

One of the following sample stages is required to perform stress measurements with GADDS:

XYZ Stage

1/4-Circle Eulerian Cradle at chi = -90 position

Two-Position Chi Stage at chi = -90 position

For all of the above stages, the sample surface must face the operator when omega=0 and face the incident beam when omega=90. For stress tensor measurements, phi rotation is required.

7.33.2 Data Collection with GADDS

Data can be collected either SingleRun with omega-scan for normal stress measurements (single phi, phi=0) or MultiRun with omega-scan for stress tensor measurements (multiple phi, e.g., phi=0, 45 and 90). All frames must have the same file name and consecutive extension numbers. For MultiRun, it is required to set the same run number for all runs in the EditRuns menu.

The psi-tilt is achieved by sample omega rotation, the so-called “iso-inclination mode.” Use the following equations to determine omega-scan angles, where (2T) is the estimated peak position:

If the detector is set at positive swing angle: omega = psi + (2T)/2.

If the detector is set at negative swing angle: omega = 180 - psi - (2T)/2.

For example, to set psi at 45, 30, 15, 0, -15, -30, -45 for iron (211) whose 2T=156 with the detector swinging negative, the omega scan values are 57, 72, 87, 102, 117, 132, 147.

7.33.3 Data Processing with GADDS

For GADDS software version 3.323 or above, the stress function is added under the Analyze menu. Follow these steps to process the data:

1. Load the first frame.
2. Select Stress under the Analyze menu.
3. In the pop-up windows, several variables must be set. Particularly: “2theta start” and “2theta end” for the peak of interest with appropriate background. “Chi start” and “Chi end” for the chi integration range. The values should be 90+/-x. x is normally set below 10 degrees. Set to 5 degrees if not sure. “Normalize intensity”—use a default value of 3. “Peak 2T”—input the estimated or pre-determined 2T peak position. This value is used to calculate psi tilt. “Filename”—the processed data will be saved in DIFFRAC*plus* format into this filename.
4. Check OK to start processing. The 2-theta and Chi range can be redefined using the mouse for each of frame. Click in the integration box for each frame.

7.33.4 Stress Calculation

DIFFRAC*plus*STRESS can open the data saved in the last step. For data format compatibility reasons, the psi-tilt of GADDS data is saved as the chi value for DIFFRAC*plus*STRESS. As such, DIFFRAC*plus*STRESS will process GADDS data as if it were collected in side-inclination mode, although the GADDS data was collected in iso-inclination mode. This will not change the stress result as long as the absorption and polarization corrections are not performed in DIFFRAC*plus*STRESS. These corrections can be made in GADDS before data processing with DIFFRAC*plus*STRESS. Verify that those correction functions are disabled when analyzing GADDS data with DIFFRAC*plus*STRESS.

7.33.5 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (2-theta start) [0.0]

Enter lower 2T of conic region in degrees.

$2 ..... (2-theta end) [30.0]

Enter upper 2T of conic region in degrees.

$3 ..... (Chi start) [0.0]

Enter lower chi of conic region in degrees.

$4 .....(Chi end) [360.0]

Enter upper chi of conic region in degrees.

/NORMAL=<n> .....(Normalize intensity) [3]

Normalize intensities: 0=none, 1=avg, 2=arc length, 3=solid angle, 4=bin method.

/STEPSIZE=<n> ...(Step size) [0.1]

Enter step size in degrees.

/2THETA=<n> .....(Peak 2T) [156.0]

Enter peak 2T for calculations.

$5 .....(Title) [$TITLE]

Enter title string or $TITLE to leave unchanged.

/FILENAME=<s> ...(File name) [stress.raw]

Enter output file name for RAW data.

7.34 Analyze > Stress > Scheme 2D

Menu Command: Analyze > Stress > Scheme 2D

Accelerator: None

User Level: 1

SLAM Syntax:

STRESS /SCHEME2D $1 /PEAK=<n> /DISTANCE=<n> $2 [/2THETA=<n>|/THETA1=<n>] [/OMEGA=<n>|/THETA2=<n>] /PHI=<n> /CHI=<n> /AXIS=<n> /WIDTH=<n> /CLEAR

Use this command to determine proper scan parameters when stress measurements are required and to determine which stress directions are properly determined.

7.34.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Output file) [$NULL]

Output file for multirun scan listing. $SCAN will automatically update directly to the SCAN /MULTIRUN menu. $NULL will skip this feature.

/PEAK=<n> .....(Stress peak) [156.0]

2T or d-spacing of desired stress peak.

/DISTANCE=<n> .. (Distance) [7.0 cm]

Detector distance in cm.

$2 ..... (# frames) [36]

Number of frames to collect.

/2THETA=<n> /THETA1=<n>(2Theta or Theta1) [-135.0 deg]

Detector swing angle in degrees.

/OMEGA=<n> /THETA2=<n>(Omega or Theta2) [0.0 deg]

/PHI=<n>..... (Phi) [0.0 deg]

/CHI=<n>..... (Chi) [90.0 deg]

The sample positioning angles in degrees.

/AXIS=<n>..... (Scan axis #) [2 - omega]

Goniometer axis for scanning: 2-omega, 3-phi, 4-chi.

/WIDTH=<n> ..... (Frame width) [5.0 deg]

Step size of scan axis between frames.

/CLEAR ..... (Pre-clear?) [Y]

Check “Y” to clear both the screen display and the output file or Scan > MultiRun list. Uncheck “N” to append to screen and output file or run list.

7.35 Analyze > Stress > Biaxial 2D • Biaxial stress measurements from frame images, Analyze > Stress > BiaxialShear2D, Analyze > Stress > Triaxial2D

Menu Command: Analyze > Stress > Biaxial 2D, Analyze > Stress > BiaxialShear2D, Analyze > Stress > Triaxial2D

Accelerator: None

User Level: 1

SLAM Syntax:

STRESS [/BIAXIAL2D | /SHEAR2D | /TRIAXIAL2D] $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n> /NUMBER=<n> /2THETA=<n> $5 /FILENAME=<s> /HKL=<s> /YOUNG=<n> /POISSON=<n> /ARX=<n> /LINESHAPE=<n> /CUTOFF=<n> /REPROCESS /BKGFIT=<s> /KALPHA2= /PHI=<n> /PSI=<n> /UNITS=<s>

Preferred stress calculation algorithm. (See the User Manual for details).

Biaxial stress solves:

$p_{11}\sigma_{11} + p_{12}\sigma_{12} + p_{22}\sigma_{22} + (1\text{-}2v)/E\ \sigma_{ph} = \ln(\sin\theta_0/\sin\theta)$

Biaxial Shear stress solves:

$p11\sigma11 + p12\sigma12 + p22\sigma22 + p13\sigma13 + p23\sigma23 + (1\text{-}2v)/E\ \sigma ph = \ln(\sin\theta0/\sin\theta)$

Triaxial stress solves:

$p11\sigma11 + p12\sigma12 + p22\sigma22 + p13\sigma13 + p23\sigma23 + p33\sigma33 = \ln(\sin\theta0/\sin\theta)$

The final stress report is somewhat different, otherwise these three commands are identical.

Biaxial stress reports:

Data collection condition	Stress report
W scan only	σ11
Chi scan only	σ22
All other cases	σ11 σ12 σ22 and σph

Biaxial Shear stress solves:

Data collection condition	Stress report
W scan only	σ11 and σ13
Chi scan only	σ22 and σ23
All other cases	σ11 σ12 σ22 σ13 σ23 and σph

Triaxial stress solves.

Data collection condition	Stress report
All cases (must scan 2 axes)	σ11 σ12 σ22 σ13 σ23 and σ33

Reprocessing Stress Data:

Frequently, obvious errors can occur and you would like to toss out specific data points from the calculation. There are two methods to reprocess data.

Method 1: Reprocess from <filename>.txt that must be created using the [Write] button. You must use the base filename with the .txt extension (defaults to edit.txt). Then use notepad to edit this file and in the last table add an addition column to reject data points. Use the letter “R” or the word “rejected” (case is not important). Finally, restart the Stress command with the reprocess option checked.

Method 2: Reprocess from <filename>.lst that is always created. This is also an ASCII file that can be edited with notepad. Any peak with “L” limit condition or missing standard deviation is rejected. Typically, peaks that are poorly refined have a large standard deviation and you may want to reject these peaks. Delete any existing <filename>.txt as these will be processed before the .lst file. Finally, restart the Stress command with the reprocess option checked.

7.35.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (2theta start) [154.5]

Enter lower 2-theta of conic region (degrees).

$2 ..... (2theta end) [157.5]

Enter upper 2-theta of conic region (degrees).

$3 ..... (Chi start) [70.0]

Enter lower chi of conic region (degrees).

$4 ..... (Chi end) [110.0]

Enter upper chi of conic region (degrees).

/NORMAL=<n>..... (Normalize intensity) [3]

Normalize intensities (0=sum, 1=avg, 2=arc, 3=solid angle, 4=bin, 5=norm bin).

/STEPSIZE=<n>…(Step size) [0.1]

Enter the step size (degrees).

/NUMBER=<n> .... (# of sub-regions) [15]

Enter the number of sub-regions to integrate.

/2THETA=<n>..... (Peak 2T or d) [156.0]

Enter unstressed 2T (or d) for triaxial tensor calculations.

$5 .....(Title) [$TITLE]

Enter title string (or $TITLE to leave unchanged).

/FILENAME=<s>...(File name) [stress.raw]

Enter output filename for RAW data.

/HKL=<s>.....(hkl) [211]

Enter hkl of line.

/YOUNG=<n>.....(Young's modulus) [210,000]

Enter Young's modulus for material.

/POISSON=<n> ....(Poisson's ratio) [0.28]

Enter Poisson's ratio for material.

/ARX=<n> .....(Arx) [1.0]

Enter anisotropicity factor (1.0=isotropic).

/LINESHAPE=<n>.(Lineshape) [4]

Enter 1=Gaussian, 2=Lorentzian, or 4=Pseudo-Voigt2.

/CUTOFF=<n> .....(Cutoff) [0]

Enter peak cutoff in percent of max (ignore peaks below cutoff).

/LINESHAPE.....(Lineshape) [4 Psuedo-Voigt 2]

Enter 0 = centroid, … Note for centroid method, you cannot refine the backgrounds, fit Kalpha2, or use the peak cutoff value, but you can subtract out a fixed background.

/REPROCESS..... (Reprocess only?) [N]

Check "Y" to skip integration of all input frames. Program will try to read the stress report file <basename>.txt (must be created with verbose output to get data table). If that fails, it will read profile fitting output <basename>.lst. Reprocessing is useful to throw out bad data points or recalculate stress from new input parameters.

/BKGFIT=<s> ..... (Background fit) [Both]

This command can handle the backgrounds during profile fitting in eight ways:

Both Initializes and refines both backgrounds.

Low Initializes and refines low (left) background; high background is fixed at initial value.

High Initializes and refines high (right) background; low background is fixed at initial value.

Neither (Init Both & Fixed) Initializes and fixes both backgrounds.

Zero & Fixed Initializes at zero and fixes both backgrounds.

Init Low & Fixed
: Initializes at low and fixes both backgrounds.

Init High & Fixed
: Initializes at high and fixes both backgrounds.

Init Avg & Fixed
: Initializes at average of low and high, and fixes both backgrounds.

/KALPHA2.....(Fit Kalpha2?) [N]

Check “Y” to fit Kalpha2 wavelength in profile fitting routine.

/PHI=<n>.....(Phi) [0.0]

/PSI=<n>.....(Psi) [90.0]

Enter the sample angles for the arbitrary stress in the stress report.

/UNITS=<s> .....(Stress units) [MPa]

Select MPa, Ksi, or Psi. 1.0 MPa = 0.145 Ksi = 145.0 Psi.

7.36 Analyze > Stress > View 2D • View biaxial stress and original frame images

Menu Command: Analyze > Stress > View 2D

Accelerator: None

User Level: 1

SLAM Syntax:

STRESS /VIEW2D $1 /DISPLAY=<n> /DATA /LINE /DELAY=<n> /DIRECTION=<s>

Use this command to display the fitted observed data and/or the calculated stress line to the original frame files for quick, visual confirmation of correctness. Can be used in movie or single frame mode.

7.36.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(First frame) [stress.000]

Enter first frame of series to display.

/DISPLAY=<n>.....(Display limit) [-1]

Enter 0 for no display, otherwise this item specifies the number of counts mapped into the maximum display memory value (for example, corresponding to white) on the display. The special value -1 directs the program to pick a reasonable value by scanning through the pixels in the frame prior to display; the special value -2 directs the program to use whatever setting is currently in effect. The default value is -1; the allowed range is from -2 to 10^6 counts. Smaller values make the displayed image look brighter; larger values make look darker.

/DATA..... (Overlay data points) [Yes]

Check “Y” to display the 2T/CH data points as “X.”

/LINE ..... (Overlay stress line) [Yes]

Check “Y” to display the calculated stress as a line.

/DELAY=<n>..... (Movie delay time) [-1.0]

Enter time in seconds between frames or -1.0 for no movie.

/DIRECTION=<s> (Movie direction) [+]

Enter either “+” or “-” for the direction through frames.

7.37 Analyze > Mapping

Menu Command: Analyze > Mapping

Accelerator: None

User Level: 1

SLAM Syntax:

MAPPING $1 /FRAME=<s> /RUN=<s> $2 /SLAM=<s>

Use this command to process a run series where each run is identically processed to obtain a “mapping parameter value” per each run. A run could be frames collected on a sample position in X and Y (or Y and Z) or a sample position in a sample library (see Collect > Scan > Grid Targets). Each resultant value across the runs is sent to and mapped in the GADDSMAP utility program. The mapping pattern will show sample variations with position or variations in samples in a sample library. Such information is frequently used for quality control.

When selected, a dialog box appears to enter the mapping parameters. You must select what parameter you want to map across all the runs. You must enter the first frame in the run series and the last run number. After clicking [OK], the frame headers of these runs will be read to determine the XY (or YZ) mapping grid. Frames must be collected on a grid, but some missing frames are allowed.

Next GADDS brings up the dialog box for inputting processing parameters needed to calculate the requested parameter to map. Which dialog box appears depends on which parameter is being mapped. For more information, see the appropriate command for this dialog box.

7.37.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (First frame) [map_0_001.gfrm]

/FRAME=<s>..... (To frame number) [001]

/RUN=<s>..... (To run number) [G]

These three parameters define the run series to process.

$2 ..... (Map parameter) [Area]

Area (integration area)

% (internal)

% (external)

% (full)

Peak 2theta

Peak height

Peak fwhm

Peak area

Biaxial Sigma 11 stress

Biaxial Sigma 12 stress

Biaxial Sigma 22 stress

Biaxial Sigma ph stress

Shear Sigma 11 stress

Shear Sigma 12 stress

Shear Sigma 22 stress

Shear Sigma 13 stress

Shear Sigma 23 stress

Shear Sigma ph stress

Triaxial Sigma 11 stress

Triaxial Sigma 12 stress

Triaxial Sigma 22 stress

Triaxial Sigma 13 stress

Triaxial Sigma 23 stress

Triaxial Sigma 33 stress

/SLAM=<s> .....() [blank]

This parameter is used in script mode. It is the script command for the processing parameters dialog box. In menu mode, just leave this blank.

8. Peaks Routines

8.1 Peaks > Mask > Create • Create a new active pixel mask for this frame

Menu Command: Peaks > Mask > Create

Accelerator: None

User Level: 1

SLAM Syntax: MASK /CREATE $1 /FILTER /BORDER=<n>

MASK /CREATE is used to create a bitmask for defining active pixels. This bitmask is used in INTEGRATE, SMOOTH, and PER_CRYSTAL commands.

The user should be aware the bitmask or the octagon mask are used exclusively. That is if the bitmask is define, the octagon mask is ignored and visa versa.

8.1.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Threshold) [1]

Threshold in counts. All Pixels whose value is below this threshold are flagged as inactive.

/FILTER ..... (Filter) [No]

Entering “Y” will filter out isolated inactive pixels and restore them to active status.

/BORDER=<n>..... (Border) [1]

Number of pixels to extend the inactive pixels regions to eliminate partially blocked pixels from the active pixel bitmask.

8.2 Peaks > Mask > Edit • Edit the active pixel mask

Menu Command: Peaks > Mask > Edit

Accelerator: None

User Level: 1

SLAM Syntax: MASK /EDIT (interactive only)

Use this command to manually edit the active pixel mask, pixel by pixel. You can turn off or on masked pixels with a click of the mouse. Hint: Zoom in on the image for better visualizing of individual pixels.

8.3 Peaks > Mask > Save • Save active pixel mask to disk file

Menu Command: Peaks > Mask > Create

Accelerator: None

User Level: 1

SLAM Syntax: MASK /SAVE $1

MASK /SAVE will store the current active bitmask to a disk file. Active bitmasks must be explicitly saved, because only the filename is stored in the frame header. One may also need to re-save the frame image, if the frame header was modified to include a new bitmask.

The user should be aware the bitmask or the octagon mask is used exclusively. That is if the bitmask is define, the octagon mask is ignored and visa versa.

8.3.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Bitmask Filename) [active.msk]

Filename of active pixel bitmask, “$NULL,” will cancel.

8.4 Peaks > Mask > Read • Read active pixel mask from disk file

Menu Command: Peaks > Mask > Create

Accelerator: None

User Level: 1

SLAM Syntax: MASK /READ $1

MASK /READ will read an active bitmask file from disk and load it as the current bitmask. The special “$NULL” can be used to define a bitmask with all active pixels.

The user should be aware the bitmask or the octagon mask are used exclusively. That is if the bitmask is define, the octagon mask is ignored and visa versa.

8.4.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Bitmask Filename) [active.msk]

Filename of active pixel map, “$NULL,” to load an all active bitmask.

8.5 Peaks > Mask > View • View active pixel mask on screen

Menu Command: Peaks > Mask > Create

Accelerator: None

User Level: 1

SLAM Syntax: MASK /VIEW $1

MASK /VIEW allows viewing the active pixels mask on top of a frame image. All inactive pixels are masked out with a dot. Active pixels are left alone. The special bitmask “$NULL” can be used to clear the mask image, while “$MASK” refers to the current bitmask.

NOTE: MASK /VIEW does not change the current active bitmask or octagon mask.

8.5.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Bitmask Filename) [$MASK]

Filename of active pixel map, “$NULL,” to clear window, “$MASK,” to view current active pixel map.

8.6 Peaks > Mask > Octagon • Alternate active pixel mask using octagon region

Menu Command: Peaks > Mask > Create

Accelerator: None

User Level: 1

SLAM Syntax: MASK /OCTAGON $1 $2 $3 $4 $5 $6 $7 $8

MASK /OCTAGON defines an octagon shaped mask which excludes pixels located on or outside the octagon from all INTEGRATE, SMOOTH, and PER_CRYSTAL commands. MASK /OCTAGON is frequently used on off-axis frames, where the beam stop does not occlude a portion of the image and on short time duration frames where the counting statistics are inadequate to properly define a bitmask of active pixels.

The user should be aware the bitmask or the octagon mask is used exclusively. That is if the bitmask is define, the octagon mask is ignored and visa versa.

8.6.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

		512-mode Defaults	1024-mode Defaults
$1	(MIN X)	[0]	[0]
$2	(MIN X+Y)	[60]	[120]
$3	(MIN Y)	[0]	[0]
$4	(MAX X-Y)	[451]	[902]
$5	(MAX X)	[511]	[1023]
$6	(MAX X+Y)	[962]	[1924]
$7	(MAX Y)	[511]	[1023]
$8	(MAX Y-X)	[451]	[902]

Enter requested values in frame pixels.

8.7 Peaks > Integrate > Chi • Perform chi integration in conic region -> F(2T)

Menu Command: Peaks > Integrate > Chi

Accelerator: None

User Level: 1

SLAM Syntax: INTEGRATE /CHI $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n>

INTEGRATE /CHI will integrate a region along the chi direction and plot the results as intensity versus 2-theta. The resulting trace may be written to a file using INTEGRATE /WRITE command, or inputted into the PEAKS /LOAD command.

The area to integrate is defined by specifying the 2-theta and chi range for the Debye-Scherrer cone. Chi zero is defined at 6 o'clock and goes CCW. Interactively, the user may redefine any of the integration region's limits by selecting the limit's line number (1 to 4) and then using the cursor keys. The current integration region limits are continuously updated and displayed on the screen. While interactively modifying an integration limit, the <ESC> key or right button will restore the limit to its original value, while the <ENTER> or left button will accepts the new value for this limit. It is also feasible to move the entire integration window by pressing the "M" key, using the cursors to position a new center of the integration window, then pressing the <ENTER> key.

Once the integration window is defined, pressing <ENTER> will start the integration calculations and display the message:

> Wait=Integrate; ESC,Other buttons=Quit

Normally, one waits for the calculations to finish and to plot the resulting data trace; however, should you wish to abort the procedure, press <ESC>. If too few data points were calculated, the command will terminate immediately. Otherwise, the message below appears:

> Warning—aborted early—Press ENTER to continue, ESC to abort.

Pressing <ESC> will terminate the INTEGRATE /CHI command immediately, while <ENTER> will accept the truncated data trace from the partially integrated window (the upper chi limit was lowered) and display the trace.

While GADDS provides several methods of converting frame images into raw spectra, you should be familiar with the differences between each method. Methods 0 and 4 are summations, while methods 1, 2, 3, and 5 are normalized to a ten pixel region.

1. Sum pixels:
2. Average pixel:
3. Arc Length: (quick and dirty)

4. Solid Angle:
5. Bin Method
6. Normalized Bin: (preferred)

Methods 0 to 3 are described later. They are quick and dirty methods. In contrast, the bin method produces the most accurate results, although at a slower pace. The bin method will produce narrower profiles (FWHMs), smoother spectra, and improved relative intensities across the spectra.

Bins are determined by the start, end and step-size of the integration. Say you requested the range 5 to 65 in 0.5 steps. The first bin covers the range 4.75 to 5.25; the second bin covers 5.25 to 5.75; …; the last bin covers the range 64.75 to 65.25. The idea is to place all of the observed intensity within each bin range into that bin. Each frame pixel covers one or more integration bins. The intensity of the each frame pixel is divided into these integration bins, using the fractional area as the weighting factor (eq. 1). The sum of all of the fractional areas for any given pixel must equal one (eq. 2).

$$I_i = \sum_{n=1}^{N} I_n A_{n,i} \qquad \text{eq. 1.}$$

$$1.0 = \sum_{i=1}^{M} A_{n,I} \qquad \text{eq. 2.}$$

WhereI = Intensity

i = integration bin number

n = frame pixel number

A = fractional area

N = total number of frame pixels

M = total number of integration bins

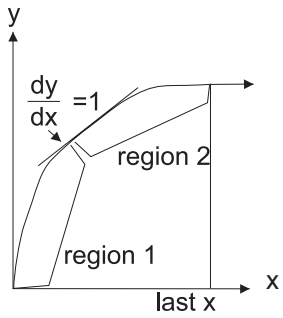
For speed considerations, the frame pixels at the edges of the integration region are not handled precisely. For chi integration, if the center of the pixel lies within the specified chi integration region, then the entire pixel is used. If the pixel center is outside region, then the entire pixel is unused. So narrow chi integration regions, less than a pixel width, should not be used for chi integration. For 2-theta integration, if the center of the pixel lies within the specified 2-theta integration region, then the entire pixel is used. If the pixel center is outside the region, but any pixel corner is inside the 2-theta region, then ¼ of the pixel is used. So narrow or zero width 2-theta integration regions can be used for 2-theta integration (needed for pole figure processing).

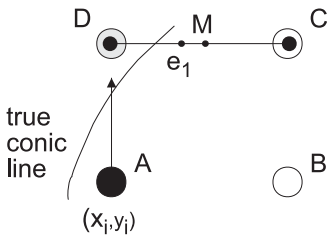
The normalized bin method varies from the above, only by normalizing each bin by the total

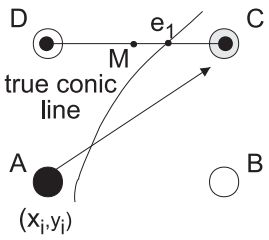
fractional area of all pixels for that bin (eq. 3). We scale the result by a factor of ten.

$$I_i = 10 \left[\sum_{n=1}^{N} I_n A_{n,i} \right] / \left[\sum_{n=1}^{N} A_{n,i} \right] \qquad \text{eq. 3.}$$

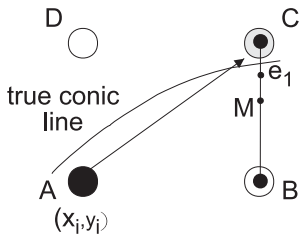
The quick and dirty methods utilizes Bresenham's Algorithm, which draws the conic lines with discrete pixels on a grid (see Figure 8.1). Its main advantage over the bin method is speed. Its disadvantages are accuracy, with broader FWHM and noisier spectra. With Bresenham's algorithm, you must select an appropriate integration step width. Too small and you integrate all the same pixels as in the previous integration step. Too large and you skip pixels between integration steps (the intensity at those pixels are never used in the spectra). Even with a good step width, the intensity at some pixels will be used for consecutive integration steps and an occasional pixel or two could be completely skipped.

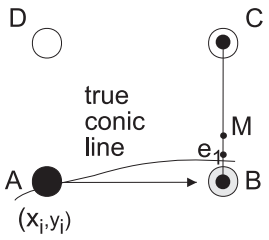






The two cases for steeply sloping regions.





The two cases for gently sloping regions.

Figure 8.1 - Bresenham's algorithm

Essentially, Bresenham bisected the problem into two cases depending upon the slope of the line. For steep slopes, the next pixel along the line always increases by one pixel in the vertical direction (Y), while the horizontal direction (X) may or may not increase by one pixel. Similarly, the converse exists for gentle slopes; the next pixel always increments in W, with or without an increment in Y. Negative slopes are handled by negating the X axis. Bresenham's algorithm adapts easily to computer graphics displays for line drawing.

The area detector image is stored as intensity values on a square pixel grid. For integrating along either 2θ or χ lines, Bresenham's algorithm is used to determine the pixels along the line, and the intensities at each pixel are summed (method=0) or averaged (method=1). These methods equally weight the intensities of all pixels.

The modified version of Bresenham's algorithm (see Figure 8.2) used by Bruker improves integration through summing the individual intensity values multiplied by a weighting factor (x1+x2), either arc length or solid angle. (While solid angle is technically more correct, in practice this weighting scheme gives nearly identical results as arc length, but is slower). This modified integration method must consider the previously chosen pixel, and so four cases arise for each slope region. The weighting given to each intensity value varies by as much as forty percent, which improves the relative integrated intensities between vertical or horizontal regions and moderately sloped regions along a Debye ring. With highly textured samples, the resultant 2θ profiles exhibit true relative intensities between peaks of varying χ positions.

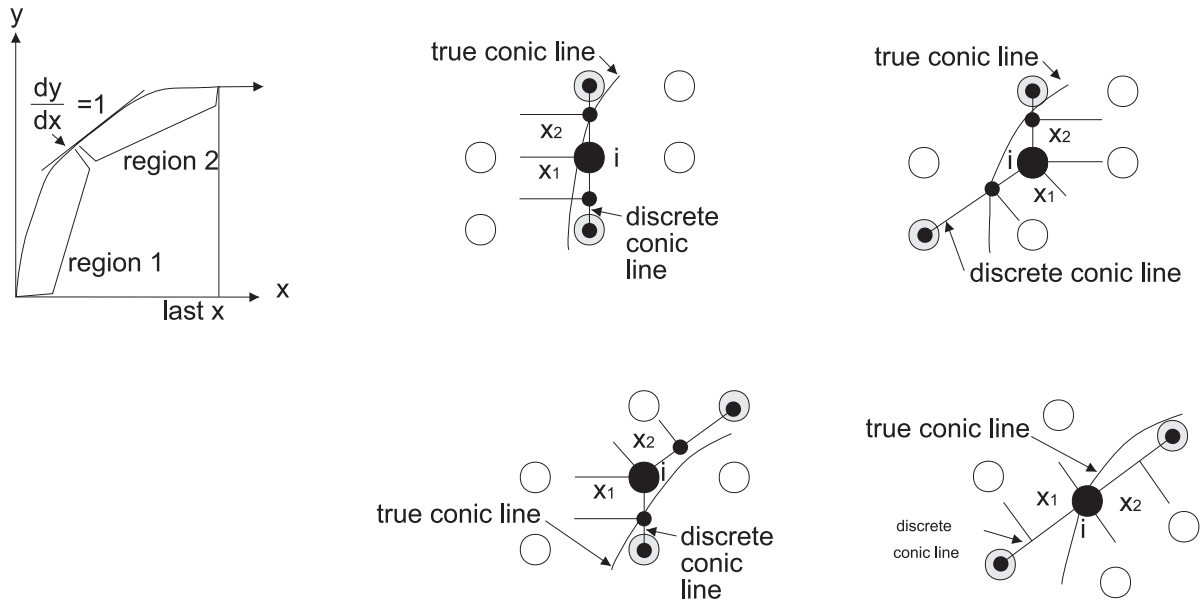


Figure 8.2 - Modified version of Bresenham's algorithm

When executed interactively, the INTEGRATE /WRITE is executed upon successful termination. For more information, see the description of the INTEGRATE /WRITE sub-command.

8.7.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(2-Theta Start) [0.00]

Enter lower 2-theta of conic region in degrees. Valid range is 0 to 179.

$2 .....(2-Theta End) [30.00]

Enter upper 2-theta of conic region in degrees. Valid range is 1 to 180.

$3 .....(Chi Start) [0.00]

Enter lower chi of conic region in degrees. Valid range is -360 to 180.

$4 .....(Chi End) [360.00]

Enter upper chi of conic region in degrees. Valid range is -180 to 360.

/NORMAL=<n> .....(Normalize intensity) [5]

When integrating pixels along a conic line segment, each pixel may be weighted by a normalization factor. Available normalizations are 0=none (sums all active pixels), 1=average pixel (sum of pixels / number of pixels), 2=arc length (sum of {pixels * arc length} / sum of arc lengths), 3=solid angle (sum of {pixels * solid angle} / sum of solid angle), 4=bin method, 5=normalized bin method. See Peaks > Integrate > Chi for full description of this normalization method.

/STEPSIZE=<n>... (Step size) [0.1]

The angle step width in degrees. The default of 0.1 works well for frames taken at 7 cm. Frames taken at 10 cm may need a smaller stepsize.

8.8 Peaks > Integrate > 2Theta • Perform 2-theta integration in conic region -> F(chi)

Menu Command: Peaks > Integrate > 2theta

Accelerator: None

User Level: 1

SLAM Syntax: INTEGRATE /2THETA $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n>

INTEGRATE /2THETA will integrate a region along the 2-theta direction and plot the results as intensity versus chi. Such chi plots are useful for examining texture effects within the data. The resulting trace may be written to a file using INTEGRATE /WRITE command, or inputted into the PEAKS /LOAD command.

The area to integrate is defined by specifying the 2-theta and chi range for the Debye-Scherrer cone. Chi zero is defined at 6 o'clock and goes CCW. Interactively, the user may redefine any of the integration region's limits by selecting the limit's line number (1 to 4) and then using the cursor keys. The current integration region limits are continuously updated and displayed on the screen. While interactively modifying an integration limit, the <ESC> key or right button will restore the limit to its original value, while the <ENTER> or left button will accepts the new value for this limit. It is also feasible to move the entire integration window by pressing the "M" key, using the cursors to position a new center of the integration window, then pressing the <ENTER> key.

Once the integration window is defined, pressing <ENTER> will start the integration calculations and display the message:

> Wait=Integrate; ESC,Other buttons=Quit

Normally, one waits for the calculations to finish and to plot the resulting data trace; however, should you wish to abort the procedure, press <ESC>. If too few data points were calculated, the command will terminate immediately. Otherwise, the message below appears:

> Warning—aborted early—Press ENTER to continue, ESC to abort

Pressing <ESC> will terminate the INTEGRATE /2THETA command immediately, while <ENTER> will accept the truncated data trace from the partially integrated window (the upper chi limit was lowered) and display the trace.

When executed interactively, the INTEGRATE /WRITE is executed upon successful termination. For more information, see the description of the INTEGRATE /WRITE sub-command.

8.8.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(2-Theta Start) [0.00]

Enter lower 2-theta of conic region in degrees. Valid range is 0 to 179.

$2 .....(2-Theta End) [30.00]

Enter upper 2-theta of conic region in degrees. Valid range is 1 to 180.

$3 .....(Chi Start) [0.00]

Enter lower chi of conic region in degrees. Valid range is -360 to 180.

$4 .....(Chi End) [360.00]

Enter upper chi of conic region in degrees. Valid range is -180 to 360.

/NORMAL=<n> .....(Normalize intensity) [3]

When integrating pixels along a conic line segment, each pixel may be weighted by a normalization factor. Available normalizations are 0=none (sums all active pixels), 1=average pixel (sum of pixels / number of pixels), 2=arc length (sum of {pixels * arc length} / sum of arc lengths), 3=solid angle (sum of {pixels * solid angle} / sum of solid angle), 4=bin method. See Peaks > Integrate > Chi for full description of this normalization method.

/STEPSIZE=<n>... (Step size) [0.1]

The angle step width in degrees. The default of 0.1 works well for frames taken at 7 cm. Frames taken at 10 cm may need a smaller stepsize.

8.9 Peaks > Integrate > Area • Perform area integration in conic region -> integer

Menu Command: Peaks > Integrate > Area

Accelerator: None

User Level: 1

SLAM Syntax: INTEGRATE /AREA $1 $2 $3 $4

Integrates total counts inside (and on) a user defined conic region. Does not subtract out background.

8.9.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(2-Theta Start) [0.00]

Enter lower 2-theta of conic region in degrees. Valid range is 0 to 179.

$2 .....(2-Theta End) [30.00]

Enter upper 2-theta of conic region in degrees. Valid range is 1 to 180.

$3 .....(Chi Start) [0.00]

Enter lower chi of conic region in degrees. Valid range is -360 to 180.

$4 ..... (Chi End) [360.00]

Enter upper chi of conic region in degrees. Valid range is -180 to 360.

8.10 Peaks > Integrate > Slice • Perform chi integration in rectangular region -> F(2t)

Menu Command: Peaks > Integrate > Slice

Accelerator: None

User Level: 1

SLAM Syntax: INTEGRATE /SLICE $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n>

INTEGRATE /SLICE will integrate a rectangular region along the chi direction and plot the results as intensity versus 2-theta. The resulting trace may be written to a file using INTEGRATE /WRITE command, or inputted into the PEAKS /LOAD command.

The area to integrate is defined by specifying the 2-theta range, chi, and height of rectangular box. Chi zero is defined at 6 o'clock and goes CCW. Interactively, the user may redefine any of the integration region's limits by selecting the limit's line number (1 to 4) and then using the cursor keys. The current integration region limits are continuously updated and displayed on the screen. While interactively modifying an integration limit, the <ESC> key or right button will restore the limit to its original value, while the <ENTER> or left button will accepts the new value for this limit.

Once the integration window is defined, pressing <ENTER> will start the integration calculations and display the message:

> Wait=Integrate; ESC,Other buttons=Quit

Normally, one waits for the calculations to finish and to plot the resulting data trace; however, should you wish to abort the procedure, press <ESC>. If too few data points were calculated, the command will terminate immediately. Otherwise, the message below appears:

> Warning—aborted early—Press ENTER to continue, ESC to abort

Pressing <ESC> will terminate the INTEGRATE /SLICE command immediately, while <ENTER> will accept the truncated data trace from the partially integrated window (the upper chi limit was lowered) and display the trace.

When executed interactively, the INTEGRATE /WRITE is executed upon successful termination. For more information, see the description of the INTEGRATE /WRITE sub-command.

8.10.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (2-Theta Start) [0.00]

> Enter lower 2-theta of conic region in degrees. Valid range is 0 to 179.

$2 ..... (2-Theta End) [30.00]

> Enter upper 2-theta of conic region in degrees. Valid range is 1 to 180.

$3 .....(Chi Angle) [90.00]

Enter chi of rectangular region in degrees. Valid range is -360 to 360.

$4 .....(Height in Pixels) [10]

Enter height in pixels of rectangular region. Valid range is 0 to {framesize-1}.

/NORMAL=<n> .....(Normalize intensity) [3]

When integrating pixels along a conic line segment, each pixel may be weighted by a normalization factor. Available normalizations are 0=none (sums all active pixels), 1=average pixel (sum of pixels / number of pixels), 2=arc length (sum of {pixels * arc length} / sum of arc lengths), 3=solid angle (sum of {pixels * solid angle} / sum of solid angle). See Peaks > Integrate > Chi for a full description of this normalization method.

/STEPSIZE=<n> ...(Step size) [0.1]

The angle step width in degrees. The default of 0.1 works well for frames taken at 7 cm. Frames taken at 10 cm may need a smaller stepsize.

8.11 Peaks > Integrate > Write • Write integration results to disk file

Menu Command: Peaks > Integrate > Write

Accelerator: None

User Level: 1

SLAM Syntax: INTEGRATE /WRITE $1 /FILENAME=<n> /FORMAT=<n> /APPEND

INTEGRATE /WRITE will output the results from either integration to a disk file format which is compatible with conventional powder diffraction data processing software. Four file formats are supported:

- PLOTSO is simple ASCII file format which is very portable to any computer platform.
- OLD_DIFFRAC-AT is the file format used by ancient PC-based software. This file format is binary and is difficult to read on non-PC platforms.
- DIFFRAC-AT is the file format used by older PC-based software. This file format is binary and is difficult to read on non-PC platforms.
- DIFFRAC*plus* is the file format used by the Bruker DIFFRAC*plus* software. This file format is binary and is difficult to read on non-INTEL platforms.

INTEGRATE /WRITE is capable of output any one of the supported file formats. All four file formats are also capable of supporting multiple ranges. To write the data to a new scan range of an existing file, set the append flag.

8.11.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Title) [auto default]

Title of plot. In SLAM mode enclose the title in quotes.

/FILENAME=<n> .. (File Name) [auto default]

Name of the RAW data file to create or append.

/FORMAT=<n> ..... (Format) [DIFFRACplus]

Enter file format as either: DIFFRAC*plus*, DIFFRAC-AT, OLD-DIFFRAC-AT, or PLOTSO. DIFFRAC*plus* is the latest file format and thus the preferred option. PLOTSO files have standard ASCII format. Non-Bruker programs should be able to read PLOTSO files (i.e., LOTUS 123, and MS EXCEL). File extensions are defaulted to *.RAW for most formats and to *.PLT for PLOTSO format.

/APPEND..... (Append as Additional Range) [Yes]

Enter “Y” to write this new data range as the next range in any existing file. If the file doesn't exists, it will be created with this data as the first and only range. Enter “N” to

delete any existing file(s) and create a new one range raw data file(s).

/SCALE .....(Scale Factor) [1.0]

Enter multiplicative scale factor or 1.0 for none. The entire range of the written raw data file will be multiplied by this scale factor.

8.12 Peaks > Integrate > Clear • Clear graph on top of image

Menu Command: Peaks > Integrate > Clear

Accelerator: None

User Level: 1

SLAM Syntax: INTEGRATE /CLEAR

INTEGRATE /CLEAR will remove the results from the previous integration from the screen without erasing the data frame.

8.12.1 Arguments

None. Command executes immediately.

8.13 Peaks > Integrate > Rectangle • Perform rectangle integration for detector testing

Menu Command: Peaks > Integrate > Rectangle

Accelerator: None

User Level: 1

SLAM Syntax: INTEGRATE /RECTANGLE $1 $2 $3 $4 /VERTICAL

Use this command to sum pixel intensities along either the vertical or horizontal directions. Useful for diagnostic purposes mainly.

8.13.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(X start) [1]

X pixel of rectangle left side.

$2 .....(X end) [510]

X pixel of rectangle right side.

$3 .....(Y start) [1]

Y pixel of rectangle bottom side.

$4 .....(Y end) [510]

Y pixel of rectangle top side.

/VERTICLE..... (Verticle Y.N) [Yes]

Check to integrate vertical, uncheck to integrate horizontal.

8.14 Peaks > Refl. Array > Threshold • Place spots/threshold in a series of frames into the array

Menu Command: Peaks > Refl. Array > Threshold

Accelerator: None

User Level: 1

SLAM Syntax:

> REFL_ARRAY /THRESHOLD $1 $2 /CONTIG=<n> /COUNTS=<n> /SIGMA=<NN> /XEXMIN=<n> /XEXMAX=<n> /RMAX=<n> /DMIN=<n> /DMAX=<n> /DBIAS=<n> [$3 $4 $5 $6 $7 $8]

This routine provides a means for automatically picking reflections from a series of data frames and placing them in the Reflection Array. The algorithm provides control over selection factors such as intensity threshold and resolution range.

Spots entered into the array in this manner always have the A flag set, and contain the goniometer setting angles, detector X,Y position, intensity normalized to 1 deg/min, and I/sigma. If the pixels above the threshold span more than one frame, the computed scan-angle centroid is more precise, and the C flag is set for that reflection. These “centered” reflections are especially suitable for autoindexing and least squares; however, if you can't find many reflections that span frames, you can set the C flags manually with the REFL_ARRAY /MODIFY command to force the autoindexing and least squares to use all the reflections found by /THRESHOLD. If a valid spatial correction is in effect (highly recommended), the X,Y values entered into the array will represent the spatially corrected X,Y position, and the S flag for that reflection will be set; otherwise, the raw X,Y will be entered and the S flag will be clear.

In the special case where you’re thresholding reflections from a single frame ($2 = 1; see below) the program automatically sets the C flags. This makes indexing from a single frame (or better, from two nearly orthogonal oscillation pictures) more convenient. When attempting to index from one or two oscillation pictures, it is best to use fairly wide frames (e.g., 0.5–1.5 degrees) to insure that changes in all three HKL indices are represented in each picture.

Normally, the setting angles for each frame are extracted directly from the frame itself; however, XENGEN-format frames taken with data collection software earlier than FRAMBO Version 2 do not contain the required information. You can still threshold frames acquired with earlier versions with use of the setting angle “override” options, described below. Make sure that these override options are all set at their default values (of 9999) unless you're processing old frames.

When invoked with the THRESHOLD option from the REFL_ARRAY submenu or when run from the command line without arguments,

REFL_ARRAY /THRESHOLD displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins refinement of the unit cell and orientation parameters; the ESC key or right mouse button returns you to the REFL_ARRAY submenu. You can interrupt thresholding in progress with the CTRL-BREAK key combination.

When thresholding starts, the program displays the name of the last frame thresholded and the number of spots found on the bottom status line. Note that if the number of spots per frame is larger than 512/N where N is the number of frames being thresholded, your threshold is too low or you're thresholding too many frames. Autoindexing and least squares run optimally if they have at least 25 and preferably 50–100 “centered” spots; more is overkill. The recommended procedure prior to indexing (but after the detector distance, flood-field correction, spatial correction, and beam center have been determined) is to threshold about half the desired number of spots from a few frames (say, 10 contiguous frames) into a blank Reflection Array, and then repeat the procedure with another series of 10 frames starting about 90 degrees in scan angle from the first set.

After all frames have been read in, the program requires a few seconds to compute integrated intensities and sort the output. Upon completion, a scrolling output window is displayed containing the resulting output text. If logging is enabled (see LOGFILE) the contents of this window are also written to the logfile. When viewing the output, pressing ENTER or the left mouse button displays a pop-up menu of options, including export of ASCII data; for example, the contents of the window could be sent to a file or printer with this function. You can also move through the window contents with the page keys, arrow keys or with mouse motion. Pressing ESC or the right mouse button exits the output window. The program then displays the prompt:

> <n> SPOTS WILL BE INSERTED IN ARRAY AT # <M>
>
> --PRESS ENTER TO CONTINUE, ESC TO QUIT

where <n> represents the number of reflections found and <M> represents the line number of the first empty record in the Reflection Array. If you press the ENTER key or left mouse button, the program stores the thresholded reflections in the array, then displays the Reflection Array in an editing window for review (see REFL_ARRAY /EDIT for description and operation of the editing window). Pressing the ESC key or right mouse button at the above prompt, or from within this editing window, returns you to the REFL_ARRAY submenu. The output window contents are described in more detail below.

If REFL /THRESHOLD was invoked from the command line, the output window is displayed subject to a 10 s timeout to allow command

scripts to run without intervention. If you do not press a key or mouse button within 10 s after the output window is displayed, the program will continue as if the ESC key had been pressed.

When invoked from the command line, REFL /THRESHOLD can take the following arguments (where <n> represents a numeric value, & indicates continuation on the next line). Optional command-line parameters are shown in square brackets. If you don't supply these parameters on the command line, the command still runs without intervention, with the default value (9999=get value from frame header) assumed:

8.14.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(First Input File Name) [FRAME.000]

Enter the file name for the first frame in the series to process. For example, if you have 15 data frames to be thresholded beginning with SAMPL.001 and ending with SAMPL.015, then you would enter “SAMPL.001” as the first frame in the series. When in the input panel, if you leave this entry blank or specify a “wildcard” filename pattern, pressing the ENTER key or the left mouse button will display a list of the current filenames matching the pattern. You can choose one from the displayed list by moving to it with the arrow/page keys or mouse and pressing ENTER or the left mouse button. You will be returned to the input panel with the selected filename filled in. If you leave this item blank, it is the same as entering a *.* wildcard pattern. Both filenames and patterns entered here are merged with the CONFIGURE /EDIT frame directory (se CONFIGURE /EDIT for a description of how this is done).

$2 ..... (# Frames to Process) [7]

Enter the number of consecutive frames to process. It is not necessary to enter all frames in a series. Try to pick number of frames and threshold that result in about 100 spots being written to the array.

/CONTIG=<n> ..... (Max Pixel Separation) [1]

Enter the maximum number of pixels of separation still considered contiguous within a given reflection. Statistical fluctuations could cause a pixel within a reflection to drop below the threshold whereas its neighbors exceed the threshold. Raising the value given here allows pixels to be considered part of the same reflection even if they are separated by below-threshold pixels. The default of 1 specifies that pixels must be contiguous, and should be satisfactory for the vast majority of cases.

/COUNTS=<n>.....(Raw Count Threshold) [50]

Process pixels that have counts equal to or greater than this value. Try to pick a value that will place about 100 reflections in the array. Note that a threshold that is low enough to accept background points as possible reflections can cause autoindexing to fail. A quick way of determining a threshold is to display a frame with the minimum display counts set to zero and the maximum display counts set to a power of 2 (for example, 64 or 128), then use the CONTRAST command to threshold the image. Move the mouse all the way to the left for maximum contrast (i.e., a sharp black-to-white transition), then move the mouse up and down until a reasonable number of spots (for example, 100 divided by the number of frames you're going to threshold) is visible. You can then estimate the threshold from the point where the black-to-white transition occurs in the color bar at the right of the screen.

/SIGMA=<n> .....(I/Sigma Threshold) [20]

Retain only those reflections with I/sigma (that is, its intensity divided by its standard deviation) at or above this value times the thermal falloff compensation derived from the value given for /DBIAS below. I/SIGMA computed for each reflection is multiplied by EXP(DBIAS * S^2) where S is sin(theta)/lambda. If the result is lower than the value specified here, the reflection is rejected.

/XEXMIN=<n> ..... (Minimum Excluded X) [0]

Exclude spots with an X-centroid between the value specified here and that specified as /XEXMAX below. This is useful for excluding the area near the beam stop. The value is in pixels in the Bruker coordinate convention with X,Y=(0,0) at the lower left of a displayed frame.

/XEXMAX=<n> ..... (Maximum Excluded X) [30]

Exclude spots with an X-centroid between the value specified as /XEXMIN above and the value specified here. This is useful for excluding the area near the beam stop. The value is in pixels in the Bruker coordinate convention with X,Y=(0,0) at the lower left of a displayed frame.

/RMAX=<n>..... (Radius Cutoff) [265]

Enter the maximum allowed distance of a reflection centroid from the detector center (in pixels). Reflections which exceed this value are rejected. Valid range is from 0 to 300.

/DMIN=<n>..... (Minimum Angstroms) [1.5]

Enter the minimum allowed interplanar spacing in Angstroms corresponding to a reflection centroid. Reflections at higher

(better) resolution than the value specified here are rejected.

/DMAX=<n> .....(Maximum Angstroms) [100]

Enter the maximum allowed interplanar spacing in Angstroms corresponding to a reflection centroid. Reflections at lower (worse) resolution than the value specified here are rejected.

/DBIAS=<n>.....(Temperature Factor) [10]

Enter the B-factor in Angstroms^2 used to bias the I/sigma threshold test as a function of resolution. I/SIGMA computed for each reflection is multiplied by EXP(DBIAS * S^2) where S is sin(theta)/lambda. If the result is lower than the value specified as /SIGMA (see above), the reflection is rejected.

$3.....(2-Theta override) [9999]

Enter the swing (2-theta setting) angle in degrees to be assumed for the frame series. The default value, 9999, specifies that the swing angle is to be extracted from the frames themselves, which is the normal mode of operation. If you're processing old XENGEN-format frames (acquired with software earlier than FRAMBO Version 2), you'll need to explicitly specify the angle here. For frames in XENGEN or BRUKER format acquired with FRAMBO V2 or higher, specify 9999.

$4 ..... (Omega override) [9999]

Enter the starting omega setting angle in degrees to be assumed for the frame series. The default value, 9999, specifies that omega is to be extracted from the frames themselves, which is the normal mode of operation. If you're processing old XENGEN-format frames (acquired with software earlier than FRAMBO Version 2), you'll need to explicitly specify the angle here. For frames in XENGEN or BRUKER format acquired with FRAMBO V2 or higher, specify 9999.

$5 ..... (Phi override) [9999]

Enter the starting phi setting angle in degrees to be assumed for the frame series. The default value, 9999, specifies that phi is to be extracted from the frames themselves, which is the normal mode of operation. If you're processing old XENGEN-format frames (acquired with software earlier than FRAMBO Version 2), you'll need to explicitly specify the angle here. For frames in XENGEN or BRUKER format acquired with FRAMBO V2 or higher, specify 9999.

$6 ..... (Chi override) [9999]

Enter the chi setting angle in degrees to be assumed for the frame series. The default value, 9999, specifies that chi is to be extracted from the frames themselves, which is the normal mode of operation. If

you're processing old XENGEN-format frames (acquired with software earlier than FRAMBO Version 2), you'll need to explicitly specify the angle here. For frames in XENGEN or BRUKER format acquired with FRAMBO V2 or higher, specify 9999.

$7 .....(Scan axis override) [9999]

Enter the scan axis number (2 for omega, 3 for phi) to be assumed for the frame series. The default value, 9999, specifies that the scan axis is to be extracted from the frames themselves, which is the normal mode of operation. If you're processing old XENGEN-format frames (acquired with software earlier than FRAMBO Version 2), you'll need to explicitly specify the axis here. For frames in XENGEN or BRUKER format acquired with FRAMBO V2 or higher, specify 9999.

$8 .....(Frame width override) [9999]

Enter the signed frame width in degrees to be assumed for the frame series. The default value, 9999, specifies that the width is to be extracted from the frames themselves, which is the normal mode of operation. If you're processing old XENGEN-format frames (acquired with software earlier than FRAMBO Version 2), you'll need to explicitly specify the width here. For frames in XENGEN or BRUKER format acquired with FRAMBO V2 or higher, specify 9999.

8.14.2 Threshold Output

An example of the output from REFL_ARRAY /THRESHOLD is shown below, resulting from thresholding of the eight myoglobin test frames supplied with the software. It begins with an overall statistical summary of the number of reflections found and their disposition. This summary contains:

FOUND

Total number of reflections above the threshold found

ON FIRST OR LAST FRAME

Reflections which have intensity on the first or last frame are rejected because their scan angle cannot be accurately determined.

IN X-EXCLUSION RANGE

This is the number of reflections rejected because their X-centroid was between the limits specified as /XEXMIN and /XEXMAX.

OUTSIDE RADIUS LIMIT

This is the number of reflections rejected because the distance of their X,Y centroid from the detector center was larger than the limit given as /RMAX.

OUTSIDE RES LIMITS

This is the number of reflections rejected because their X,Y-centroid was outside of the resolution limits specified as /DMIN and /DMAX.

< I/SIGMA THRESHOLD

This is the number of reflections rejected because their (I/SIGMA) * EXP(DBIAS * S^2) was below of the threshold specified as /SIGMA.

ORPHAN PIXELS

This is the number of reflections rejected because there was only a single pixel over the threshold.

BIFURCATED

This is the number of spots where the 2D intensity on one frame merges with the 2D intensity of more than one spot on an adjacent frame. These reflections are rejected.

TOTAL # USEABLE

Number of non-rejected reflections found.

CENTERED FOR LS

The number of reflections with the C flag set. These are reflections whose intensity spanned more than one frame, and are especially suitable for autoindexing or least squares (LS).

TOTAL # UNUSED

Number of rejected reflections

Following the overall statistics is a reflection-by-reflection summary. For each reflection, a line contains (in order) the X,Y and scan-angle centroids (X and Y are in pixels, and scan angle is in degrees), the integrated intensity normalized to 1 deg/min, the intensity divided by its standard deviation, the resolution of the reflection in Angstroms, and a hexadecimal code where each set bit indicates a status condition. Conditions 4 and 8 (code 000C hex when combined) are desirable; the others cause the reflection to be rejected. Bit assignments in the status code are:

Bit #	Value (Hex)	Meaning
0	1	Reflection rejected if set
1	2	Reflection is bifurcated
2	4	Found a close 2D spot on adjacent frame
3	8	Reflection spans frames
4	10	Orphan pixel
5	20	Excluded by X limits
6	40	Excluded by resolution limits
7	80	Excluded by radius limit
8	100	Excluded by I/sigma limit

Example output follows:

Example 8.1 - REFL_ARRAY /THRESHOLD Output from Eight Myoglobin Test Frames

Reflection disposition:
found = 133
on first or last frame = 33
in X-exclusion range = 5
outside radius limit = 10
outside res. limits = 0
< I/sigma threshold = 0
orphan pixels = 11
bifurcated = 0
Total # useable = 107
“centered” for LS = 26
Total # unused = 26

X	Y	Rot	Inorm	#Sig	D	Code
82.9	51.2	-0.3	627	112	4.1	000C
33.3	99.1	-0.4	468	97	5.4	000C
142.1	309.5	-0.4	344	83	4.2	000C
82.9	196.2	-0.6	379	87	5.6	000C
130.0	127.2	-0.6	285	76	4.1	000C
156.7	28.7	-0.7	223	67	3.2	000C
164.6	264.0	-0.7	228	68	4.0	000C
198.8	241.4	-0.7	205	64	3.5	000C
95.1	77.1	-0.6	175	59	4.2	000C
96.6	357.5	-0.6	179	60	4.6	000C
177.8	104.2	-0.3	142	53	3.4	000C
269.2	173.1	-0.3	97	44	2.8	000C
145.1	403.4	-0.7	121	49	3.6	000C
222.9	151.2	-0.7	77	39	3.2	000C
94.6	149.6	-0.4	81	40	4.9	000C
219.5	450.4	-0.6	49	31	2.8	000C
190.3	80.3	-0.6	51	32	3.2	000C
192.9	29.7	-0.7	47	31	3.0	000C
34.9	313.0	-0.4	71	38	6.8	000C
58.8	195.7	-0.3	63	36	6.3	000C
119.6	333.3	-0.3	53	33	4.4	000C
141.2	196.4	-0.3	52	32	4.3	000C
281.8	150.3	-0.4	22	21	2.7	000C
107.0	287.4	-0.7	32	26	5.0	000C
322.7	376.5	-0.3	14	17	2.4	000C
155.1	79.3	-0.6	10	14	3.5	000C
107.2	52.7	-0.8	355	85	3.8	0005
141.2	173.6	-0.8	369	86	4.2	0001
164.8	286.4	-0.8	334	82	3.9	0001
83.4	287.8	-0.2	325	81	5.5	0005
164.4	219.1	-0.8	246	70	4.0	0005
117.8	173.3	-0.1	230	68	4.6	0001
165.5	127.6	-0.3	178	60	3.7	0000
175.7	196.5	-0.1	177	60	3.8	0001
70.6	75.7	-0.2	191	62	4.5	0005
143.7	53.8	-0.1	135	52	3.5	0001
210.9	285.8	-0.2	98	44	3.4	0001
167.7	378.3	-0.5	99	45	3.5	0000
267.9	3.1	-0.9	63	36	2.5	0001
224.1	330.9	-0.3	84	41	3.2	0000
134.1	428.5	-0.2	93	43	3.6	0001
210.3	196.4	-0.3	85	41	3.4	0000
263.7	400.4	-0.7	56	34	2.7	0000
82.8	219.2	-0.1	87	42	5.7	0001
352.0	51.8	-0.5	36	27	2.2	0000
33.9	195.3	-0.3	90	43	7.2	0000
82.9	101.5	-0.8	75	39	4.6	0000
177.6	331.6	-0.8	65	36	3.6	0000
176.6	308.8	-0.3	65	36	3.7	0000
176.1	173.8	-0.7	60	35	3.7	0000
329.7	240.1	-0.1	37	27	2.5	0001
202.8	377.3	-0.5	50	32	3.2	0000
58.2	100.7	-0.5	60	35	5.0	0000
83.8	311.2	-0.7	60	35	5.4	0000
106.5	242.1	-0.4	57	34	5.1	0000
225.0	353.8	-0.8	39	28	3.1	0001
180.7	401.7	-0.6	38	28	3.3	0000
215.7	55.4	-0.4	33	26	2.9	0000
199.2	285.9	-0.9	39	28	3.5	0001
284.2	352.7	-0.6	27	23	2.7	0000
108.7	380.6	-0.2	41	29	4.2	0005
142.1	103.7	-0.5	38	28	3.8	0000
304.1	240.0	-0.6	25	23	2.6	0000

294.8	126.9	-0.7	23	21	2.6	0000
321.4	102.0	-0.8	20	20	2.4	0005
236.8	353.7	-0.3	24	22	3.0	0000
257.1	285.0	-0.2	24	22	2.9	0001
190.1	354.3	-0.5	27	23	3.4	0000
400.8	98.7	-0.3	13	16	2.1	0000
300.1	503.1	-0.5	16	18	2.3	0000
211.5	308.2	-0.4	26	23	3.3	0000
256.9	196.0	-0.4	21	21	2.9	0000
234.9	128.2	-0.8	21	21	3.0	0000
200.4	128.1	-0.4	23	22	3.3	0000
296.8	353.0	-0.2	17	18	2.6	0005
132.4	380.0	-0.8	26	23	3.9	0005
325.7	53.4	-0.8	11	15	2.3	0000
304.2	262.2	-0.5	13	16	2.6	0000
303.9	217.5	-0.7	12	16	2.6	0000
290.0	424.7	-0.9	11	15	2.5	0001
257.5	173.6	-0.8	12	16	2.9	0000
106.4	219.3	-0.7	18	19	5.1	0000
210.6	173.7	-0.8	14	17	3.3	0005
315.9	217.4	-0.4	10	14	2.5	0000
106.7	264.7	-0.5	16	18	5.1	0000
316.2	239.9	-0.3	8	13	2.5	0000
210.8	218.8	-0.2	11	15	3.4	0001
234.9	151.0	-0.2	10	14	3.1	0001
60.6	407.7	-0.9	13	16	4.6	0001
182.7	2.8	-0.5	9	13	2.9	0000
269.6	150.3	-0.7	8	13	2.8	0000
316.3	262.0	-0.3	7	12	2.5	0000
436.9	191.6	-0.2	4	9	2.0	0001
157.7	426.6	-0.8	9	14	3.4	0001
258.4	307.4	-0.5	8	12	2.9	0000
328.4	217.5	-0.2	6	11	2.5	0001
73.4	432.3	-0.7	10	14	4.2	0000
145.8	1.4	-0.7	8	13	3.2	0000
59.9	312.0	-0.5	11	15	6.0	0000
231.6	4.0	-0.2	5	10	2.7	0001
307.2	126.6	-0.4	4	9	2.5	0000
209.7	476.2	-0.3	5	10	2.8	0000
292.0	262.0	-0.9	4	9	2.7	0001
244.6	240.8	-0.5	5	10	3.1	0000
257.0	218.1	-0.2	4	9	3.0	0001
213.3	103.9	-0.6	5	10	3.1	0000
198.6	218.8	-0.9	5	10	3.5	0001
379.1	50.9	-0.3	2	7	2.1	0010
337.2	400.8	-0.8	3	7	2.3	0010
312.7	503.5	-0.2	2	7	2.2	0011
334.0	102.0	-0.7	2	6	2.3	0010
270.4	329.3	-0.4	3	7	2.8	0010
303.5	195.3	-0.9	2	6	2.6	0011
244.7	218.5	-0.6	3	7	3.1	0010
260.4	104.3	-0.6	2	6	2.8	0010
250.3	377.0	-0.5	2	6	2.8	0010
147.2	454.3	-0.6	2	7	3.3	0010
72.0	25.8	-0.3	2	7	3.9	0010
23.8	435.2	-0.6	170	59	4.7	002C
7.9	98.7	-0.8	299	78	5.9	0025
22.8	362.3	-0.2	97	44	6.1	0021
8.8	194.9	-0.6	88	42	8.5	0020
9.7	314.0	-0.8	13	16	7.8	0020
-2.6	362.4	-0.6	773	125	6.8	008C
48.6	434.3	-0.5	396	89	4.5	008C
61.8	459.2	-0.5	179	60	4.0	008C
95.7	26.0	-0.7	117	49	3.7	008C
136.7	480.4	-0.3	77	39	3.2	008C
86.4	457.2	-0.8	687	118	3.8	0085
-3.9	146.8	-0.2	288	76	7.6	0085
35.3	409.2	-0.9	117	49	5.0	0081
38.3	459.1	-0.5	26	23	4.3	0080
75.5	483.8	-0.9	11	15	3.7	0081

8.15 Peaks > Refl. Array > Pick • Select spots from currently displayed frame to put in array

Menu Command: Peaks > Refl. Array > Pick

Accelerator: None

User Level: 1

SLAM Syntax:

REFL_ARRAY /PICK $1 $2 $3 $4
/START=<n> /QUADRANT=<n>
/FRAME_HALFWIDTH=<n>

This option provides an interactive means for adding reflections to the array. This is useful in cases where a known reflection has fallen below threshold during automatic picking, or when you want to isolate specific reflections to see if there is a satellite or twinning in the sample. This command is very similar to GRAPH /ROCKING, except that the computed 3D intensity-weighted centroid coordinates and setting angles are entered into the Reflection Array on completion.

Before running REFL_ARRAY /PICK, a set of data frames must be collected with fixed step size in any angle (a single frame is sufficient, but the centroid in scan angle will not be precisely determined, and the rocking curve will not be displayed). Use the DISPLAY or LOAD command to display the central frame about which you want the rocking curve to be computed. Then, invoke REFL_ARRAY /PICK, where a rectangular cursor like the one in CURSORS /BOX is used to select a region within the data frame. From this, the program calculates the background-subtracted intensity for that region in each frame. If /FRAME-HALFWIDTH is greater than zero (that is, if intensity was obtained from more than a single frame) the program also displays the results in a plot of intensity versus scan angle. Background-subtracted intensity is determined in the same way as for CURSORS /BOX. The background is computed as the average of the points on the perimeter of the box, excluding those points which are more than 3 standard deviations above the mean. You have to be careful to choose the correct box size, since in some cases the X,Y centroid of the x-ray reflection may change as a function of scan angle.

When invoked with the PICK option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /PICK displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins interactive region-of-interest selection with a box cursor. The ESC key or right mouse button returns you from the input panel to the REFL_ARRAY submenu.

When you're selecting a region-of-interest, a rectangular cursor from 2x2 to 128x128 pixels in size appears in the detector frame area, and can be moved or re-sized under control of the mouse and/or keyboard arrow keys. The arrow

keys are very useful for precise, 1-pixel adjustments. Pressing the ENTER key or left mouse button computes the intensity versus scan angle curve and draws it on the screen. Pressing the ESC key or the right mouse button toggles between position-change mode and size-change mode where the lower left corner of the box remains anchored while the upper left corner moves under mouse control. If you want to exit without computing, drawing the graph, and entering the reflection into the array, use CTRL-BREAK. Depending on the number of frames specified with the FRAME HALFWIDTH argument (see below) the rocking curve can take several seconds to compute.

The lineweight of the cursor can be increased from the default thickness of 1 pixel by defining the environment variable SAXI$CURSWEIGHT with an integer value from 2 to 7. In general, SAXI$CURSWEIGHT=3 is a good value to use if you want thick cursors. Odd values are better than even ones, since the extra thickness is then added symmetrically about the true cursor position.

On completion, the setting angles, the X,Y and scan-angle centroids, the intensity and I/sigma are entered into the Reflection Array in the specified record number, or in the next available record number if specified as zero. The A flag is set in the new Reflection Array entry. If the scan-angle centroid was computed from intensity on more than one frame, the C flag is set. If a valid spatial correction is in effect, the corrected X,Y are placed in the Reflection Array and the S flag is set, otherwise the raw X,Y are stored and the S flag is clear. If a valid orientation matrix is in effect, the nearest integer HKL indices are also entered into the array and the H flag is set.

The output statistics written to the status area in the middle right of the screen, and to the output logfile if logging is enabled, are detailed in the description of the GRAPH /ROCKING command.

By providing arguments on the command line, you can direct the REFL_ARRAY /PICK computations and graphing to be performed once at a single specified position, after which control returns immediately to the command line.

If logging is turned on (see the LOGFILE command for more information), the quantities computed, for the final position of the cursor prior to exiting the command, are written to the output logfile. If scripting is enabled (again, see LOGFILE), a non-interactive REFL_ARRAY /PICK command corresponding to the final cursor position is written to the output script file.

8.15.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(X-Origin) [256]

The X-coordinate of the lower left of the box defining the region-of-interest in pixels. The range is from 0 to {framesize-1}; default value is 256.

$2 .....(Y-Origin) [256]

The Y-coordinate of the lower left of the box defining the region-of-interest in pixels. The range is from 0 to {framesize-1}; default value is 256.

$3 .....(Width) [16]

The width of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 16.

$4 .....(Height) [16]

The height of the box defining the region-of-interest in pixels. The range is from 0 to 128; default value is 16.

/START=<n> .....(Reflection #) [0]

This specifies the position in the Reflection Array into which the new reflection is to be stored. The first line in the Reflection Array is numbered 1. If you specify a value of zero here (the default), the new reflection will be placed in the first available empty line of the array.

/QUADRANT=<n> (Quadrant) [0]

This parameter specifies whether you want the graph to appear covering the entire data frame (enter “0”), or just one of the four quadrants (enter 1 through 4 as appropriate). The default value is 0 (full frame window). Quadrants are 0 = full window, 1 = lower left, 2 = lower right, 3 = upper left, and 4 = upper right.

/FRAME_HALFWIDTH=<n>(Frame Halfwidth) [5]

Enter the number of frames ON EACH SIDE of the currently displayed frame to be included in the rocking curve. Make sure that you don't exceed the number of frames actually available for processing in either direction. If FRAME_HALFWIDTH is zero, intensity will be taken from only the frame which is currently displayed. The scan-angle centroid will not be precisely determined in this case, and the C flag will not be set for the new record inserted into the reflection array. In this case, a rocking curve is not displayed (and response is therefore much faster).

8.16 Peaks > Refl. Array > Index • Autoindex to compute HKL's of angles-only reflections

Menu Command: Peaks > Refl. Array > Index

Accelerator: Ctrl+I

User Level: 1

SLAM Syntax:

> REFL_ARRAY /INDEX $1 /AAX=<n> /BAX=<n> /CAX=<n> /U1=<n> /U2=<n> /U3=<n> /FCELL=<n> /SIGA=<n> /NOREDUCE /VERBOSE /FGROUP=<n> /HKLTOL=<n> /FFIT=<n>

REFL_ARRAY /INDEX is used following REFL_ARRAY /THRESHOLD (and/or /PICK) to determine HKL indices for those reflections in the array which have at least the A and C flags set, that is, those reflections which contain setting angles, X, Y and span more than one frame (are "centered"). Autoindexing determines, in addition to HKL indices for each reflection, a rough crystal orientation and, unless specified otherwise, the reduced primitive unit cell.

There are two ways to perform indexing depending on the setting of the /NOREDUCE qualifier described below. The normal method determines the reduced primitive unit cell, whose axis lengths must fall within the ranges specified in the input (if you don't know the axis lengths, specify large ranges). Following this method of autoindexing, you should run REFL_ARRAY / BRAVAIS to determine the correct Bravais lattice based on the metric symmetry of the reduced primitive cell; for example, if you have a centered lattice, /BRAVAIS will determine the parameters of the centered cell and will transform the reflection indices to the centered-cell indices. Following the Bravais lattice determination, you would then run REFL_ARRAY / LEASTSQ to refine the unit cell parameters, crystal orientation and detector positional corrections.

The second indexing method, used when /NOREDUCE is set, suppresses the conversion to the reduced primitive cell. In this case, the program looks for a solution which fits both the input axis length ranges AND the input cell angle ranges. The method can be useful, for example, for indexing a known centered unit cell directly on the centered lattice. Following indexing by this /NOREDUCE method, you will typically bypass the Bravais lattice step and run REFL_ARRRAY /LEASTSQ to refine the cell, orientation, etc. However, if you do use the Bravais lattice option after indexing by the /NOREDUCE method, be sure to specify the correct lattice type in the /BRAVAIS input panel. For example, if you index on a known C-centered lattice, but specify a P (primitive) input lattice in the /BRAVAIS panel, the Bravais lattice output will probably not be what you intended. This /NOREDUCE indexing method should be used ONLY when you're sure you already know the

correct unit cell, since it bypasses a very important step in the unit cell determination. Remember that errors in an initial determination of unit cell from a few precession pictures are fairly common—the normal indexing method followed by the Bravais lattice determination should always be used in early stages of a problem to check the initial choice of unit cell.

The Reflection Array can hold a maximum of 512 reflections; however, autoindexing and determination of orientation requires only a small fraction of this number. Usually, 25 reflections is the bare minimum you'll need, with 50–100 reflections about optimal. While determination of orientation from just a few contiguous frames is possible (for example, the FRAMBO and SADIE verification tests determine the orientation of a myoglobin crystal from eight contiguous frames), you'll get much more precise cell parameters if you threshold a few frames taken 90 degrees or so in scan angle from the first set, adding them to the Reflection Array prior to indexing.

If you can't obtain enough reflections with the C flag set, you can set this flag with the /MODIFY sub-command; however, the precision of the resulting cell parameters and orientation will not be as good as if centered reflections were used.

Autoindexing is performed with the algorithm developed by Sparks, operating on difference vectors derived from the input reflections. Difference vectors are classified into groups based on a specified input tolerance. Any group formed from fewer than $1 difference vectors (where $1 is specified on input as defined below) is ignored. Up to 100 such groups are used by the program. This is a very reliable indexing technique. If indexing on difference vectors fails, the program tries indexing on the full vectors; however, the difference vector approach is more reliable and if it fails, the full vector approach will seldom succeed. If for some reason, the program cannot find a solution, check for one of the following:

1. Prior to taking data on a new sample (including new flood-field and spatial corrections), make sure you have entered the correct sample-detector distance and correct X,Y beam center in the CONFIGURE /EDIT panel. (REFL_ARRAY /INDEX displays the current X,Y beam center coordinates in its input panel title bar for your review). Don't guess at the beam center; measure it from an image taken with after removing or repositioning the beam stop (make sure the direct beam is suitably attenuated before trying to record it or you could damage the detector!) The 0.060" aluminum cover plate shipped with the detector is good for this purpose with a sealed tube, or with a rotating anode run at low power setting (5 KW or less with 0.3 x 3mm filament and 0.3 mm collimator; less if your beam is larger). The ADD command is useful for accumulating a direct-beam image.

Always take another image WITH THE ALUMINUM COVER PLATE IN PLACE after replacing/repositioning the beam stop to make sure it is properly re-located. If you need to make positional adjustments, use the ADD command with realtime display enabled and a /RESET interval of 1 to a few seconds for coarse positioning. You may than want to take some longer frames to perform fine adjustments based on the background recorded immediately around the beam stop after removing the cover plate.

Remember, if your specified beam center coordinates are in error by more than half the smallest center-to-center spot spacing, the chances for mis-indexing increase substantially.

2. You must use the same flood-field correction for taking the data frames from which spots are extracted as for taking the fiducial plate image used as input to the spatial correction. Take the brass plate image AFTER the flood-field.
3. A good, recently determined spatial correction, computed from a fiducial-plate frame taken at the SAME distance as the frames from which the Reflection Array spots were obtained must be installed, preferably prior to thresholding frames to populate the Reflection Array.
4. When using frames written in XENGEN format by earlier versions of the software, the setting angles contained in the frame may not be correct. In particular, frames taken with phi scans on a 4-circle goniometer may be incorrectly interpreted as omega scans. The setting angles in the reflection array may thus show the scan angle in the OMEGA position instead of the PHI position, with the result that the sense of the scan angle will be reversed from its true direction (OMEGA is a right-handed rotation and PHI is left-handed). Autoindexing does not work correctly unless the sense of the scan angle is correct. If this problem occurs, use the /MODIFY sub-command to negate the scan angle values or to move the omega values into the phi field, then zero the omega values (see REFL_ARRAY /MODIFY). Frames written in XENGEN format by earlier versions of the software can contain zero for the swing angle. Again, you can use /MODIFY to insert the correct values in the Reflection Array.
5. Make sure you haven't used too low a threshold in the REFL_ARRAY /THRESHOLD command. The Reflection Array should contain the positions of strong spots, not those of high background points.

When invoked with the INDEX option from the REFL_ARRAY submenu or when run from the command line without arguments,

REFL_ARRAY /INDEX displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins refinement of the unit cell and orientation parameters; the ESC key or right mouse button returns you to the REFL_ARRAY submenu. You can interrupt autoindexing progress with the CTRL-BREAK key combination.

When autoindexing starts, the program displays the message “AUTOINDEXING...” on the bottom status line. Indexing should usually be completed within 10 to 30s. Upon completion, a scrolling output window is displayed containing the resulting output text. If logging is enabled (see LOGFILE) the contents of this window are also written to the logfile. When viewing the output, pressing ENTER or the left mouse button displays a pop-up menu of options, including export of ASCII data; for example, the contents of the window could be sent to a file or printer with this function. You can also move through the window contents with the page keys, arrow keys or with mouse motion. Pressing ESC or the right mouse button exits the output window, continuing with the REFL_ARRAY /INDEX command. This first output window contains the results of the indexing and reduced primitive unit cell determination, and is presented for review PRIOR to re-indexing the Reflection Array. It is described in more detail below. When you've reviewed the output and exited the window, following prompt is displayed.

RE-INDEX REFLECTION ARRAY: ARE YOU SURE? (Y OR ENTER=YES; N OR ESC=NO)

Press the Y key, the ENTER key or the left mouse button to write HKL indices into the reflections in the array and set the H flag of each reflection, otherwise press the N key, ESC key, or right mouse button to quit autoindexing and return to the REFL_ARRAY submenu without changing the Reflection Array.

If you've chosen to continue, the program updates the Reflection Array HKL indices and flags, then displays a second scrolling output window containing least-squares statistics related to the differences between observed and calculated HKL indices and scan angle, including histograms of the distributions of these differences. This is very similar to the output from REFL_ARRAY /LEASTSQ; but is derived from a relatively crude linear least squares and will show substantially larger deviations. It is described in more detail below. When you exit this second output window (with the ESC key or right mouse button), the program returns to the REFL_ARRAY submenu (to the BRAVAIS subcommand, since it's usually invoked next).

If REFL /INDEX was invoked from the command line, each output window is displayed subject to a 10 s timeout to allow command scripts to run without intervention. If you do not press a key or mouse button within 10 s after the output window is displayed, the program will continue as if

the ESC key had been pressed. Similarly, the prompt RE-INDEX REFLECTION ARRAY... described above will in that case time out after 10 s as if the ENTER key had been pressed.

8.16.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

/AAX=<n> .....(Expected A-Axis Length) [80.00]

A trial A-axis vector is accepted only if its length is in the range AAX * MAX(1-FCELL,0.01) to AAX * (1+FCELL). The allowed input range is 1-2500 Angstroms and the default value is 80 A. If you know the axis length, enter it here and make FCELL small, otherwise, make the best guess you can. You can use the CURSORS /VECTOR and CURSORS /CIRCLE commands to derive approximate unit cell axis lengths.

/BAX=<n> .....(Expected B-Axis Length) [80.00]

A trial B-axis vector is accepted only if its length is in the range BAX * MAX(1-FCELL,0.01) to BAX * (1+FCELL). The allowed input range is 1-2500 Angstroms and the default value is 80 A. If you know the axis length, enter it here and make FCELL small, otherwise, make the best guess you can. You can use the CURSORS /VECTOR and CURSORS /CIRCLE commands to derive approximate unit cell axis lengths.

/CAX=<n>..... (Expected C-Axis Length) [80.00]

A trial C-axis vector is accepted only if its length is in the range CAX * MAX(1-FCELL,0.01) to CAX * (1+FCELL). The allowed input range is 1-2500 Angstroms and the default value is 80 A. If you know the axis length, enter it here and make FCELL small, otherwise, make the best guess you can. You can use the CURSORS /VECTOR and CURSORS /CIRCLE commands to derive approximate unit cell axis lengths.

/U1=<n> ..... (Expected Alpha Cell Angle) [90.00]

Specifies the alpha unit cell angle in degrees when a known unit cell is assumed. This value is used ONLY when assuming a known unit cell; if ASSUME KNOWN UNIT CELL is specified as “N” on the input panel or /NOREDUCE is absent in command line mode, this value is ignored.

/U2=<n> ..... (Expected Beta Cell Angle) [90.00]

Specifies the beta unit cell angle in degrees when a known unit cell is assumed. This

value is used ONLY when assuming a known unit cell; if ASSUME KNOWN UNIT CELL is specified as “N” on the input panel or /NOREDUCE is absent in command line mode, this value is ignored.

/U3=<n> .....(Expected Gamma Cell Angle) [90.00]

Specifies the gamma unit cell angle in degrees when a known unit cell is assumed. This value is used ONLY when assuming a known unit cell; if ASSUME KNOWN UNIT CELL is specified as “N” on the input panel or /NOREDUCE is absent in command line mode, this value is ignored.

/FCELL=<n>.....(Axis Length Deviation) [0.75]

Specifies the fractional range of axis lengths which will be accepted for trial A,B, and C axis solutions. A trial axis vector is accepted only if its length is in the range AX * MAX(1-FCELL,0.01) to AX * (1+FCELL) where AX is one of the lengths specified above for /AAX, /BAX or /CAX. The allowed input range is 0.0-2.0 and the default value is 0.75. If you know the axis lengths, enter them as /AAX, /BAX, /CAX make FCELL small (for example, 0.1), otherwise, make the best guesses you can. You can use the CURSORS /VECTOR and CURSORS /CIRCLE commands to derive approximate unit cell axis lengths.

/SIGA=<n> ..... (Cell Angle Deviation) [0.1]

Specifies the fractional range of cell angles which will be accepted for trial solutions when a known unit cell is assumed. This value is used ONLY when assuming a known unit cell; if ASSUME KNOWN UNIT CELL is specified as “N” on the input panel or /NOREDUCE is absent in command line mode, this value is ignored.

A trial cell angle is accepted only if its length is in the range ANGLE * MAX(1-FCELL,0.01) to ANGLE * (1+FCELL) where ANGLE is one of the lengths specified above for /U1, /U2 or /U3. The allowed input range is 0.0-2.0 and the default value is 0.1.

/NOREDUCE..... (Assume Known Unit Cell (Y/N) ?) [No]

If specified as “Y” on the input panel, or as /NOREDUCE in command line mode, this qualifier suppresses the normal computation of the reduced primitive cell. Instead, the program attempts to find a solutions only for the input A, B, C, ALPHA, BETA, GAMMA values as described above. This is NOT recommended for general operation, since it bypasses a very important step in determination of the correct unit cell. However, in cases which are difficult to index, the additional constraints supplied by the known cell angles (used only when /NOREDUCE is in effect) may help, and in cases of

known cells with centered lattices, /NOREDUCE enables you to index on the centered lattice directly and bypass the extra Bravais lattice transformation step (again, NOT a good thing to do unless you're very sure that your input cell is the correct one).

/VERBOSE.....(Verbose Output (Y/N) ?) [Yes]

Specifies that “long-form” indexing output is desired. If this qualifier is set (i.e., “Y” in the input panel, or present on the command line), the first output window contains lists of the difference vectors and full vectors, and the second output window contains a reflection-by-reflection listing of observed versus calculated HKL's and scan angles; otherwise these lists are not written. The default in the input panel is “Y.”

$1 .....(Minimum # Vectors in Group) [2]

The small integer value you specify here determines how many difference vectors with nearly identical components must be found before the difference vectors will be included in the autoindexing. The vectors in any cluster which does not contain at least this number of difference vectors are ignored. The default of 2 should be satisfactory in most cases. If you supply a value of 1, every difference vector will be included in the calculations. As you specify higher values, you increase the confidence level that an observed group corresponds to a true reciprocal-lattice difference vector; however, you at the same time reduce the number of groups available for autoindexing. Valid range is 1–999; however, you'll want to stay at the lower end of this range.

/FGROUP=<n>..... (Length Fraction for Grouping) [0.3]

Specifies how closely the components of difference vectors must agree before they will be placed in the same group. Difference vectors which belong to the same group are averaged together, and the autoindexing is actually performed on the groups, not on the individual difference vectors. The value given here divided by the largest allowed unit cell axis length (computed from /AAX, /BAX, /CAX, and /FCELL below) represents the maximum allowed distance between the endpoints of two difference vectors (assuming they're at a common origin). If the distance between a difference vector endpoint and that of the current group average is larger than this value, it is not included in the group (and in fact starts a new group). If the distance is within this limit, the difference vector is averaged into the group. The default of 0.3 should be satisfactory in most cases; that is, if two difference vector endpoints are identical within about 1/3 of the

shortest possible difference vector, they are included in the same group.

/HKLTOL=<n> .....(Fractional HKL Deviation) [0.1]

Difference vector groups whose calculated HKL indices are integers within this specified tolerance are considered to be “fit” by the current axial vector solution. For each difference vector group, the difference between H, K, or L index calculated from the trial axis vector solution and the nearest integer to that index is computed. If the absolute value of the difference is within the /HKLTOL value, the solution fits that difference vector group. In order for an axis-vector solution to be accepted, it must fit at least FFIT * N difference vector groups, where FFIT is described below, and N is the total number of difference vector groups included in the indexing. The default value of 0.1 should be suitable in most cases, although if you have large unit cell axis lengths (say, > 250 A), you may want to increase it, for example, to 0.2. Valid input range is 0-1, although it is not a good idea to increase this parameter to much above 0.25.

/FFIT=<n> .....(Fraction which must be fit) [0.8]

A trial axis vector is accepted only if the number of difference groups it fits is at least FFIT * N where FFIT is the value specified here and N is the total number of difference vector groups included in the indexing. The default value of 0.8 should be suitable in most cases. If the program cannot find a solution and you've checked the spatial correction, beam center, etc. as described above, you might try decreasing this number (e.g., to 0.7). Valid input range is 0-1, but if you have to reduce this number to 0.5 or lower to find a solution, something is wrong.

8.16.2 Autoindexing Output

Two examples of the output from REFL_ARRAY /INDEX is shown below. Both have the /VERBOSE qualifier set. Example 1 is the first output window from indexing of the eight myoglobin test frames. If you're familiar with Bruker's scintillation counter software, this output is similar. The indexing was performed with 26 “centered” reflections extracted with a /THRESHOLD subcommand, as performed by the FVERIFY.SLM test sequence supplied with the program; however, the indexing here was performed specifying /AAX=90 /BAX=90 /CAX=45 /FCELL=0.1. The output and indexing time in this case are significantly shorter than those obtained in the test sequence, which specifies /AAX=80 /BAX=80 /CAX=80 /FCELL=0.75.

The first output line contains the axis length limits in Angstroms used to filter trial axis vector solutions in the order minimum, maximum A; minimum, maximum B; minimum, maximum C; followed by the maximum HKL difference vector

index used to compute test solutions. These values are computed from the input /AAX /BAX /CAX and /FCELL.

Next is a list of the trial axis vector solutions. Each record consists of two or more lines. The first line contains the solution number, the axis length in angstroms, a figure of merit (actually a residual—lower values are better) indicating the rms deviation from integer HKL indices calculated from the solution combined with a measure of the vector length, three integers which define the direction of the axis (this is the integer triple described by Sparks in Computational Crystallography, D. Sayre, ed., Oxford (1982) pp. 1–18), and a bit mask containing a 1 for each difference vector group which is fit by the solution and a 0 for each group that is not fit. The first line holds mask elements for up to 50 groups; if the number of groups is larger, the mask is continued on the second line immediately below the first 50 elements.

Starting at the second line of each record (the third if the bit mask requires a second line) is a list of angles between the solutions. The numbers are in degrees, with the first number in the list representing the angle from the current solution to solution #1; the second, to solution #2, and so on. Angles near 90 degrees are highlighted with a trailing “*”; angles near 60 or 120 degrees, with a “#”.

Following the list of axis vectors is the chosen triple of solutions for the three crystallographic axes, derived from the three non-coplanar axis vectors with best (lowest) figures-of-merit. The shortest solutions with good integerness of calculated HKL indices have the best figures-of-merit. In addition to the solution number and length of each axis chosen, the XYZ components of each axis vector are displayed.

If the program was not able to find an acceptable set of three solutions from its first group of trial solutions (generated from a basis set consisting of the three shortest non-coplanar difference vector groups), the output will contain the message

RETRYING WITH NEXT SHORTEST VECTOR

followed by another listing of axis vector solutions. If you see this message (even several occurrences of it) followed by successful indexing, it is no cause for concern. If necessary, the program continues to step through the difference vector groups generating trial solutions from a new basis set of three such groups until a solution is found or until the number of groups has been exhausted. If this occurs, the output will contain the lines

INDEXING FAILED ON DIFFERENCE VECTORS

RE-TRYING WITH FIRST 100 FULL VECTORS

and a final attempt at indexing on the full vectors is made.

Following the axis vector solution, a unit cell reduction by the method of Buerger is performed. The output contains the resulting reduced primitive unit cell, with parameters in the order A,B,C (Angstroms), ALPHA, BETA, GAMMA (degrees).

If verbose output has been specified, a list of the difference vector groups follows. A line for each group contains the group number, its length in Angstroms, its reciprocal-lattice components, and the number of difference vectors in the group.

A linear least squares is then performed to refine the parameters of the reduced primitive cell with, the refined parameters displayed in the same order, followed by the unit cell volume in cubic Angstroms). These values and their standard deviations are automatically transferred to the /BRAVAIS sub-command input panel, for subsequent determination of the /BRAVAIS lattice based on the metric symmetry of the reduced primitive cell.

If verbose output was specified, the least squares result is followed by a list of the input full vectors with their calculated HKL indices. A line for each vector contains the vector number, the number of the vector closest to it (i.e., the one which yielded the smallest difference vector), the calculated HKL indices expressed as real numbers (if these values are not close to being integers, something is wrong; most should be within 0.1 of an integer value), and the corresponding reciprocal lattice vector components.

Example 2 below is sample output from the same indexing run displayed in the second output window following re-indexing of the Reflection Array. The output results from a rough linear least-squares refinement of the reduced primitive unit cell to the indexed full vectors. It is similar to the output produced by REFL_ARRAY / LEASTSQ, although the refinement will not be as precise.

First are several tabular histograms, showing the distribution of the unsigned differences between observed and calculated values of H,K,L, scan angle (always labeled OMEGA, even if the scan angle was actually PHI), and detector X,Y position. In all cases, the more closely bunched toward the left side of the histogram the differences are, the better the refinement. Scan angle differences are in degrees, and X,Y differences are in pixels. Following the histograms are the overall average and rms differences for these same quantities, H,K,L, scan angle, X, and Y. The myoglobin example shown below is a very good one. Often the numbers are two or three times higher. The AVG values indicate any systematic bias in the results. Unlike the case for REFL_ARRAY /LEASTSQ, the AVG values will probably be significant here; however if they are large compared with the corresponding RMS values, you might suspect mis-indexing or misalignment of the system. In such a case, make

sure you have a good spatial correction and correct estimates for the detector distance and beam center entered in the CONFIGURE /EDIT panel.

Following the overall statistics is a reflection-by-reflection summary of the agreement for each reflection in the reflection array. Each record consists of two lines, the first containing the reflection as it's entered in the reflection array (i.e., the “observed” values), and the second containing the differences for HKL, scan angle (always converted into omega rotation) and detector X,Y with the sense OBSERVED - CALCULATED. This output shows both those reflections included in the least squares, and those not included (for example, reflections without the C flag set). It also shows computed HKL indices for reflections which do not have the H flag set. It does not include reflections which do not have the A flag set, since there are many possible combinations of setting angles and detector X,Y which could correspond to given HKL indices.

The two example outputs follow (neither case assumes a known unit cell):

Example 8.2 - Output from indexing of 8 Myoglobin Test Frames, prior to re-indexing the Reflection Array

```
Axis limits, max index:    81.000  99.000  81.000  99.000  40.500  49.500   13

 #   Length    FOM   H 1H 2H 3 Reflections fit
Angles between solutions

 1   46.159    0.01    1   1   0     1111111111111111

 2   92.542    0.01    0   1   1     1111111111111111
 89.4*

 3   92.318    0.02    2   2   0     1111111111111111
  0.0  89.4*

 4   91.833    0.01    1   1   2     1111111111111111
 90.0*119.6# 90.0*

 5   92.707    0.03    1   2   3     1111111111111111
 89.4* 59.4# 89.4* 60.2#

Predicted reduced primitive axes are:
Soln#        X             Y             Z          Length
  4      -87.10253   -29.05033    -1.61254    91.83340
  2      -68.84866    61.83576    -0.53702    92.54236
  1        0.90663    -0.11663   -46.14998    46.15903

Reduced primitive cell is:
   91.833    92.542    46.159    89.398    89.984    60.372

Difference Vectors:
   #       Length          X1          X2          X3    Freq
   1    40.05527    -0.00803    -0.00913    -0.02180    2
   2    32.87223    -0.00410    -0.02093    -0.02170    2
   3    30.28461    -0.01281    -0.03043    -0.00017    2
   4    25.39675    -0.01247    -0.03035    -0.02177    2
   5    22.04425    -0.01167     0.00270    -0.04375    2
```

6	18.34492	-0.01719	-0.05173	-0.00059	2
7	18.29090	-0.00113	-0.03306	0.04353	2
8	17.00628	-0.01710	-0.05170	-0.02218	2
9	16.32388	-0.00953	-0.04254	0.04304	2
10	14.31518	-0.01803	-0.05208	0.04292	2
11	13.87408	-0.02895	-0.04912	-0.04410	2
12	12.60927	-0.02206	-0.07317	0.02118	2
13	11.18752	-0.03342	-0.07032	-0.04390	2
14	9.18217	-0.03102	-0.08251	0.06396	2
15	9.03692	-0.01905	-0.00642	-0.10882	2
16	7.90768	-0.01505	-0.06411	0.10796	2

Least squares cell parameters:

92.865	91.946	46.174	89.264	89.442	59.640	340159.50

Full vectors:

#	NEAR	H	K	L	X1	X2	X3
1	9	-8.99	6.99	7.99	-0.04561	-0.16710	-0.17374
2	20	-5.99	6.01	5.98	-0.02503	-0.12757	-0.12977
3	21	-9.98	10.99	-2.99	-0.04181	-0.22498	0.06442
4	20	-7.01	8.99	1.99	-0.02324	-0.17308	-0.04331
5	15	-9.98	9.99	4.99	-0.04328	-0.21235	-0.10873
6	26	-13.00	9.00	9.00	-0.07110	-0.22841	-0.19636
7	3	-11.01	11.99	-1.00	-0.04587	-0.24611	0.02100
8	7	-13.00	13.00	-0.01	-0.05838	-0.27656	-0.00078
9	2	-9.01	7.99	7.02	-0.04215	-0.17936	-0.15221
10	24	-8.02	9.02	-5.00	-0.03361	-0.18313	0.10781
11	26	-12.99	11.00	5.99	-0.06419	-0.25246	-0.13093
12	14	-18.00	14.00	3.02	-0.09522	-0.33492	-0.06701
13	10	-10.99	9.99	-7.01	-0.05529	-0.22290	0.15082
14	11	-15.00	12.98	4.00	-0.07382	-0.29497	-0.08783
15	4	-7.99	9.00	4.01	-0.03086	-0.18211	-0.08697
16	13	-16.01	11.00	-9.01	-0.09371	-0.28161	0.19354
17	11	-14.00	10.99	7.00	-0.07223	-0.26154	-0.15278
18	6	-15.00	9.99	9.00	-0.08397	-0.25896	-0.19665
19	0	-5.00	7.01	-3.01	-0.01564	-0.13087	0.06517
20	19	-6.00	8.00	2.01	-0.01865	-0.15188	-0.04339
21	10	-8.99	9.99	-4.01	-0.03773	-0.20412	0.08625
22	4	-9.97	11.00	2.02	-0.04029	-0.22467	-0.04399

23	12	-19.00	14.00	4.00	-0.10323	-0.34409	-0.08877
24	19	-7.99	9.99	-1.98	-0.02880	-0.19450	0.04293
25	16	-21.98	13.99	-6.00	-0.13114	-0.37279	0.12776
26	5	-12.02	10.02	7.01	-0.05949	-0.23122	-0.15272

Example 8.3 - Output from indexing of 8 Myoglobin Test Frames, after reindexing the Reflection Array (Truncated)

Histograms:

	.00	.05	.10	.15	.20	.25	.30	.35	.40	.45	+Inf
H	26	0	0	0	0	0	0	0	0	0	0
K	26	0	0	0	0	0	0	0	0	0	0
L	26	0	0	0	0	0	0	0	0	0	0
Omega	26	0	0	0	0	0	0	0	0	0	0

	0.00	0.25	0.50	0.75	1.00	1.25	1.50	1.75	2.00	2.25	+Inf
X	20	6	0	0	0	0	0	0	0	0	0
Y	20	5	1	0	0	0	0	0	0	0	0

	H	K	L	Omega	X	Y
AVG	0.001	-0.002	0.001	-0.002	0.039	0.038
RMS	0.010	0.011	0.009	0.017	0.215	0.227

#	Flags	H	K	L	2-Theta	Omega	Phi	Chi	X	Y	Inorm	I/Sig
1	ACHS	-9	7	8	-30.000	-0.271	0.000	0.000	82.85	51.23	626.60	112
		-.01	-.01	+.02		0.006			0.00	0.40		
2	ACHS	-6	6	6	-30.000	-0.443	0.000	0.000	33.26	99.06	467.95	97
		+.00	-.02	+.02		-0.016			0.23	0.64		
3	ACHS	-10	11	-3	-30.000	-0.448	0.000	0.000	142.13	309.54	344.28	83
		-.01	+.00	+.00		-0.006			-0.22	-0.06		

.
.
.
etc.

8.17 Peaks > Refl. Array > Bravais • Determine Bravais lattice and perform HKL transformations

Menu Command: Peaks > Refl. Array > Bravais

Accelerator: Ctrl+B

User Level: 1

SLAM Syntax:

> REFL_ARRAY /BRAVAIS $1 $2 $3 $4 $5 $6 $7 /SIGA=<n> /SIGB=<n> /SIGC=<n> /SIGMA=<n> /SIGBEST=<n>

REFL_ARRAY /BRAVAIS determines possible Bravais lattices corresponding to the specified input unit cell parameters and standard deviations, based strictly on the metric symmetry. Possible solutions are ranked according to degree of symmetry and a goodness-of-fit. The highest-symmetry solution whose goodness-of-fit is better than an input threshold is flagged as the most likely solution. You can accept that solution or one of the other possible solutions, in which case the reflections in the Reflection Array will be automatically re-indexed according to the selected unit cell.

Normally, you will invoke this command immediately after autoindexing the Reflection Array with the REFL_ARRAY /INDEX command. REFL_ARRAY /INDEX automatically stores its resulting reduced primitive unit cell parameters and their standard deviations in the /BRAVAIS input panel, and you can usually invoke /BRAVAIS without changing any of the input panel values.

The goodness-of-fit is a measure of how well a trial Bravais lattice fits the input unit cell parameters. Lower values are better. The scale is arbitrary (this is NOT a true least-squares goodness-of-fit; don't expect values near 1), but in general good solutions will have values less than 10. The input panel allows you to set two different thresholds on the goodness-of-fit. The first is the threshold below which a solution is listed in the output. The second is the threshold below which a solution can be flagged as the “best” solution. The highest symmetry solution whose goodness-of-fit is below this second threshold is marked as the best solution. The default values are 20 and 6 respectively for these thresholds, and they should work well in most cases.

The possible Bravais lattices determined by the program are:

Program Output	Description
CUBIC F	Face-centered cubic
CUBIC I	Body-centered cubic
CUBIC P	Primitive cubic
RHOMBOHEDRAL (OBV);	
HEXAGONAL R SETTING	Rhombohedral on hexagonal axes
TRIGONAL P (NO C-AXIS SYMMETRY);	
HEXAGONAL P (C-AXIS SYMMETRY)	Trigonal/hexagonal
TETRAGONAL I	Body-centered tetragonal
TETRAGONAL P	Primitive tetragonal
ORTHORHOMBIC F	Face-centered orthorhombic
ORTHORHOMBIC I	Body-centered orthorhombic
ORTHORHOMBIC C	C-centered orthorhombic
ORTHORHOMBIC P	Primitive orthorhombic
MONOCLINIC C	C-centered monoclinic
MONOCLINIC P	Primitive monoclinic
TRICLINIC P	Primitive triclinic

If for some reason you need to use a different, non-standard setting, you can use REFL_ARRAY /TRANSFORM to transform the HKL indices in the reflection array prior to running the /LEASTSQUARES sub-command.

When invoked with the BRAVAIS option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /BRAVAIS displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins refinement of the unit cell and orientation parameters; the ESC key or right mouse button returns you to the REFL_ARRAY submenu.

When refinement starts, the program displays the message “PERFORMING LATTICE SEARCH” on the bottom status line. The determination should usually be completed within a second or two. Upon completion, a scrolling output window is displayed containing the resulting output text. If logging is enabled (see LOGFILE) the contents of this window are also written to the logfile. When viewing the output, pressing ENTER or the left mouse button displays a pop-up menu of options, including export of ASCII data; for example, the contents of the window could be sent to a file or printer with this function. You can also move through the window contents with the page keys, arrow keys or with mouse motion. Pressing ESC or the right mouse button exits the output window, continuing with the /BRAVAIS sub-command. The output is described in more detail below.

After you exit the output window, an input window appears requesting you to enter the solution number of the Bravais lattice you want to use, with a default value corresponding to the solution labelled as “best” (that solution is preceded in the output window by the characters “>>>”). If you enter a non-zero solution number,

pressing the ENTER key or left mouse button selects the input solution number, and re-indexes the reflections in the Reflection Array to correspond to the selected Bravais lattice, then returns to the REFL_ARRAY submenu with the LEASTSQ option highlighted (since that's usually the next operation). If you enter a solution number of zero and press ENTER or the left button, the program returns to the submenu without re-indexing the array. Pressing ESC or the right mouse button in the input window returns you to the /BRAVAIS scrollable output window for reviewing the output prior to selecting a solution.

If REFL /BRAVAIS was invoked from the command line, the output window is displayed subject to a 10 s timeout to allow command scripts to run without intervention. If you do not press a key or mouse button within 10 s after the output window is displayed, the program will continue as if the ESC key had been pressed. In command line mode, the “best” solution is always selected—no second input window is displayed for selecting a solution number.

8.17.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Lattice Type) [P]

Usually the unit cell parameters you supply in this input panel correspond to the reduced primitive cell determined by REFL_ARRAY /INDEX, which are automatically transferred from /INDEX to the /BRAVAIS input panel. While you'll normally use the default input panel values set up be the /INDEX sub-command, you can also perform Bravais lattice determination by directly entering unit cell parameters on the input panel. If you know that the parameters you enter here correspond to a non-primitive lattice, enter the known lattice type here. Valid types are:

P: Primitive

A: A-centered

B: B-centered

C: C-centered

I: Body-centered

F: Face-centered

R: Rhombohedral

If you change this entry, it is a good idea to reset it to P when you exit. The /INDEX subcommand does NOT automatically update this item when it exits. The default is P.

$2 ..... (Current A Axis Length) [10.0]

Specifies the A-axis length in Angstroms of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the

reduced primitive cell when you run /INDEX. Default is 10. Valid input range is 1 to 2500.

$3 .....(Current B Axis Length) [10.0]

Specifies the B-axis length in Angstroms of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 10. Valid input range is 1 to 2500.

$4 .....(Current C Axis Length) [10.0]

Specifies the C-axis length in Angstroms of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 10. Valid input range is 1 to 2500.

$5 .....(Current Alpha Cell Angle) [90.0]

Specifies the ALPHA unit cell angle in degrees of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 90. Valid input range is 0 to 179.

$6 ..... (Current Beta Cell Angle) [90.0]

Specifies the BETA unit cell angle in degrees of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 90. Valid input range is 0 to 179.

$7 ..... (Current Gamma Cell Angle) [90.0]

Specifies the GAMMA unit cell angle in degrees of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 90. Valid input range is 0 to 179.

/SIGA=<n> ..... (Standard Deviation of A) [0.03]

Specifies the A-axis standard deviation in Angstroms of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 0.03. Valid input range is 0 to 999.

/SIGB=<n> .....(Standard Deviation of B) [0.03]

Specifies the B-axis standard deviation in Angstroms of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 0.03. Valid input range is 0 to 999.

/SIGC=<n> .....(Standard Deviation of C) [0.03]

Specifies the C-axis standard deviation in Angstroms of the input unit cell to be tested for correspondence with other lattices. This item is automatically filled in with the value from the reduced primitive cell when you run /INDEX. Default is 0.03. Valid input range is 0 to 999.

/SIGMA=<n> .....(Max Sigmas for any SOLN) [20]

Solutions with goodness-of-fit below this value are listed in the output window. Those with goodness-of-fit above the value are rejected. The default of 20 should be satisfactory for most purposes. Valid input range is 0 to 999.

/SIGBEST=<n> .....(Max Sigmas for best SOLN) [6]

Solutions with goodness-of-fit below this value are candidates for the “best” solution, indicated in the output window with the characters “>>>”. The highest-symmetry solution with goodness-of-fit below this value is flagged as the “best” solution. The default of 6 should be satisfactory for most purposes. Valid input range is 0 to 999.

8.17.2 Bravais Lattice Output

An example of the /BRAVAIS output window contents is shown below in EXAMPLE 1. It contains a summary of the values on the input panel followed by the number of solutions found with goodness-of-fit within the /SIGMA threshold. Next is a list of the solutions. Solutions are grouped according to lattice type, with each group preceded by a line containing one of the Bravais lattice types listed above. Higher-symmetry Bravais lattices are listed before those with lower symmetry. Each solution is displayed on two lines. The first line contains the solution number, its goodness-of-fit (labeled #SIG), its unit cell parameters in the order A, B, C (Angstroms), alpha, beta, gamma (degrees). The second line contains the rows of the 3 x 3 transformation matrix which would transform the HKL indices from the input lattice to the lattice corresponding to the solution. The rows are separated by slashes; thus, using the standard mathematical convention, the nine elements on the third line are in the order T11,T12,T13/ T21,T22,T23/ T31,T32,T33. If you stack these rows above one another (the first row on top), the resulting matrix will pre-multiply a column

HKL vector in the input cell to give a column
HKL vector in the new cell.

Example 8.4 - Bravais Lattice Output for Myoglobin Test Data

```
#Sigmas for acceptance of any soln, best soln:      20.0       6.0
Input lattice type:  P
Input cell and standard deviations:
      92.865  91.946  46.174  89.264  89.442  59.640   340159.50
       0.476   0.494   0.036

Number of solutions =   14

     #   #Sig    A            B            C          Alpha       Beta        Gamma
TRIGONAL P (NO C-AXIS SYMMETRY); HEXAGONAL P (C-AXIS SYMMETRY)
>>> 1   2.98    91.906      91.946     46.174    90.736      89.827      119.323
 -1.00   1.00   0.00/        0.00      -1.00      0.00/        0.00        0.00     1.00/

ORTHORHOMBIC C
     2   2.55    92.865     158.674    46.174    90.527      90.558      89.971
 -1.00   0.00   0.00/        1.00       -2.00      0.00/        0.00        0.00     1.00/

     3   2.98    91.906     160.341    46.174    89.255      89.827      90.661
  1.00  -1.00   0.00/       -1.00      -1.00      0.00/        0.00        0.00    -1.00/

     4   3.02    91.946     160.272    46.174    89.776      90.736      90.689
  0.00  -1.00   0.00/        2.00      -1.00      0.00/        0.00        0.00     1.00/

MONOCLINIC C
     5   1.31   158.674     92.865      46.174    89.442      90.527      90.029
  1.00  -2.00   0.00/        1.00       0.00       0.00/        0.00        0.00     1.00/

     6   1.72    91.946     160.272    46.174    90.224      90.736      89.311
  0.00   1.00   0.00/        2.00      -1.00      0.00/        0.00        0.00    -1.00/

     7   1.74   160.341     91.906      46.174    89.827      90.745      89.339
  1.00   1.00   0.00/        1.00      -1.00      0.00/        0.00        0.00    -1.00/

     8   2.19    92.865     158.674    46.174    90.527      90.558      89.971
 -1.00   0.00   0.00/        1.00       -2.00      0.00/        0.00        0.00     1.00/
```

```
    9  2.45   91.906   160.341    46.174   89.255     90.173     89.339
 1.00 -1.00   0.00/      1.00       1.00     0.00/       0.00       0.00    1.00/

   10  2.96  160.272    91.946    46.174   90.736     90.224     89.311
-2.00  1.00   0.00/      0.00      -1.00     0.00/       0.00       0.00    1.00/

MONOCLINIC P
   11  2.55   91.906    46.174    91.946   90.736    119.323     89.827
 1.00 -1.00   0.00/      0.00       0.00    -1.00/       0.00       1.00    0.00/

TRICLINIC P
   12  0.00   46.174    91.906    91.946   60.677     89.264     89.827
 0.00  0.00  -1.00/      1.00      -1.00     0.00/       0.00      -1.00    0.00/

   13  2.62   46.174    91.906    92.865  120.317     90.558     90.173
 0.00  0.00  -1.00/     -1.00       1.00     0.00/       1.00       0.00    0.00/

   14  2.62   46.174    91.946    92.865   59.640     89.442     89.264
 0.00  0.00  -1.00/      0.00      -1.00     0.00/      -1.00       0.00    0.00/
```

8.18 Peaks > Refl. Array > LeastSq • Determine orientation and refined cell parameters

Menu Command: Peaks > Refl. Array > LeastSq

Accelerator: Ctrl+L

User Level: 1

SLAM Syntax:

> REFL_ARRAY /LEASTSQ $1 $2 $3 $4 $5 $6 $7 /DXC=<n> /DYC=<n> /DISTANCE=<n> /ROLL=<n> /YAW=<n> /U1=<n> /U2=<n> /U3=<n> /HKLTOL=<n> /HALFWIDTH=<n> /MASK=<n> /PARNAME=<n>

REFL_ARRAY /LEASTSQ determines and refines the crystallographic orientation matrix, unit cell parameters, and detector positional corrections given a valid list of indexed x-ray spots in the Reflection Array. Its output contains the orientation matrix, the refined parameters and their standard deviation, refinement and agreement statistics, and a reflection-by-reflection list of observations versus least-squares calculated values.

Usually, the reflection array will have been populated through a previous REFL_ARRAY /THRESHOLD or /PICK, followed by REFL_ARRAY /AUTOINDEX to index the array, then REFL_ARRAY /BRAVAIS to determine the Bravais lattice and perform any required transformation of HKL indices. (However, all of this can be done only after you have a good spatial correction computed, and accurate values for the detector distance and X,Y beam center stored in the CONFIGURE /EDIT input panel). This leaves the array in a state where least squares can be performed.

The Reflection Array can hold a maximum of 512 reflections; however, determination of orientation requires only a small fraction of this number. Usually, 25 reflections is the bare minimum you'll need, with 50–100 reflections about optimal. While determination of orientation from just a few contiguous frames is possible (for example, the FRAMBO and SADIE verification tests determine the orientation of a myoglobin crystal from eight contiguous frames), you'll get much more precise cell parameters if you threshold a few frames taken 90 degrees or so in scan angle from the first set, adding them to the Reflection Array prior to indexing.

The least squares can incorporate crystal-system constraints if desired. By default, the program performs a quick linear least squares (of the type used in the P3 program) which determines unit cell parameters and orientation, but doesn't refine any of the detector positional corrections or apply constraints. The result (coupled with guesses of zero for the small detector positional corrections) is used as an initial guess for a nonlinear refinement which incorporates detector positional corrections and constraints. While crystal-system constraints are useful if you want to obtain the best unit cell parameters,

you should usually NOT use constraints to determine the matrix to be used for data collection or data reduction; the unconstrained matrix is usually better for this purpose. The default is unconstrained refinement.

When invoked with the LEASTSQ option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /LEASTQ displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins refinement of the unit cell and orientation parameters; the ESC key or right mouse button returns you to the REFL_ARRAY submenu. You can interrupt a refinement in progress with the CTRL-BREAK key combination; however, the current orientation matrix (e.g., for use by the CURSORS commands for computing HKL indices) at that point is undefined.

When refinement starts, the program displays the message “REFINING...” on the bottom status line. Refinement should usually be completed within 10 or 15s. Upon completion, a scrolling output window is displayed containing the resulting output text. If logging is enabled (see LOGFILE) the contents of this window are also written to the logfile. When viewing the output, pressing ENTER or the left mouse button displays a pop-up menu of options, including export of ASCII data; for example, the contents of the window could be sent to a file or printer with this function. You can also move through the window contents with the page keys, arrow keys or with mouse motion. Pressing ESC or the right mouse button exits the output window, returning you to the REFL_ARRAY submenu. The output is described in more detail below.

If REFL /LEASTSQ was invoked from the command line, the output window is displayed subject to a 10 s timeout to allow command scripts to run without intervention. If you do not press a key or mouse button within 10 s after the output window is displayed, the program will continue as if the ESC key had been pressed.

Upon completion, the program updates the values in the input panel to their refined values (which you'll see if you re-run REFL /LEASTSQ, for example, to apply a different set of constraints.)

8.18.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (LSQRS/Constraint Type (0-9)) [1]

Specifies the type of crystal-system constraints to be applied. Types are:

0—Perform only the linear least squares; don't proceed with non-linear refinement

1—Linear least squares followed by unconstrained non-linear refinement

2—Linear least squares followed by non-linear refinement with monoclinic-C constraints (alpha=beta=90)

3—Linear least squares followed by non-linear refinement with monoclinic-B constraints (alpha=gamma=90)

4—Linear least squares followed by non-linear refinement with monoclinic-A constraints (beta=gamma=90)

5—Linear least squares followed by non-linear refinement with orthorhombic constraints (alpha=beta=gamma=90)

6—Linear least squares followed by non-linear refinement with tetragonal constraints (A=B, alpha=beta=gamma=90)

7—Linear least squares followed by non-linear refinement with trigonal/hexagonal constraints (A=B, alpha=beta=90, gamma=120)

8—Linear least squares followed by non-linear refinement with rhombohedral constraints (A=B=C, alpha=beta=gamma)

9—Linear least squares followed by non-linear refinement with cubic constraints (A=B=C, alpha=beta=gamma=90)

If you negate constraint type 1–9, the preceding linear least squares is suppressed, and initial guesses are obtained directly from the values in the input panel. This might save a few seconds if you're re-running the previous least-squares (which updated the input panel parameters to their refined values on previous exit) with a different constraint type.

The default, 1, should be satisfactory for most purposes.

$2 ..... (A Axis Length) [10.0]

Initial guess for the A-axis length in Angstroms on entry, updated to the refined value on exit. Note that if the constraint type ($1) is 1–9, the value you start with here doesn't matter, since the program will perform a linear least squares to compute initial guesses for refinement. Valid range is 1-9999 Angstroms.

$3 ..... (B Axis Length) [10.0]

Initial guess for the B-axis length in Angstroms on entry, updated to the refined value on exit. (See comments for $2 above).

$4 ..... (C Axis Length) [10.0]

Initial guess for the C-axis length in Angstroms on entry, updated to the refined value on exit. (See comments for $2 above).

$5 ..... (Alpha Cell Angle) [90.0]

Initial guess for the alpha unit cell angle in degrees on entry, updated to the refined

value on exit. Valid range is 1–179 degrees. (See comments for $2 above).

$6 .....(Beta Cell Angle) [90.0]

Initial guess for the beta unit cell angle in degrees on entry, updated to the refined value on exit. Valid range is 1–179 degrees. (See comments for $2 above).

$7 .....(Gamma Cell Angle) [90.0]

Initial guess for the gamma unit cell angle in degrees on entry, updated to the refined value on exit. Valid range is 1–179 degrees. (See comments for $2 above).

/DXC=<n> .....(X Beam Center Correction) [0.0]

Initial guess for the CORRECTION to the detector beam center X-coordinate in pixels. Zero is usually a good value. Note that if the constraint type ($1) is 1–9, the value you start with here doesn't matter, since the program will set the initial guesses for the detector positional corrections to zero when it performs the linear least squares. This entry is updated with its refined value on exit. Valid range is -256 to 256.

/DYC=<n> .....(Y Beam Center Correction) [0.0]

Initial guess for the CORRECTION to the detector beam center X-coordinate in pixels. Zero is usually a good value. (See comments for /DXC above).

/DISTANCE=<n> .. (Detector Distance Correction) [0.0]

Initial guess for the CORRECTION to the detector distance in CM. Zero is usually a good value. Valid range is -10 to 10 CM. (See comments for /DXC above).

/ROLL=<n>..... (Detector Roll Angle) [0.0]

Initial guess for the detector roll angle in degrees. Zero is usually a good value. Roll is defined as right-handed rotation of the detector about the goniometer X-axis (the direct beam axis) when the swing angle is zero. At zero roll, the detector Y-axis is parallel to the goniometer Z-axis. Valid range is -60 to 60 degrees. (See comments for /DXC above).

/YAW=<n> ..... (Detector Yaw Angle) [0.0]

Initial guess for the detector yaw angle in degrees. Zero is usually a good value. Yaw is defined as right-handed rotation about the detector Y-axis (the vertical axis). At zero yaw, the detector X-axis is parallel to (but reversed in direction from) the goniometer Y-axis. Valid range is -60 to 60 degrees. (See comments for /DXC above).

/U1=<n> .....(1st U-Matrix Eulerian Angle) [0.0]

Initial guess for the first Eulerian angle in degrees. The Eulerian angles define the orientation of the crystal axes relative to the goniometer XYZ axes when the goniometer angles have been driven to zero. They define the unitary component of the orientation matrix (i.e., they define the U matrix in Busing and Levy's terminology). The first Eulerian angle is a rotation about Z (analogous to the omega angle on a 4-circle goniometer); the second is a rotation about X' (analogous to chi), and the third is a rotation about Z'' (analogous to phi). Note that if the constraint type ($1) is 1–9, the value you start with here doesn't matter, since the program will get the initial guesses for the Eulerian angles from the linear least squares. This entry is updated with its refined value on exit. Valid range is -360 to 360 degrees.

/U2=<n> .....(2nd U-Matrix Eulerian Angle) [0.0]

Initial guess for the second Eulerian angle in degrees. (See comments for /U1 above).

/U3=<n> .....(3rd U-Matrix Eulerian Angle) [0.0]

Initial guess for the third Eulerian angle in degrees. (See comments for /U1 above).

/HKLTOL=<n>..... (Max Allowed HKL Deviation) [0.25]

When the least squares is begun, a comparison between the HKL values in the reflection array and HKL's computed based on the setting angles and detector X,Y is made for each reflection. Any reflection with a calculated index which deviates from the value in the array by more than the tolerance specified here is removed from the least squares, by clearing its H flag. The following prompt is issued when any reflections are outside the tolerance (where <n> is the number of reflections removed):

<n> REFLECTION(S) REMOVED FROM LS (OUTSIDE HKL TOL)

--PRESS ENTER TO CONTINUE, ESC TO QUIT

Pressing ENTER or the left mouse button continues with the refinement; pressing ESC or the right mouse button returns you to the REFL_ARRAY submenu (however, the H flags of the out-of-tolerance reflections remain cleared; you can restore them with a /MODIFY command). If the command was started from a script or from the command line, this prompt will time out in 10s (if it receives no response before then) assuming an ENTER response, to allow scripts to run without intervention.

The default of 0.25 should be satisfactory in most cases. Valid range is 0.1 to 999; this quantity is dimensionless.

/HALFWIDTH=<n>(Frame Halfwidth) [0.125]

Specifies half the scan width per frame in degrees (on average) of the frames from which the records in the reflection array were extracted. This value is used to determine the weighting of observed X,Y positions versus that of observed scan angle in the least squares. That is, the non-linear least squares minimizes the residual

sum[Wxy * (Xobs-Xcalc)^2 + Wxy * (Yobs-Ycalc)^2 + Wz * (Zobs-Zcalc)^2]

where Xobs and Xcalc are the observed and calculated detector X, Yobs and Ycalc are the observed and calculated detector Y, and Zobs and Zcalc are the observed and calculated scan angle for each spot. The relative weights Wxy and Wz are determined according to:

Wxy = 1./(Exy)^2 and Wz = 1./(0.5 * H)^2

where Exy is an estimate of the positional standard deviation of a reflection and H is the frame halfwidth specified here (0.25 of the frame width appears to be a fair estimate for the expected rms error in scan angle).

A smaller value for the halfwidth will give more weight to the scan angle information; a larger value gives it less weight. The valid range is 0.001 to 9999. The scan angle information is very powerful in determining a correct solution, and it is probably better for the value you enter here to be too low than too high. The default is 0.125 (corresponding to 0.25 degree frames).

/MASK=<n>..... (Constraint Mask) [0]

Specifies that certain variables are to be held fixed in the non-linear refinement. The default value of 0 frees all variables, allowing the refinement to proceed normally, and should be satisfactory in almost all cases. The value you specify here is a decimal integer corresponding to a bit mask, where a set bit fixes its assigned parameter and a clear bit frees the parameter. The bit/parameter assignments are:

Bit#	Value	Parameter
0	1	Detector X positional correction
1	2	Detector Y positional correction
2	4	Detector distance correction
3	8	Detector roll
4	16	Detector yaw
5	32	Unit cell axis lengths
6	64	Unit cell angles

For example, if you specify a value of 96 (=32 + 64), the program would refine the

crystal orientation and detector parameters, leaving the unit cell parameters (axis lengths and angles) fixed. Note that if you wanted them to remain fixed at the values specified in the input panel rather than at the initial guesses computed by the linear least squares, you would have to specify a negative value for the constraint type (see $1 above).

/PARNAME=<n> ...(Output Parameter Filename) [newfram0.p4p]

Specifies the filename to which the orientation matrix and refined parameters are written. This file can be read by ASTRO. It is an ASCII file which can be typed, edited, and transferred to other computer types (as long as the transfer software handles any differing end-of-line conventions correctly). By convention, these filenames end with a ._pr extension. The base name of the file defaults to the base name of the last set of frames processed with REFL_ARRAY /THRESHOLD if any, otherwise to NEWFRAM0. An example of a ._pr file is:

NAME:swmyo1

WAVE: 1.541840

ORT1: -0.008553 -0.012507 0.000284

ORT2: -0.009394 0.002745 0.000005

ORT3: -0.000143 -0.000237 -0.021975

DIST: 12.000000

DETP: 4.5299 0.5312 -0.2006 0.0000 0.1999 0.0029

XCYC: 255.000000 242.000000

Each line contains a 5-character item name followed by data in free format. The items are:

NAME: The data set name, usually the base name of the frames processed in the last REFL_ARRAY /THRESHOLD command

WAVE: X-ray wavelength in Angstroms

ORT1,2,3: Rows of the orientation matrix. The storage convention is that, as written here, you could use the matrix to pre-multiply a column HKL vector (in the standard mathematical notation) to give a column reciprocal lattice vector.

DIST: Nominal detector distance, CM

DETP: The six positional corrections. In order they are:
Detector X positional correction (pixels)
Detector Y positional correction (pixels)
Detector distance correction (CM)
Detector pitch (deg)
Detector roll (deg)
Detector yaw (deg)

XCYC: Raw X,Y pixel coordinates of the direct beam at swing angle of zero.

The matrix determined by FRAMBO is a true orientation matrix; that is, it is independent of the starting goniometer angles of the scan series used to determine it. While it cannot be used directly by XENGEN, in many cases it is possible to use the Eulerian

angles output by FRAMBO's least squares to derive initial pseudo-goniostat angles for the XENGEN REFINE program. The following relationships apply ONLY IN THE CASE WHERE THE STARTING GONIOMETER OMEGA, PHI, AND CHI FOR THE FRAME SERIES INPUT TO THE SPOTS PROGRAM ARE ALL ZERO. Note that a 3-circle goniometer is always at chi=45 degrees. Below OMEGA(X), PHI(X) and CHI(X) represent the XENGEN pseudo-goniostat omega, phi, and chi, respectively.

The /U1 Eulerian angle in FRAMBO is equivalent to -PHI(X)

The /U2 Eulerian angle in FRAMBO is equivalent to 180 + CHI(X)

The /U3 Eulerian angle in FRAMBO is equivalent to OMEGA(X)

If your starting frame angles were different from zero, you can use the XENGEN NEWRUN program to compute the pseudo-goniostat angles in the following steps:

- Use REFINE to create a .upr file containing zero-setting-angle pseudo-goniostat angles according to the relationships above.
- Run NEWRUN. Enter 0 0 0 for the old setting angles, and the omega, chi, phi starting angles of your frame series for the new setting angles.
- NEWRUN will print the values of the pseudo-goniostat angles at your starting setting angles.

  Since the parameters used in the least squares refinement are different in FRAMBO from those in XENGEN, there is no guarantee that pseudo-goniostat angles derived from FRAMBO's Eulerian angles will be close enough to permit REFINE to run. We are not recommending that you try to use FRAMBO's indexing and least squares instead of the autoindexing in REFINE on a regular basis; the relationships between the angles are described above because they may occasionally be useful under special circumstances.

8.18.2 Least Squares Output

An example of the output frame REFL_ARRAY /LEASTSQ is shown below. It begins with the orientation matrix (in the same convention as described above for the ._pr file) and the refined unit cell parameters. The unit cell parameters are listed horizontally in the order A, B, C, ALPHA, BETA, GAMMA, VOLUME, with lengths in Angstroms, angles in degrees, and the volume in cubic Angstroms. Below each cell parameter is its estimated standard deviation.

Next are several tabular histograms, showing the distribution of the unsigned differences between observed and calculated values of H,K,L, scan angle (always labeled OMEGA,

even if the scan angle was actually PHI), and detector X,Y position. In all cases, the more closely bunched toward the left side of the histogram the differences are, the better the refinement. Scan angle differences are in degrees, and X,Y differences are in pixels. Following the histograms are the overall average and rms differences for these same quantities, H,K,L, scan angle, X, and Y. The myoglobin example shown below is a very good one. Often the numbers are two or three times higher. The AVG values indicate any systematic bias in the results; if these values are a substantial fraction of the corresponding RMS values, you might suspect mis-indexing or mis-alignment of the system. In such a case, make sure you have a good spatial correction and correct estimates for the detector distance and beam center entered in the CONFIGURE /EDIT panel.

Next are the five refined detector positional corrections, with the X and Y beam center correction in pixels, the detector distance correction in CM and the angular corrections in degrees. In this example, our estimate of the X beam center was just a guess, and was not very good as the result indicates. Depending on the smallest inter-spot separation on the input frames, you may not be able to get away with this poor an estimate (off by 4 pixels) in your own data sets. You should try to specify the beam center to better than half the smallest center-to-center spot separation.

The refined Eulerian angles come next, with the three values in order corresponding to /U1, /U2, and /U3 in degrees.

A line containing overall refinement statistics follows, with values of the starting and ending residual, goodness of fit, number of refinement cycles actually performed, and a completion code. The residuals give an indication of the amount of improvement made by the non-linear refinement relative to the initial guesses computed by the linear least squares. Usually the residual improves by a factor of two or more. The goodness of fit is relative to an estimated 0.2-pixel error in detector X,Y position of a reflection centroid, and an estimated 0.25 frame-width error in scan angle. If the goodness of fit is less than 1.0, the refinement is better overall than these nominal estimates; values higher than 1.0 indicate that the fit is not as good. The completion code is for diagnostic use by Bruker. It is normally 0; if it is nonzero and the number of refinement cycles is listed as 20, it indicates that the solution might benefit from additional cycles of refinement. In this situation, negate the CONSTRAINT TYPE (see description of the $1 argument) and re-rerun the least squares, and the refinement will continue where it left off. Other cases where the completion code is non-zero indicate that no further improvement in the residual can be made even though some of the gradients are non-zero, and indicates that we've probably underestimated the magnitude of round-off errors in the compu-

tations (the solution, however, should still be valid). Please notify Bruker if you see many non-zero completion codes.

Following the overall statistics is a reflection-by-reflection summary of the agreement for each reflection in the reflection array. Each record consists of two lines, the first containing the reflection as it's entered in the reflection array (i.e., the “observed” values), and the second containing the differences for HKL, scan angle (always converted into omega rotation) and detector X,Y with the sense OBSERVED - CALCULATED. This output shows both those reflections included in the least squares, and those not included (for example, reflections without the C flag set). It also shows computed HKL indices for reflections which do not have the H flag set. It does not include reflections which do not have the A flag set, since there are many possible combinations of setting angles and detector X,Y which could correspond to given HKL indices. Use the /HCALC sub-command if you need to determine angles corresponding to specific HKLs.

An example output (truncated after the first few reflections) for least squares on reflections from the series of eight contiguous test frames produced with a hexagonal myoglobin crystal is shown below. The refinement was unconstrained. The cell parameters in this example are not very good, and their standard deviations are correspondingly large. They would be better if we thresholded an additional set of frames starting at a scan angle 90 degrees or so away from the first eight prior to indexing and least squares.

Example 8.5 - Least Squares Output from the Eight Test Frames

```
Orientation Matrix:
 -0.00855331 -0.01250697  0.00028393
 -0.00939403  0.00274520  0.00000470
 -0.00014339 -0.00023734 -0.02197455

Lattice parameters & Standard deviations:
  90.8317   90.1132   45.5042   90.314   89.964   119.944    322733.90
   0.9975    1.8806    0.4779    0.348    0.091     0.238     13974.49

Histograms:
         .00  .05  .10  .15  .20  .25  .30  .35  .40  .45  +Inf
       H  26    0    0    0    0    0    0    0    0    0
       K  26    0    0    0    0    0    0    0    0    0
       L  26    0    0    0    0    0    0    0    0    0
   Omega  26    0    0    0    0    0    0    0    0    0

        0.00  0.25  0.50  0.75  1.00  1.25  1.50  1.75  2.00  2.25  +Inf
       X    22     4     0     0     0     0     0     0     0     0
       Y    25     1     0     0     0     0     0     0     0     0

                    H         K         L     Omega         X         Y
      AVG       0.000     0.000     0.000     0.000     0.000     0.000
      RMS       0.012     0.006     0.006     0.014     0.147     0.137
Detector corrections:  X-Cen   Y-Cen      Dist      Roll     Yaw
                       4.530  -0.531  -0.201   0.200   0.003

Eulerian angles:     -95.154 178.930 -37.169

Nonlinear refinement:   StartingRes      FinalRes         GOF   #Cycles    Code
                        6.49567E-01    2.76423E-01    0.44          4         0

  # Flags     H  K  L   2-Theta   Omega     Phi      Chi        X       Y  Inorm   I/Sig
  1 ACHS   16 -7  8  -30.000   -0.271   0.000   0.000  82.85  51.23  626.60  112
           +.02-.01+.01             0.004                    -0.26   0.15

  2 ACHS   12 -6  6  -30.000   -0.443   0.000   0.000  33.26  99.06  467.95   97
           +.01+.00+.01            -0.022                    -0.14   0.28
```

```
3 ACHS   21 -11  -3 -30.000  -0.448   0.000   0.000 142.13 309.54  344.28   83
        +.01+.00+.00           -0.012                      -0.16   0.02
                                .
                                .
                                .
                                .
                               etc.
```

8.19 Peaks > Refl. Array > Edit • View/modify the reflection array

Menu Command: Peaks > Refl. Array > Edit

Accelerator: Ctrl+E

User Level: 1

SLAM Syntax: REFL_ARRAY /EDIT

When you select EDIT from the REFL_ARRAY submenu the system displays a “scrollable” window listing all of the reflections currently in the reflection array. You can add to, delete from, or reorganize the list as desired by using the appropriate screen-editing functions. This is very useful for making minor corrections, changes, and deletions; however, some of the other sub-commands, such as /SORT and /MODIFY can operate globally on the entire array, and provide a faster method for making more extensive changes.

REFL_ARRAY /EDIT is an interactive command only. You can invoke it from the command line, but it will not proceed without intervention. There is no built-in 10s timeout on REFL_ARRAY /EDIT like there is on other scrolling output windows. The command line syntax is:

REFL_ARRAY /EDIT

Some of the other sub-commands, such as /MODIFY automatically invoke /EDIT on completion (but only when they have been invoked from the REFL_ARRAY submenu) so you can review the results. Operation in such a case is the same as described here.

Like other scrollable windows, the REFL_ARRAY /EDIT window displays the ASCII “icon” |/\\/| at the left of the title bar. You can move through the text in the array with the page keys, arrow keys, or mouse motion. If you press the ESC key or right mouse button, the program will return to the REFL_ARRAY submenu. If you press the ENTER key or left mouse button when in the scrolling edit window, the program displays a pop-up menu of editing functions. You can then use the cursor keys or mouse to select a specific function to implement. Press ENTER or the left mouse button again to execute it, or ESC/right button to return to the editing window.

The functions in the pop-up menu are as follows:

Exit

Return to REFL_ARRAY submenu, saving changes to array. The ESC key or right mouse button performs the same function when you're in the editing window.

Edit

Edit displayed lines, using mouse or cursor to move between lines.

UpPage

Move up one page (screen) in list of reflections. The PgUp key (Prev on VAX) per-

forms the same function when you're in the editing window.

DownPage

Move down one page (screen) in list of reflections. Note that you cannot move down past the end of the list. The PgDn key (Next on VAX) performs the same function when you're in the editing window.

Top

This moves you to the first line in the reflection array. The key combination CTRL-PgUp has the same effect when you're in the editing window.

Bottom

This moves you to the last line in the reflection array. The key combination CTRL-PgDn has the same effect when you're in the editing window.

Write

Writes all lines or selected lines to an ASCII file on disk for storage and future use. If a range of lines has been highlighted with SELECT (see below) only the highlighted range is written to the file, otherwise the entire array is written.

Read

Appends lines from a disk file (for example, created by WRITE) to the end of the array. You can use the Cut and Paste functions to move the new lines elsewhere if necessary.

Select

This function is used to highlight (select) a range of lines in the array, permitting writing, cutting, copying and pasting a specified range. Pressing the F7 key has the same effect when you're in the editing window.

Cut

This removes a selection from the array and places it in the paste buffer. Use PASTE to reinsert the line(s) that were cut. Pressing the F8 key has the same effect when you're in the editing window.

Store

Makes a copy of the current selection (this is the same as CUT, but does not remove the selected text from the array) and places it in the paste buffer. Pressing the F9 key has the same effect when you're in the editing window.

Paste

Inserts the contents of the paste buffer ahead of the current line. Pressing the F10 key has the same effect when you're in the editing window. If there aren't enough free lines in the array, the paste will not be performed.

The items in the Reflection Array have the following definition:

FLAGS

The status of a reflection is indicated by a series of single-character flags that are displayed in this field. There are four possible flags, having the following meanings. The flags always appear in sorted order, ACHS, ACS, AH, etc. with no intervening spaces. If you're entering or changing the flags in the /EDIT sub-command, you can enter the flags in a different order, but make sure that there are no imbedded spaces.

A This reflection record includes the goniometer settings angles and the the X,Y position of the reflection relative to detector origin (in the standard Bruker pixel coordinate convention). This flag is automatically set by REFL_ARRAY /THRESHOLD and /PICK when they enter a new reflection into the array. If this flag is not set, the /INDEX and /LEASTSQ sub-commands ignore the reflection.

H This reflection record includes the HKL indices. Autoindexing automatically sets this flag when it computes the HKL indices. If this flag is not set, REFL_ARRAY /LEASTSQ ignores the reflection.

C This reflection is “centered” in scan angle; that is, there was sufficient information to determine the centroid in scan angle to better than 1 frame width. REFL_ARRAY /THRESHOLD and /PICK automatically set this flag if the spot intensity (e.g., for those pixels above the threshold) spanned more than one frame. If the reflection appeared on only one data frame it, the C flag is not set. In a case where there are too few spots spanning frames, you can use the /MODIFY sub-command to add the C flag to all reflections in the set. In general, it doesn't affect the autoindexing capability of the program to do this; however, the RMS deviation in the scan angle (as output by the /LEASTSQ sub-command) is typically much larger when these spots are included, and the orientation and cell parameters may not be as precise.

S Indicates that the values of the X,Y spot positions in this reflection record have been corrected with a valid spatial correction (obtained by processing a brass fiducial plate image with the SPATIAL /NEW, /PROCESS or /LOAD command). REFL_ARRAY /THRESHOLD and /PICK automatically set this flag and store the corrected X,Y values if a spatial correction was in effect

when they were executed. If this flag is absent, REFL_ARRAY /INDEX and /LEASTSQ assume that the X,Y values in this record are raw values, and explicitly correct them in the course of their computations.

X Display angles in XSCANS conventions with X,Y at detector center, instead of goniometer settings and X,Y pixel location.

H,K,L

The HKL crystallographic indices. /INDEX automatically computes these indices and stores them in the array. /BRAVAIS and /TRANSFORM transform these indices among different unit cell possibilities and conventions. If HKL indices are not available for a reflection /LEASTSQ ignores it.

2-THETA, OMEGA, PHI, CHI

The goniometer setting angles. /THRESHOLD and /PICK automatically enter these values into the array based on the angles found in the frame headers. If the C flag is set, the scan angle (omega or phi) will typically be set to the intensity-weighted centroid value computed by /THRESHOLD or /PICK; otherwise, the scan angle is set to that corresponding to the frame on which the spot was located. If angles are not available for a reflection, /INDEX and /LEASTSQ ignore it.

X,Y

These are the X- and Y-centroids of the reflection on this line in the Bruker pixel coordinate convention. /THRESHOLD and /PICK automatically enter these values into the array. If a spatial correction is in effect at the time, the entered X,Y values are corrected for spatial distortion and the S flag is set; otherwise, raw X,Y values are entered and the S flag is not set. If X and Y are not available for a reflection, /INDEX and /LEASTSQ ignore it.

INORM

This is the normalized intensity for the reflection. /THRESHOLD and /PICK automatically enter this value into the array. The intensity is normalized to 1 deg/min scan velocity.

I/SIGMA

This is the ratio of the reflection intensity to its standard deviation. /THRESHOLD and /PICK automatically enter this value into the array. /THRESHOLD uses I/SIGMA (modified by a specified sin(theta) bias) as a sort key, and reflections entered automatically be /THRESHOLD are thus approximately in order of decreasing I/SIGMA (with “centered” reflections coming before “uncentered” reflections).

8.19.1 Line Editing

You can edit text within a line with the same functions used to edit text in an input panel. The data you enter on each line is read, validated and reformatted according to the flags you supply at the beginning of the line. For a given combination of flags, the program expects there to follow a certain number of numeric values in free separated by spaces. If the number of items or their type doesn't agree with the flag settings, the program issues and error message and asks you to re-enter the line. Modifying the A and H flags from with REFL_ARRAY /EDIT (as opposed to /MODIFY) can be a tricky process and is therefore not recommended.

8.20 Peaks > Refl. Array > Modify • Alter specified item for a range of reflections in the array

Menu Command: Peaks > Refl. Array > Modify

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /MODIFY $1 $2 /FIELD=<n> /VALUE=<s>

This option lets you make global changes to all or part of a specified column in the Reflection Array. It is possible to add and subtract flags from a range of lines, set a particular column to a constant value, negate the values in a column, or transfer the values from one column into another column.

When invoked with the MODIFY option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /MODIFY displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button performs the specified modifications, then displays the resulting array in an editing window for review, identical to the REFL_ARRAY /EDIT window (see REFL_ARRAY /EDIT). Pressing ESC or the right mouse button in the editing window or in the input panel returns you to the REFL_ARRAY submenu.

8.20.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (First Reflection #) [1]

This is the line where you want the selection range to start. Line numbers start at 1. For example, if you want to modify only reflections 5 through 7, you would enter “5” in the FIRST REFLECTION # parameter. Default is 1. Valid range is 1–512.

$2 ..... (Last Reflection #) [512]

This is the line where you want the range to end. Line numbers start at 1. To continue the previous example, if you want to modify only reflections 5 through 7, you would enter “7” in the LAST parameter. Default is 1. Valid range is 1–512.

/FIELD=<n>.....(Field to Modify) [1]

Specify which field (column) you want to change. You specify the field by its column number. Default is 1. Valid range is 1–12. Field numbers are:

Field #	Description
1	Flags (for example, ACHSX)
2	H index
3	K index
4	L index
5	2-Theta setting (swing) angle
6	Omega setting angle
7	Phi setting angle
8	Chi setting angle
9	Detector X pixel coordinate
10	Detector Y pixel coordinate
11	Intensity
12	I/sigma

/VALUE=<s> .....(New Value) [-C]

Enter the value to which the entries in the specified column and range of lines are to be set. REFL_ARRAY /MODIFY also supports the following “special” values:

+f, -f where f is one of the flag characters A C H or S. This sets or clears the specified flag, leaving the state of the other flags unaffected for each reflection. The field # must be 1 if you use this option.

- Negates all the numeric values in the specified range. The field number must be 2–8 (i.e., only applies to HKL indices and setting angles).

#N where N is the number of a field in the same group. This copies the values from column #N into the column being modified. This works within two different groups of columns, the HKL group (#2–4) and the setting angle group (#5-8). Thus, if the value you specified for /FIELD is 7, only #5, #6, #7, or #8 is a valid copy operation; #2 would not work in this case.

Examples:

1. Set the C flags of all reflections in the array, leaving all the other flags intact:

REFL_ARRAY /MODIFY 1 512 /FIELD=1 /VALUE=+C

2. Change the scan angle extracted from a frame series from omega to phi, effectively reversing the sense of the scans (assuming all the existing phi values in the array are the same):

REFL_ARRAY /MODIFY 1 512 /FIELD=7 /VALUE=#6

REFL_ARRAY /MODIFY 1 512 /FIELD=6 /VALUE=0.0

3. Change the swing angle for reflections 107–200 to -30 degrees:

REFL_ARRAY /MODIFY 107 200 /FIELD=5 /VALUE=-30.0

8.21 Peaks > Refl. Array > Sort • Sort all or part of array on a specified parameter

Menu Command: Peaks > Refl. Array > Sort

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /SORT $1 $2 /FIELD=N /DESCENDING

This command lets you sort the reflection array, or a specified range of lines within the array, in ascending or descending order. The array may be sorted on any of the 12 Reflection Array columns:

FLAGS, H, K, L, 2THETA, OMEGA, PHI, CHI, X, Y, INORM, I/SIGMA

This provides a means for organizing the array in a manner more suitable for publication (e.g., placing it in hkl order; 001 002 003...), or that will facilitate editing, problem diagnosis, etc.

When invoked with the SORT option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /SORT displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button begins the sort; the ESC key or right mouse button returns you to the REFL_ARRAY submenu. When sorting starts, the program displays the message

“SORTING...” on the bottom status line. Sorting should be completed within a few seconds. On completion the program displays the resulting array in an editing window for review, identical to the REFL_ARRAY /EDIT window (see REFL_ARRAY /EDIT). Pressing ESC or the right mouse button in the editing window returns you to the REFL_ARRAY submenu.

When you sort on one of the HKL indices, the program automatically performs secondary and tertiary sub-sorts on the other two indices. For example, if you sort on H, the program performs that sort, then sorts on K for each H, and on L for each K. The result would look something like this:

H K L
0 0 1
0 0 2
0 0 3
0 1 0
0 1 1
0 1 2
1 0 0
1 0 1
1 0 2
1 0 3
1 1 0
1 1 3
1 1 5
etc.

Similarly, if you sort on one of the scan angles, sub-sorts are performed on the other scan angles. The sub-sorts are performed in the following order:

Specified Sort Key	Secondary Sort	Tertiary Sort	Quaternary Sort
H	K	L	None
K	L	H	None
L	H	K	None
2-Theta	Omega	Phi	Chi
Omega	2-Theta	Phi	Chi
Phi	2-Theta	Omega	Chi
Chi	2-Theta	Omega	Phi

8.21.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (First Reflection #) [1]

This is the Reflection Array line where you want the sort range to start. The first line is numbered 1. For example, if you want to sort only reflections 9 through 50, you would enter “9” as the $1 parameter.

$2 ..... (Last Reflection #) [512]

This is the line where you want the sort range to end. To continue the previous example, if you want to sort only reflections 9 through 50, you would enter “50” in the LAST parameter.

/FIELD=<n> .....(Sort Field) [1]

Specifies number of the column you want to sort on. Column numbers are:

Field #	Description
1	Flags (for example, ACHSX)
2	H index
3	K index
4	L index
5	2-Theta setting (swing) angle
6	Omega setting angle
7	Phi setting angle
8	Chi setting angle
9	Detector X pixel coordinate
10	Detector Y pixel coordinate
11	Intensity
12	I/sigma

/DESCENDING .....(Descending (Y/N) ?) [No]

If you enter Y for this item on the input panel, or if this qualifier is present on the command line, the sort is in descending order, otherwise it is in ascending order.

8.22 Peaks > Refl. Array > Transform • Transform HKLs in array according to specified 3x3 matrix

Menu Command: Peaks > Refl. Array > Transform

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /TRANSFORM $1 $2 $3 $4 $5 $6 $7 $8 $9

REFL_ARRAY /TRANSFORM lets you enter the nine elements of a specific HKL transformation matrix, and transforms the HKL indices of all indexed reflections (i.e., those whose H flag is set) in the Reflection Array by that matrix. The input matrix pre-multiplies a column HKL vector formed from each input HKL to yield a column vector containing the transformed HKL. You would use this function, for example, if you needed to use a non-standard space group setting (e.g., orthorhombic with the B axis longest), to transform the indices to correspond to the desired setting prior to performing least squares.

When invoked with the TRANSFORM option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /TRANSFORM displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button performs the specified transformation; the ESC key or right mouse button returns you directly to the REFL_ARRAY submenu without updating the matrix. Following a successful transformation, the program displays the resulting Reflection Array in an editing window for review, identical to the REFL_ARRAY /EDIT window (see REFL_ARRAY /EDIT). Pressing ESC or the right mouse button in the editing window returns you to the REFL_ARRAY submenu.

8.22.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

Note that the element order on the input panel corresponds to the standard mathematical convention (e.g., (1,3) is 3rd column on 1st row). It has nothing to do with FORTRAN storage conventions. As entered, the matrix will pre-multiply a column HKL vector to give a transformed column HKL vector.

$1 ..... (Matrix(1,1)) [1.0]

Value for row 1, column 1 of orientation matrix

$2 ..... (Matrix(1,2)) [0.0]

Value for row 1, column 2 of orientation matrix

$3 .....(Matrix(1,3)) [0.0]

Value for row 1, column 3 of orientation matrix

$4 .....(Matrix(2,1)) [0.0]

Value for row 2, column 1 of orientation matrix

$5 .....(Matrix(2,2)) [1.0]

Value for row 2, column 2 of orientation matrix

$6 .....(Matrix(2,3)) [0.0]

Value for row 2, column 3 of orientation matrix

$7 .....(Matrix(3,1)) [0.0]

Value for row 3, column 1 of orientation matrix

$8 .....(Matrix(3,2)) [0.0]

Value for row 3, column 2 of orientation matrix

$9 .....(Matrix(3,3)) [1.0]

Value for row 3, column 3 of orientation matrix

8.23 Peaks > Refl. Array > Matrix • Enter an orientation matrix (e.g., from external program)

Menu Command: Peaks > Refl. Array > Matrix

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /MATRIX $1 $2 $3 $4 $5 $6 $7 $8 $9

REFL_ARRAY /MATRIX lets you enter the nine elements of a specific orientation matrix. The resulting matrix is treated as if it had been determined by REFL_ARRAY /LEASTSQUARES. In general, this is not as accurate as running REFL_ARRAY /LEASTSQUARES, since the latter simultaneously refines both the matrix elements and the detector positional corrections—here, we're only entering a matrix. Nevertheless, if you have an existing matrix (for example, from P3 or XSCANS), REFL_ARRAY /MATRIX could allow you to immediately index a few spots on a frame and run least squares without the need for autoindexing.

When invoked with the MATRIX option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /MATRIX displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button installs the specified orientation matrix and returns you to the REFL_ARRAY submenu; the ESC key or right mouse button returns you directly to the REFL_ARRAY submenu without updating the matrix.

When REFL_ARRAY /MATRIX updates the orientation matrix, it also extracts the unit cell parameters from the matrix and places them in the REFL_ARRAY /BRAVAIS and /LEASTSQUARES input panels as defaults (in the case of the /LEASTSQUARES panel, the Eulerian angle defaults are also extracted from the input matrix). You can use this feature to compute the cell parameters and Eulerian angles corresponding to a given orientation matrix.

8.23.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

Note that the element order on the input panel corresponds to the standard mathematical convention (e.g., (1,3) is 3rd column on 1st row). It has nothing to do with FORTRAN storage conventions. As entered, the matrix will pre-multiply a column HKL vector to give and column reciprocal-lattice vector. The matrix must conform to the common convention used in FRAMBO, P3, XSCANS, ASTRO, GADDS, etc.:

$1 ..... (Matrix(1,1)) [1.0]

Value for row 1, column 1 of orientation matrix

$2 .....(Matrix(1,2)) [0.0]

Value for row 1, column 2 of orientation matrix

$3 .....(Matrix(1,3)) [0.0]

Value for row 1, column 3 of orientation matrix

$4 .....(Matrix(2,1)) [0.0]

Value for row 2, column 1 of orientation matrix

$5 .....(Matrix(2,2)) [1.0]

Value for row 2, column 2 of orientation matrix

$6 .....(Matrix(2,3)) [0.0]

Value for row 2, column 3 of orientation matrix

$7 .....(Matrix(3,1)) [0.0]

Value for row 3, column 1 of orientation matrix

$8 .....(Matrix(3,2)) [0.0]

Value for row 3, column 2 of orientation matrix

$9 .....(Matrix(3,3)) [1.0]

Value for row 3, column 3 of orientation matrix

8.24 Peaks > Refl. Array > Hcalc • Compute X, Y, and scan angle for specified HKL

Menu Command: Peaks > Refl. Array > Hcalc

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /HCALC $1 $2 $3 $4 $5 $6 $7 $8 $9

Given an orientation matrix, specified HKL indices, a scan axis, and setting angles for the other axes, REFL_ARRAY /HCALC computes the detector X and Y in pixels and the scan angle at which the reflection will be observed. You must already have computed a valid orientation matrix with REFL_ARRAY /LEASTSQ prior to executing this command.

In general, there are two solutions. Depending on the angle between the scan axis and reciprocal-lattice vector, the setting angles you specify for the non-scan axes, and the current detector distance, one, both, or none of the solutions may be observable. The program displays the results in a scrollable output window.

When invoked with the HCALC option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /HCALC displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button solves for the positions at which the specified HKL can be observed; the ESC key or right mouse button returns you directly to the REFL_ARRAY submenu. Following a successful computation, a scrolling output window is displayed containing the resulting output text. If logging is enabled (see LOGFILE) the contents of this window are also written to the logfile. When viewing the output, pressing ENTER or the left mouse button displays a pop-up menu of options, including export of ASCII data; for example, the contents of the window could be sent to a file or printer with this function. You can also move through the window contents with the page keys, arrow keys or with mouse motion. Pressing ESC or the right mouse button exits the output window, returning you to the REFL_ARRAY submenu. The output is described in more detail below. In GADDS, the program will prompt you on the bottom status line as to whether you want to drive to one of the solutions; for example,

> DRIVE TO SOLN #1 AT -30.00 150.62 0.00 0.00? (Y OR ENTER=YES; N OR ESC=NO)

If you answer one of these prompts with the Y key, ENTER key, or left mouse button, GADDS attempts to drive the goniometer to that position. If you answer with the N key, ESC key, or right mouse button, the goniometer remains where it is. The operation in SADIE is the same, except that the drive prompts are not issued.

In some cases, no rotation about the specified scan axis exists which will place the specified

HKL in the diffracting condition. If this occurs, the program displays the message

REFLECTION NOT OBSERVABLE --
PRESS ENTER OR MOUSE TO RETURN

Pressing the ENTER key or left mouse button returns you to the input panel (or to the command line if the command was invoked from there).

8.24.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(H) [0]

Enter the H index of the reflection whose position is to be computed. Default is 0 and valid range is -9999 to 9999. Real values may be used; they are not rounded to integer values prior to computing the position.

$2 .....(K) [0]

Enter the K index of the reflection whose position is to be computed. Default is 0 and valid range is -9999 to 9999. Real values may be used; they are not rounded to integer values prior to computing the position.

$3 .....(L) [2]

Enter the L index of the reflection whose position is to be computed. Default is 2 and valid range is -9999 to 9999. Real values may be used; they are not rounded to integer values prior to computing the position.

$4 ..... (Scan Axis #) [2]

Enter the axis number (2 for omega or 3 for phi) of the axis whose position (to place the specified HKL in the diffracting condition, if possible) is to be computed. The values that you specify below for the other three goniometer axes are kept fixed for the purposes of computation. The value that you supply below for this scan axis makes no difference.

$5 ..... (2-Theta) [0.00]

Enter the detector swing angle in degrees at which the scan angle and detector X,Y of the specified HKL reflection are to be computed. Default is zero and valid range is -360 to 9999.

$6 ..... (Omega) [0.00]

Enter the omega goniometer angle in degrees at which the scan angle and detector X,Y of the specified HKL reflection are to be computed. If you've specified a scan axis of 2 (see above), any valid value is OK here. Default is zero and valid range is -360 to 9999.

$7 ..... (Phi) [0.00]

Enter the phi goniometer angle in degrees at which the scan angle and detector X,Y of

the specified HKL reflection are to be computed. If you've specified a scan axis of 3 (see above), any valid value is OK here. Default is zero and valid range is -360 to 9999.

$8 .....(Chi) [0.00]

Enter the chi goniometer angle in degrees at which the scan angle and detector X,Y of the specified HKL reflection are to be computed. Default is zero and valid range is -360 to 9999.

$9 .....(Frame Size) [512]

Enter number of linear pixels in a frame, 512 or 1024.

8.24.2 HCALC Output

Example 8.6 below is an output window from REFL_ARRAY /HCALC. The output window starts with a line containing the input HKL indices, followed by the two solutions, if available. The three non-scan axes will contain the same values as you specified in the input panel. The value of the scan axis that would place the specified HKL in the diffracting condition in degrees is also shown. The X,Y position in pixels (in the Bruker convention with (0,0) at the left of a displayed frame) is shown both in spatially corrected coordinates (X(cor),Y(cor)) and in raw coordinates (X(raw),Y(raw)). If the corrected coordinates are too far outside the detector active area for raw coordinates to be computed, the X(raw), Y(raw) columns contain the text “OUTSIDE DETECTOR AREA.”

Example 8.6 - REFL_ARRAY /HCALC Output

```
Calculated positions for HKL =  16.00  -7.00   8.00:

Soln #  2Theta   Omega     Phi     Chi  X(cor)  Y(cor)  X(raw)  Y(raw)
     1  -30.00   15.45    0.00    0.00 -632.24  548.21: outside detector area
     2  -30.00  162.07    0.00    0.00  175.03  427.07  173.71  425.44

Determine desired solution (1 or 2).  Press ESC to continue ...
```

8.25 Peaks > Refl. Array > Clear • Erase the reflection array and current orientation matrix

Menu Command: Peaks > Refl. Array > Clear

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /CLEAR

Use this command to erase the reflection array that is currently in use and to delete the orientation matrix associated with it. This is useful if you're starting analysis of a new sample, have (for example) used too low a threshold in specifying spots for the array and wish to start over, or if you suspect twinning and would like to calculate the orientation matrices for different sets of reflections to test the crystal quality.

When you invoke CLEAR from the REFL_ARRAY submenu or specify REFL_ARRAY /CLEAR on the command line, the program issues the warning on the bottom status line:

> ERASE REFLECTION ARRAY: ARE YOU SURE? (Y or ENTER=YES; N or ESC=NO)

Press the Y key, Enter key, or left mouse button to erase the array and return control to the program, or the N key, ESC key, or right mouse button to return without erasing the array. If you've invoked REFL_ARRAY /CLEAR from the command line, this prompt will time out in 10s, assuming a “Y” answer, allowing script files to run unattended. If you however press a key within the 10s period, the wait for timeout is cancelled, and the program will take the action you've just specified.

8.25.1 Arguments

None. Command executes immediately.

8.26 Peaks > Refl. Array > Load • Read in orientation matrix from existing .p4p or ._pr file

Menu Command: Peaks > Refl. Array > Load

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /LOAD $1 $2 $3

When invoked with the LOAD option from the REFL_ARRAY submenu or when run from the command line without arguments, REFL_ARRAY /LOAD displays an input panel where you can view/modify the arguments described below. When in the panel, pressing the ENTER key or left mouse button performs the load command. Pressing ESC or the right mouse button returns you to the REFL_ARRAY submenu.

8.26.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(Filename) [lys.p4p]

Enter name of P4P or LS parameter (*._pr) file to load. If extension is omitted, GADDS will try P4P, then _PR.

$2 ..... (Overwrite Reflections?) [No]

Check to overwrite reflection array list with list in P4P/LS file.

$3 ..... (Overwrite Crystal Info?) [No]

Check to overwrite Project > Edit crystal info items.

8.27 Peaks > Refl. Array > Rspace • Reciprocal space viewing for interactive indexing

Menu Command: Peaks > Refl. Array > RSpace

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /RSPACE

Rspace command is designed to perform interactive indexing on an HKL list consisting of multiple domains. These domains can be either the same structure with different orientations, or different structures.

Rotate

Use Rotate to view the HKL reflections in reciprocal space. The idea is to rotate the view until the reciprocal space planes line-up. All reflections lining up on planes are from a single domain.

Zero all angles

Rotate to initial position. Sort of a return to starting point.

Set plane

Select points on a plane. These points are assigned to a group (up to five groups may be used). Typically used after rotating until reflections line up on planes.

Zoom in (2x)

Select new center of rotation, the zoom by a factor of 2.

Zoom out

Zoom out by a factor of 2.

Delete group

Assigns all points of a group to the global group. The reflections are not deleted, so it reverses the effects of “Set plane.”

Write group

Write a group to a file. This file can be read under Refl_array /Edit and then indexed.

Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

None..... () []

Due to the interactive nature of this command, /RSPACE cannot be executed in SLAM mode.

8.28 Peaks > Refl. Array > CDF Search • Search the CDF database for structure with specified unit cell

Menu Command: Peaks > Refl. Array > CDF Search

Accelerator: None

User Level: 1

SLAM Syntax:

REFL_ARRAY /CDF $1 $2 $3 $4 $5 $6 $7 $8 /FORMULA=<s> /TYPE=<s> /FILE=<s> /VERBOSE

REFL_ARRAY /CDF (CDF Search on the submenu) lets you search the NIST Crystal Data File for any published lattice parameters that match the lattice parameters for your crystal. Supports either the ICDD Crystal Data or the newer NIST Crystal Data 1999 database.

Before CDF search may be used, the CDF index file must be generated by running \saxi\gadds32\indxtl.exe. INDXTL requires a couple of files as input:

SAXI$CDCODE:codens.dat

SAXI$CDROM:crystal.dat

And generates as output the index file:

SAXI$CDF:cryidx.bin

INDXTL takes a long time to run, so be patient.

8.28.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (A Axis Length) [10.0]

$2 ..... (B Axis Length) [10.0]

$3 ..... (C Axis Length) [10.0]

$4 ..... (Alpha Cell Angle) [90.0]

$5 ..... (Beta Cell Angle) [90.0]

$6 ..... (Gamma Cell Angle) [90.0]

These are the 6 unit cell parameters you want to find matching entries for. Normally they will be those for the mounted crystal, but you may enter parameters for any unit cell. The values in the input panel are automatically updated with the results of the REFL /BRAVAIS or REFL /LEASTSQ whenever these commands are run.

$7 ..... (Decimal Fraction Deviation) [0.01]

The program searches for any unit cell with axis lengths in the range of (1 - d) * input axis length to (1 + d) * input axis length. The variable d is the DECIMAL FRACTION DEVIATION. A value of 0.01 is a good value for the first search.

$8 .....(Lattice Centering Type) [P]

Enter the lattice type (P,A,B,C,I,F or R), where P=Primitive, A, B or C=Edge-centered, I=Body-centered, F=Face-centered, or R=Rhombohedral. The input panel value is automatically updated with the results of the REFL /BRAVAIS or REFL /LEASTSQ whenever these commands are run.

/FORMULA=<s> ...(Chemical Formula) [?]

This item is currently unused; in a later version the program may allow selection by chemical formula.

/TYPE=<s> .....(Search Type) [BOTH]

The NIST Crystal Data File is divided into Organic and Inorganic structures. Choose Organic, Inorganic or Both.

/FILE=<s> .....(Output File Name) [hits.out]

The information from the NIST Crystal Data File for each match that is found is written to an output file, in addition to being displayed on the screen. Enter a file name for this file.

/VERBOSE.....(Verbose Output) [N]

Controls the amount of information sent to the output file. Choose Y to put the entire CDF record(s) out to the output file.

8.28.2 CDF-Search Algorithm

The current version of the NIST Crystal Data File contains unit cell parameters for over 144,000 crystals whose lattice parameters have been published. This file is not included with GADDS. It can be obtained, in CD-ROM format, from:

NIST

Need address here.

An index file containing reduced cell axial lengths and cell volumes was prepared to enable the search algorithm to search the CD-ROM very efficiently. INDXTL, a program that builds this index, is included in the GADDS distribution.

From the input lattice parameters and lattice type, the reduced unit cell parameters are calculated. The index file is searched for all possible matches that have a, b, c and volume within the DECIMAL FRACTION DEVIATION. For each match, the corresponding NIST Crystal Data File record is read. If the cell angles are within the prescribed limits, all information for that record is written to a match file. The matches are then sorted by a goodness-of-fit parameter (the best matches will be first) and written to the output file.

The search algorithm takes only a few seconds to complete. If you get too few matches, increase the DECIMAL FRACTION DEVIATION.

If you get too many matches, decrease the DECIMAL FRACTION DEVIATION. The output information includes the reduced unknown cell, the reduced Crystal Data Cell, the chemical name and the literature reference.

8.29 Peaks > Refl. Array > Save • Save the reflection array in a .p4p file

Menu Command: Peaks > Refl. Array > Save

Accelerator: None

User Level: 1

SLAM Syntax: REFL_ARRAY /SAVE

Save the current reflection array and other relevant information in a P4P file for use by other programs such as SHELXTL. While Least-Squares will automatically create a P4P file, after manual editing of the reflection list, you may wish to update the P4P file.

The file name is taken from the current data set name. As the command executes you will see the messages:

OK to create: XXXX.P4P? Yes No

Overwrite XXXX.P4P? Yes No

Created: | Updated: XXX.P4P.

8.29.1 Arguments

None. Command executes after confirmation.

9. Special Routines

9.1 Special > PDF2 > View • View PDF2 card on screen

Menu Command: Special > PDF2 > View

Accelerator: None

User Level: 1

SLAM Syntax: PDF2 /VIEW $1 /NBS*AIDS /TYPE=<n>

The PDF2 /VIEW command can scroll through selected PDF patterns in either “pretty” format or in the native NBS*AIDS format.

9.1.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(PDF Number) [33-1161]

The PDF number is defined by a set number and a pattern number. These numbers can be separated by a space, a comma, or a dash. (i.e., “33 1161”, “33,1161”, or “33-1161” are all valid PDF numbers.

/NBS*AIDS ..... (Format) [No]

Information about each diffraction pattern is stored in NBS*AIDS format on the CD-ROM (see the ICDD-JCPDS NBS*AIDS83 manual for more details). Users can choose to view the complete NBS*AIDS image format or view the “pretty” format which is much easier to read. The output is in 80 columns.

/TYPE=<n>..... (Data Type) [3]

The D/I table can be outputted as either:

0 = author's reported method (original data as reported in literature)

1 = theta values in degrees

2 = 2-theta values in degrees

3 = d-spacings in Angstroms

4 = sin(theta) ^{2}

5 = Q values

9.2 Special > PDF2 > Print • Print PDF2 card to printer or file

Menu Command: Special > PDF2 > Print

Accelerator: None

User Level: 1

SLAM Syntax: PDF2 /PRINT $1 $2 /NBS*AIDS /TYPE=<n> /CARD

PDF2 /PRINT command can print any selected PDF patterns in either “pretty” format, the native NBS*AIDS format, or the standard JCPDS card image in 128 column format.

9.2.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (PDF Number) [33-1161]

The PDF number is defined by a set number and a pattern number. These numbers can be separated by a space, a comma, or a dash. (i.e., “33 1161”, “33,1161”, or “33-1161” are all valid PDF numbers.

$2 ..... (Print Device) [SAXI$PRINTER]

Enter either the filename or device which is to receive the printout. The default device is SAXI$PRINTER, which you can define as a logical name to point to a file or device if desired. For example, the DOS command

SET SAXI$PRINTER=PRN would direct output to a parallel printer. Alternatively, you can just enter the output name directly in the input panel, for example, PRN. If you specify a filename, the system “prints to disk” creating a file with that filename on the system hard disk which may later be output directly to a printer without having to run GADDS. Under DOS, a command like COPY /B <filename> PRN would copy your output file to a parallel LaserJet printer.

/NBS*AIDS.....(Format) [No]

Information about each diffraction pattern is stored in NBS*AIDS format on the CD-ROM (see the ICDD-JCPDS NBS*AIDS83 manual for more details). Users can choose to view the complete NBS*AIDS image format or view the “pretty” format which is much easier to read. The output is in 80 columns.

/TYPE=<n> .....(Data type) [3]

The D/I table can be outputted as either:

0 = author's reported method (original data as reported in literature)

1 = theta values in degrees

2 = 2-theta values in degrees

3 = d-spacings in Angstroms

4 = $\sin(\text{theta})^2$

5 = Q values

/CARD ..... (Card format ?) [No]

An alternative format is the standard JCPDS card image format, where the output is similar to the “pretty” format but the d-spacing table is positioned to the right of the name, cell, and comments boxes. This output is in 128 column format. If selected /CARD will override the /NBS*AIDS switch.

9.3 Special > PDF2 > Display • Graph PDF2 card above frame image as Debye-Scherrer rings

Menu Command: Special > PDF2 > Display

Accelerator: None

User Level: 1

SLAM Syntax: PDF2 /DISPLAY $1 /DASHED

PDF2 /DISPLAY will draw the PDF pattern's d-lines on top of any displayed frame image for quick pattern matching or verification.

9.3.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 .....(PDF Number) [33-1161]

The PDF number is defined by a set number and a pattern number. These numbers can be separated by a space, a comma, or a dash. (i.e., “33 1161”, “33,1161”, or “33-1161” are all valid PDF numbers.

/DASHED .....(Dashed lines?) [No]

Defines whether the PDF pattern lines are drawn using a solid or dashed conic lines on top of the frame image.

9.4 Special > PDF2 > Search • Search PDF2 by mineral, inorganic, or organic name

Menu Command: Special > PDF2 > Search

Accelerator: None

User Level: 1

SLAM Syntax: PDF2 /SEARCH $1 /MINERAL /INORGANIC /ORGANIC

Perform an ASCII search on various indexes on the PDF2 CDROM. The search is case-insensitive. Wildcard characters are not permitted. The inputted search text must match the first letters of the index keys to be considered a hit. Thus, “Quartz” will match all keys starting with “Quartz.”

```
05-0490 D QUARTZ
33-1161   QUARTZ
** end ** Return to main menu
```

You can display any hit by selecting that line and [OK]. To exit select the last line “** end ** Return to main menu” and [OK].

9.4.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Search string) [Quartz]

Enter search string (up to 40 characters); may truncate.

/MINERAL ..... (Mineral index) [Yes]

“Y” to search mineral name index file: PDF2$KEY:pdf2.s04.

/INORGANIC..... (Inorganic index) [No]

“Y” to search inorganic name index file: PDF2$KEY:pdf2.s03.

/ORGANIC ..... (Organic index) [No]

“Y” to search organic name index file: PDF2$KEY:pdf2.s09.

9.5 Special > PDF2 > Clear • Clear PDF2 overlay graph

Menu Command: Special > PDF2 > Clear

Accelerator: None

User Level: 1

SLAM Syntax: PDF2 /CLEAR

PDF2 /CLEAR command will clear the graphics overlay plane while preserving the displayed frame image. Thus, any pattern displayed with PDF2 /DISPLAY command can be quickly cleared.

9.5.1 Arguments

None. Command executes immediately.

9.6 Special > Commandmode • Switch between command line and menu mode

Menu Command: Special > Commandmode

Accelerator: Ctrl+K

User Level: 1

SLAM Syntax: MENUMODE

The MENUMODE command requires no arguments. It toggles back and forth between menu mode and command line / command file mode.

When operating the system in menu mode, the software is programmed to automatically prompt you for input of options and arguments via dialog boxes when a menu item is selected. This is particularly useful when first learning the system, or when you do not wish to either memorize the parameters for all commands or continually refer to this manual. On the other hand, the command mode allows you to execute command scripts, which can be used, for example, to automate repetitive tasks.

Special > Command Line makes both these operating modes available. To go from menu mode to command line mode, click the Special > Command Line menu item. To return to menu mode from command line mode, enter the following command at the prompt:

```
GADDS> MENUMODE
```

If you start GADDS with the /LOCK qualifier, all commands in the Level menu are disabled (grayed) including Special > Command Line. However, SLAM command scripts can still be executed from the User menu.

For more information on command line and command file (scripts) see the GADDS User's Manual: Scripts section.

9.6.1 Arguments

None. Command executes immediately.

9.7 Special > System • Suspend program and invoke the Command Prompt processor

Menu Command: Special > System

Accelerator: None

User Level: 1

SLAM Syntax: SYSTEM $1

Use the SYSTEM command to spawn either a single command or a session. Spawning a single command permits the execution of external programs, such as a temperature controller software, without leaving the GADDS environment. If the spawn command is non-interactive, it may even be used within a script file.

Spawning a session allows the execution of one or numerous programs in the native operating system command interpreter (e.g., CMD.EXE) by temporarily returning you to that environment. The GADDS software is kept resident in the operating system, and when you are finished with the system level program(s) you can quickly return to the configuration existing when you selected SYSTEM without having to save or reload the configuration file, display or other parameters.

Under NT, use the syntax “CMD /K <command>” to execute the <command> in a Command Prompt window (DOS emulator), “CMD” or “CMD /K” to execute a session, or “<program>” to execute a specific program. (To return to GADDS type “exit” at the prompt.) GADDS will confirm your request with the message:

Suspend GADDS while spawning another task?

Continue and GADDS closes the logfile and autoscript file, then minimizes the GADDS window while the spawn tasks runs. When the spawned task finishes and exits, the GADDS window is restored, and the logfile and autoscript file(s) are restored/reactivated.

9.7.1 Arguments

Each argument is listed below by its SLAM command line name, followed by its dialog box prompt in parentheses:

$1 ..... (Command) []

> “<program>” to spawn a single program, “CMD /K <command>” to spawn a single command (for example dir), or “CMD /K:” to spawn a command prompt session.

9.8 Special > Spawn PROFILE^{plus} • Spawn PROFILE^{plus} (or TOPAS P) with current spectra

Menu Command: Special > Spawn PROFILE-plus

Accelerator: None

User Level: 1

SLAM Syntax: SPAWN

Use this command to spawn (start as separate task) the profile fitting package with the current integrated spectra. Either TOPAS2, TOPAS P or PROFILE^{plus} can be spawned. By default the program is found in either:

- GADDS$SYSTEM: directory
- PROF$SYSTEM: directory
- <Drive>\Topas2P directory
- <Drive>\TopasP directory
- <Drive>\Profile directory
- <Drive>\DiffPlus directory

So if the program cannot file the executable, define the environment variable PROF$SYSTEM: to point to the directory specification.

9.8.1 Arguments

None. Command executes immediately.

9.9 Special > Redraw • Redraw current screen (e.g., if corrupted by window manager)

Menu Command: Special > Redraw

Accelerator: None

User Level: 1

SLAM Syntax: REDRAW

Use this command to force GADDS to redraw the screen. Useful whenever the screen becomes corrupted. Only the current frame image, display header, and goniometer status windows are redrawn when you choose this command. Any information displayed in the previous quadrants and the statistics window are lost, as is any overlay graphics.

9.9.1 Arguments

None. Command executes immediately.

9.10 Special > Level 1, Special > Level 2, and Special > Level 3 • Switch to simple, advanced or administrator menu interface

Menu Command: Special > Level 1, Level 2 or Level 3

Accelerator: None

User Level: 1

SLAM Syntax: LEVEL1 LEVEL2 LEVEL3

GADDS's menu bar can be switched between an abbreviated form (which contains only those commands needed for routine diffraction problems) and those needed for expert diffractionists. Additionally, the detector administrator account will see a third level for the full set of commands needed for calibration and management of the system in addition to data collection. The abbreviated form is the “Special > Level 1” menu bar, the full form is the “Special > Level 2” menu bar, and the administration form is the “Special > Level3” menu bar. You can use these commands to switch between the two (or three) menu bars. You can also use the startup qualifiers /LEVEL2, /LEVEL3, and /LOCK to start GADDS at a specific user level, and/or disable the Level menu commands, locking GADDS at the startup user level. See Startup Qualifiers, Section 1.3 for more information.

9.10.1 Arguments

None. Command executes immediately.

10. User Task Routines

10.1 User > * • Execute user task

Menu Command: User > * (user defined)

Accelerator: Ctrl+F1 through Ctrl+F12

User Level: 1

SLAM Syntax: None

Up to sixteen user-defined commands, called User Tasks, may be added to the User menu on the menu bar by modifying GADDS$SYS-DATA:usertask.ini. When GADDS is started, it reads this file to modify the menu bar to add all the defined user tasks. When a user task is selected, GADDS reads this file again to retrieve the parameter prompts, parameter help line, and the script filename. The script associated with the selected task is then executed. Up to 10 parameters may be added to any user task, and they are treated as replaceable parameters within the script file. If no parameters are associated with the user task, then the task begins executing immediately.

Instructions on modifying usertask.ini file are found in the header of that file. The following example (corresponding to one section of the GADDS$SYSDATA:usertask.ini file) defines user task number 12 to execute the SLAM command script d:\frames\scripts\process.slm:

[12]

menu=”My Collect”

help=”My favorite data collection process”

slam=”D:\frames\scripts\process”

prompt=”Filename”,”Enter filename specification”

prompt=”Title”,”Enter title string”

11. Help Routines

11.1 Help > Software Reference • Display Software Reference online documentation

Menu Command: Help > Software Reference

Accelerator: None

User Level: Ctrl+H

SLAM Syntax: HELP /REFERENCE or HELP

Spawns or displays the GADDS Software Reference Manual. This is either a PDF document, a windows help file, or ASCII *._TP files located in the GADDS$SYSTEM: directory. The Acrobat reader must be installed to display PDF files.

11.1.1 Arguments

None. Command executes immediately.

11.2 Help > User's guide • Display User's Manual online documentation

Menu Command: Help > User's Guide

Accelerator: None

User Level: Ctrl+M

SLAM Syntax: HELP /USERGUIDE

Spawns or displays the GADDS User's Manual. This is either a PDF document, a windows help file, or ASCII *._TP files located in the GADDS$SYSTEM: directory. The Acrobat reader must be installed to display PDF files.

11.2.1 Arguments

None. Command executes immediately.

11.3 Help > Mapping • Display online documentation for GADDSmap

Menu Command: Help > Mapping program

Accelerator: None

User Level: None

SLAM Syntax: HELP /MAP

Spawns or displays the GADDSmap online documentation. This is either a PDF document or a windows help file. The Acrobat reader must be installed to display PDF files.

11.3.1 Arguments

None. Command executes immediately.

11.4 Help > About • Display program, trademark, copyright, and license information

Menu Command: Help > About

Accelerator: None

User Level: 1

SLAM Syntax: ABOUT

Displays the program's version number, copyright notice, trademarks, license information, and developer names.

For information about the goniometer, see Edit > Configure > ShowModel, Section 4.5.

11.4.1 Arguments

None. Command executes immediately.

11.5 Help > Errata • Display changes to printed documentation

Menu Command: Help > Errata

Accelerator: None

User Level: 1

SLAM Syntax: HELP /ERRATA

Displays the online errata for the printed GADDS manuals

11.5.1 Arguments

None. Command executes immediately.

11.6 Help > Releases notes • Display release notes

Menu Command: Help > Release notes

Accelerator: None

User Level: 1

SLAM Syntax: HELP / RELNOTES

Displays the program's online release notes.

11.6.1 Arguments

None. Command executes immediately.

12. SLAM Routines

Most SLAM commands have been discussed in earlier sections with headings corresponding to the menu bar (where menu commands equivalent to the SLAM commands can be found). Some SLAM commands are unique to command mode and are fully discussed in this section. All SLAM commands are listed in Appendix G for reference.

12.1 Echo

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: ECHO /OUT=<s> /APPEND /WAIT=<n> $1 $2 $3 .... $8 $9 $0

ECHO is available only on the SLAM command line (that is, at the GADDS> prompt) and is used for writing command scripts. For example, it can be used to write a specific set of PLOTSO directives into a file for subsequent screen display with the GRAPH /FILE command, all from within the SLAM command script.

Each argument is listed below by its command line name.

$1, $2 ... $9, $0

Enter the text strings to be written to the output file. If your text contains slashes or more than ten separate blank-delimited words, enclose the text in double quotes.

/OUT=<s>

Enter the name of the output file to receive the text.

/APPEND

If this qualifier is given, the text gets appended to the output file if the file already exists, otherwise a new output file is created to receive the text. If this qualifier is omitted,

the output file is overwritten if it already exists.

/WAIT=<n>

Enter a value to represent the number of seconds to wait after text is displayed. The script will continue after this number of seconds or when you press a key, whichever occurs first. The valid value range is -1 to $1.0x10^{10}$ seconds. A value of -1 will wait indefinitely until you press a key.

Example:

The following commands direct GADDS to display double-height text in its image area, then to wait for 16 seconds (or a keyboard key) before continuing:

```
echo /out=wrtext.tmp "!@!C1,2"

echo /app /out=wrtext.tmp "!@!A .1 .75" "In this example, we determine"

echo /app /out=wrtext.tmp "!@!A .1 .70" "the structure of a small compound,"

echo /app /out=wrtext.tmp "!@!A .1 .65" "the YLID (C[11] H[10] N[2] S)."

graph /file /quad=0 wrtext.tmp

wait 16.
```

12.2 Menumode

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: MENUMODE

MENUMODE is available in command line mode at the GADDS> prompt. Use this command to exit command mode and to return to menu mode. MENUMODE takes no arguments.

12.3 Quit

Menu Command: App menu Close, Close box

Accelerator: Alt+F4 (NT only)

User Level: Command, All

SLAM Syntax: QUIT

QUIT is available in command line mode at the GADDS> prompt, or from the application menu or close box on the title bar. Whereas File > Exit GADDS updates the configuration file before returning to the operating system, QUIT does not save the configuration, but instead throws away any changes you've made since starting the program. QUIT takes no arguments.

12.4 Peaks

While the TOPAS software package sports superior profile fitting algorithms, GADDS still has some primitive profile fitting features. If your profile fitting needs are minimal, the GADDS PEAKS command may be sufficient for your needs.

To access PEAKS:

1. Go to Special > Command Mode.
2. Select Peaks. A pop-up menu of all the PEAKS commands will appear.
3. Type MENUMODE (or MENU) to exit command mode and return to menubar control.

If you constantly use these old PEAKS commands, add them to your “usertasks.” The provided file “usertask.pks” is a good start. Replace your “usertask.ini” with this file (rename to usertask.ini). Then you will see these old Peaks commands under the “User” heading.

NOTE: If you cancel or get an error message, the message is displayed below and the program stays in command mode (you must type “menu”). While it is possible to write script files with error handling so “MENUMODE” is always executed, then you don’t see an error message.

PEAKS has twelve subcommands:

EXIT	Close the PEAKS submenu and return to the GADDS menu
AUTO	Automatically locate and refine peaks
CLEAR	Clear pattern/graphs in selected quadrant(s)
LOAD	Load *.PKS file
MANUAL	Manually select peak positions and parameters
POSTER	Annotate screen before printing
PROFILE	Define peak profile shapes
REFINE	Refine peak parameters after manual editing
SAVE	Save peak table to disk file
SIMULATE	Simulate peak profile shapes
VIEW	View the current peak parameter table
ZOOM	Select new plotting limits

When you start PEAKS from the command line, you need to specify one of these subcommands as a qualifier (if not, the submenu appears and GADDS waits until you have made a selection). To select one of these options, highlight it with the arrows or mouse. A help message appears on the bottom status line describing the action taken by the selected item. To start the selected option, press ENTER. To exit and return to the menu bar, select EXIT or press ESC.

PEAKS uses profile analysis to produce very accurate peak positional, intensity, and FWHM data. Also, standard deviations of peak parameters can be obtained. At least once after installation and prior to executing either PEAKS/AUTO or PEAKS/REFINE, you must generate the required peak profile(s) by running PEAKS/PROFILE. These profile lineshapes are used in the least squares refinement of all peak parameters. During the least squares refinement, any peak parameter may be fixed or variable (refined).

Representative profile lineshapes can be either collected data or simulated data using mathematical functions. PEAKS/SIMULATE allows you to use a Cauchy (Lorentian), Gaussian, modified Cauchy, asymmetrical Cauchy, Pseudo-Voigt, Pearson VII, or split Pearson VII function to model the profile shape.

PEAKS/PROFILE creates the profile lineshape file by allowing you to select one or more representative lineshapes at various 2θ positions. Each lineshape should be an isolated peak and the profile fitting algorithm works best with lineshapes taken at low, medium and high 2θ angles. The α_2 contribution must be either consistently present or consistently absent from all peak profiles. All profiles are stored in a special format of DIFFRAC-AT raw data structure and the individual profile shapes can be displayed with PEAKS/LOAD.

PEAKS/AUTO analyzes a diffraction pattern by searching for peaks, resolving overlapping peaks, and refining the position, intensity and FWHM of all peaks. If the selected profile lineshapes have α_2 removed, AUTO can refine both the α_1 and α_2 lines simultaneously, providing the resolution of the overlapped α_2 line with an unrelated α_1 line, as in the “five fingers of quartz” region. AUTO first dissects the scan range into multiple regions which include data points of at least BKGDSIG standard deviations above background. Each region must start in background and end in background or the peak(s) are not found (in this case, you must use PEAKS/MANUAL to locate peaks). Each region has a maximum number of steps (currently 1024) and a maximum number of allowed peaks (15). You may have to manually manipulate regions with numerous overlapping peaks.

For each region, the background is assumed to be a linear function in 2θ. Least squares estimates of the left and right backgrounds are per-

formed. With the removal of background, the largest remaining sample point is compared to PEAKSIG times the standard deviation of that point. Values greater than this quantity result in a peak being added. Least squares estimates are performed on peak position, FWHM and intensity, as well as the backgrounds. GADDS then reiterates, identifying and removing the largest peak from the remaining data until either 15 peaks are found or the largest residual intensity is below PEAKSIG times standard deviation. The standard deviations generated by AUTO are measures of the precision of the refined parameters. Systematic errors such as 2θ zero error, sample positional error, and absorption must be taken into account.

PEAKS/MANUAL is used to interactively choose peaks and their parameters. The most frequent use of MANUAL is to correct any shortcomings of PEAKS/AUTO, which is known to have difficulties whenever the scan range begins or ends within a peak and with extremely complicated patterns with more than 15 overlapping peaks. MANUAL lets you enter all peak and background data, as well as variables you want to refine. After entering or modifying peaks parameters with MANUAL, PEAKS/REFINE performs a least squares fit of all variable parameters. Very accurate results can be obtained from user-specified peaks.

The final peak parameter table can be saved to an ASCII file with PEAKS/SAVE. Also, PEAKS/VIEW re-lists the current peak parameter table on the screen. The ASCII peak parameter files consist of three sections:

- General header with file, date, title, wavelengths, and range.
- Peak data table with ds, 2Ts, Is, Irel, and FWHMs.
- Background data table with 2T start and end of each region and backgrounds.

Full visual screen control is accomplished with PEAKS/CLEAR. Screen text windows can be cleared; or the raw data trace, peak profiles, or both can be cleared from any quadrant. Additional options permit the destruction of the raw or peak data from internal memory.

12.4.1 PEAKS/AUTO

AUTO analyzes a diffraction pattern, searching for peaks, resolving overlapping peaks, and refining the position, intensity and FWHM of all peaks. If the selected profile lineshapes have α_2 removed, AUTO can refine both the α_1 and α_2 lines simultaneously, providing resolution of the overlapped α_2 line with an unrelated α_1 line as in the “five fingers of quartz” region. AUTO first dissects the scan range into multiple regions which include data points of at least BKGDSIG standard deviations above background. Each region must start in background and end in background or the peak(s) are not found (in this case, you must use PEAKS/MANUAL to locate peaks). Each region has a maximum number of steps (currently 1024) and a maximum number of allowed peaks (15). You may have to manually manipulate regions with numerous overlapping peaks.

For each region, the background is assumed to be a linear function in 2θ. Least squares estimates of the left and right backgrounds are performed. With the removal of background, the largest remaining sample point is compared to PEAKSIG, multiplied by the standard deviation of that point. Values greater than this quantity result in a peak being added. Least squares estimates are performed on peak position, FWHM and intensity, as well as the backgrounds. GADDS then reiterates, identifying and removing the largest peak from the remaining data until either 15 peaks are found or the largest residual intensity is below PEAKSIG times standard deviation.

The standard deviations generated by AUTO are measures of the precision of the refined parameters. Systematic errors such as 2θ zero error, sample positional error, and absorption must be taken into account. During the least squares, the refined parameters are background, peak 2θ, peak-intensities, and the FWHM. The FWHM are grouped (variable, but all peaks within a region possess the same FWHM); however, during the final refinement, the FWHM are set to variable. If the least squares fails to converge, the FWHM are fixed and a final refinement is performed.

PEAKS/MANUAL is used to interactively choose peaks and their parameters. The most frequent use of PEAKS/MANUAL is to correct any shortcomings of PEAKS/AUTO, which is known to have difficulties whenever the scan range begins or ends within a peak and with extremely complicated patterns with more than 15 overlapping peaks. PEAKS/MANUAL lets you enter all peak and background data, as well as variables which you wish to refine. See *Applied Crystallography* by J. Taupin (1973) volume 6, page 266.

When started from the command line, PEAKS/ AUTO takes the following arguments:

```
PEAKS /AUTO $1 /FWHM=[n] /PEAKSIG=[n] /
BKGDSIG=[n] /VERBOSE /GRAPH /SPLIT=[n]
&
/FLAG=[n] /RATIO=[n] $2 $3
```

where the arguments are:

$1	(CALIBRATION FILE) Calibration file containing representative profile lineshapes.
BKGDSIG=[n]	(BKGD) Background significance used to determine regions containing peaks.
PEAKSIG=[n]	(PEAK SIGNIFICANCE) Peak significance to adding new peaks.
FWHM=[n]	(INITIAL FWHM) Initial FWHM is used to: • Determine minimum size of region (removes spurious background points). • Capture tails of peaks by extending regions twice the FWHM. • Attempt to resolve peaks with a FWHM 1.75*input as two overlapping peaks. • Set initial FWHM of new peaks before refinement.
VERBOSE	(VERBOSE OUTPUT Y/N) Non-verbose output lists only the resulting peak parameters. Verbose output lists regions, refinements with standard deviations, and the final peak parameter table.
GRAPH	(GRAPH PEAKS Y/N) Check the box to draw the resulting fitted peak profiles.
FLAG=[n]	(NUMBER OF WAVELENGTHS) [Default: 1] Flag = 1 or 2. Determines the number of wavelengths present. NOTE: If the profile shapes contain a1 and a2 lines, FLAG must be set to “1”.
SPLIT=[n]	(ALPHA-1/ALPHA-2 SPLIT) [Default: 0.0] Alpha-1 to alpha-2 split at true zero. May be non-zero for incident beam monochromator systems.
RATIO=[n]	(ALPHA-1/ALPHA-2 RATIO) [Default: 0.5] Alpha-1/alpha-2 intensity ratio.
$2	(2THETA BEGIN) Starting 2θ for peak fitting.
$3	(2THETA END) Ending 2θ for peak fitting.

12.4.2 PEAKS/CLEAR

Full visual screen control is accomplished with CLEAR. Screen text windows can be cleared. Also, the raw data trace, the peak profiles, or both, can be cleared from any quadrant. Additional options let you destroy raw or peak data from internal memory.

When started from the command line, PEAKS/CLEAR takes the following arguments:

```
PEAKS /CLEAR $1 /DATA_SAVE /TRACE_SAVE
/PEAKS_SAVE /FIT_SAVE /SCREEN_SAVE
```

where the arguments are:

$1	(SCREEN QUADRANT) Quadrant to clear: 1 = none 0 = full 1-4 = respective quadrants 5-6 = top or bottom half of screen
DATA_SAVE	(PRESERVE RAW DATA Y/N) Check the box to preserve raw data in internal memory.
TRACE_SAVE	(PRESERVE RAW TRACE Y/N) Check the box to preserve graphic raw data trace.
PEAKS_SAVE	(PRESERVE PEAK DATA Y/N) Check the box to preserve peak parameters in internal memory.
FIT_SAVE	(PRESERVE PROFILES Y/N) Check the box to preserve graphic peak profiles.
SCREEN_SAVE	(PRESERVE TEXT SCREENS Y/N) Check the box to preserve text screens.

12.4.3 PEAKS/LOAD

Raw data traces must be displayed with INTEGRATE or PEAKS/LOAD, which can read either a DIFFRAC-AT v1 or v2 file, DIFFRAC-5000 file, or a PLOTSO file, regardless of which computer platform is being operated. GADDS can directly read DIFFRAC-5000 files, on which only ranges in the first series are accessible.

When started from the command line, PEAKS/LOAD takes the following arguments:

```
PEAKS /LOAD $1 /RANGE=[n] /QUADRANT=[n]
```

where the arguments are:

$1	(INPUT FILENAME) DIFFRAC-AT v1/v2, DIFFRAC-5000 or PLOTSO file containing raw data. The file format does not need to be specified, PEAKS/LOAD automatically determines which file format is being read.
RANGE=[n]	(INPUT RANGE) Scan range to read. On DIFFRAC-5000 files, only ranges in the first series can be accessed.
QUADRANT=[n]	(DISPLAY QUADRANT) Specifies the quadrant to display the raw data trace:
	0 = full screen
	1-4 = respective quadrants
	5-6 = top or bottom half of screen

12.4.4 PEAKS/MANUAL

MANUAL is used to interactively choose peaks and their parameters. The most frequent use of MANUAL is to correct any shortcomings of PEAKS/AUTO, which is known to have difficulties whenever the scan range begins or ends within a peak, and with extremely complicated patterns with more than 15 overlapping peaks. MANUAL lets you enter all peak and background data, as well as variables which you wish to refine. At least once after installation and before executing MANUAL, you must run PEAKS/PROFILE to generate the required peak profile(s) file. These profile lineshapes are used to overlay the manually inserted peaks overtop the displayed raw data pattern. After entering or modifying peaks parameters with MANUAL, PEAKS/REFINE performs a least squares fit of all variable parameters. Very accurate results can be obtained from user-specified peaks.

MANUAL can be used in interactive mode only. When you choose PEAKS/MANUAL from the menu bar, a vertical cursor appears. Within the statistics window is the wavelength, 2θ, d-spacing, and intensity for the current cursor position. If the cursor resides within a peak region, the region start/end and backgrounds area also displays in the statistics window. The peak parameters (2T, d, I, FWHM) of the nearest peak within the peak region are also displayed.

MANUAL has four options. Press ENTER or the left mouse button to display the submenu, or press the first letter of the subcommand to directly enter that option. Choices are:

ADD	Add a new peak. All peak parameters are defaulted using values obtained at the current cursor position and a pop-up entry menu appears. Upon exiting, the peak is saved and a peak profile is drawn.
DELETE	Delete the peak nearest the current cursor position. No further arguments are required. The peak profile is also deleted.
MODIFY	Modify a peak's current parameters. A menu appears with the current peak parameters. Upon exiting, the peak profile is erased and redrawn with the new parameters.
REGION	Add or modify a region's current parameters. A menu appears with the current (or defaulted) region parameters. Upon exiting, all peaks within the region are erased and redrawn with the new region parameters.

If you try to add a peak before you specify a peak region, both REGION and ADD are executed.

When started from the command line, PEAKS/MANUAL takes no arguments and can only be run in interactive mode. Command line syntax is:

```
PEAKS /MANUAL
```

12.4.5 PEAKS/POSTER

With this command, you can interactively annotate plots or frame images. PEAKS/POSTER has seven subcommands:

EXIT	Close the POSTER submenu and return to GADDS menu
DRAW	Draw various objects on screen
EDIT	Edit current annotations
CLEAR	Clear annotations within rectangular region
LABEL	Label spots/peaks using d, I, HKL, TH, 2T, etc.
SAVE	Save annotations to PLOTSO file
TEXT	Position text on screen

When you choose PEAKS/POSTER from the menu bar, GADDS displays a pop-up submenu containing these subcommands. When you start PEAKS/POSTER from the command line, no qualifiers are allowed. The submenu appears and GADDS waits until you have made a selection. PEAKS/POSTER runs in interactive mode only. To select one of the options, highlight it with the arrows or mouse. A help message appears on the bottom status line describing the action taken by the selected item. Press ENTER to run the selected item. To exit or return to the menu bar, select EXIT or press ESC.

PEAKS/POSTER/DRAW

When you choose PEAKS/POSTER/DRAW from the menu bar, GADDS displays a pop-up submenu containing these subcommands:

EXIT	Close the DRAW submenu and return to the POSTER menu
ARROW	Draw an arrow pointer
BOX	Draw a rectangular box
CIRCLE	Draw an ellipse
DOT	Draw a single dot
LINE	Draw a straight line
STYLE	Switch between solid and dashed line styles

PEAKS/POSTER/DRAW/ARROW

PEAKS/POSTER/DRAW/ARROW is used to draw an arrow. When selected, a crosshair is visible. To draw an arrow:

1. Use the mouse to position the crosshairs at the point of the arrow to be drawn and press ENTER. The crosshairs are replaced with an arrow that has the point anchored at the selected position and the tail at the cursor position.
2. Position the tail of the arrow and press ENTER. The arrow is drawn and a crosshairs cursor appears to position the next arrow.
3. When you are finished, press ESC to return to the DRAW menu.

PEAKS/POSTER/DRAW/BOX

PEAKS/POSTER/DRAW/BOX is used to draw a rectangular box. When selected, a crosshair cursor is visible. To draw a box:

1. Use the mouse to position the crosshairs at a corner of the box to be drawn.
2. Press ENTER to anchor the corner. The crosshairs are replaced with a rectangular box with one corner at the anchored point just selected and the other corner at the current cursor position.
3. Position the second box corner and press ENTER. The box is drawn and a crosshairs cursor appears to position the next box.
4. When you are finished, press ESC to return to the Poster menu.

PEAKS/POSTER/DRAW/CIRCLE

PEAKS/POSTER/DRAW/CIRCLE is used to draw an ellipse. When selected, a crosshair cursor appears. To draw a circle:

1. Use the mouse to position the crosshairs at the center of the ellipse and press ENTER to anchor this spot. The crosshairs are replaced with an ellipse drawn with the center anchored and the width and height selected from the cursor.
2. Move the mouse until the width and height are correct and press ENTER. The ellipse is drawn, and a crosshairs cursor appears to position the ellipse center.
3. When you are finished, press ESC to return to the POSTER menu.

PEAKS/POSTER/DRAW/DOT

PEAKS/POSTER/DRAW/DOT is used to draw a single dot. When selected, a crosshair cursor appears. To draw a dot:

1. Use the mouse to position the crosshairs at the point you want to draw the dot and press ENTER. A dot is drawn and the crosshairs remain to position the next dot.
2. When you are finished, press ESC to return to the POSTER menu.

PEAKS/POSTER/DRAW/LINE

PEAKS/POSTER/DRAW/LINE is used to draw a line segment between two points. When selected, a crosshairs cursor is visible. To draw a line segment:

1. Position the crosshairs at the start of the line segment to anchor the segment and press ENTER. The crosshairs are replaced with a line segment between the anchored point and the current cursor position.
2. Position the line segment end point and press ENTER. The line segment is drawn and a crosshairs cursor appears to position the next line.
3. When you are finished, press ESC to return to the POSTER menu.

PEAKS/POSTER/DRAW/STYLE

PEAKS/POSTER/DRAW/STYLE is used to toggle between drawing objects with a solid line and drawing objects with a dashed line style. The current style is displayed in the submenu title bar.

PEAKS/POSTER/EDIT

All poster annotations are stored in a PLOTSO file format. These commands can be edited with a simple screen editor. After exiting EDIT, the graphics plane is erased and the poster annota-

tions are redrawn. This erases all graphs displayed before starting PEAKS/POSTER.

PEAKS/POSTER/CLEAR

PEAKS/POSTER/CLEAR is used to clear a rectangular region. When selected, a crosshair cursor appears. To clear a region:

1. Position the crosshairs at a corner of the box to be erased.
2. Press ENTER to anchor the corner. The crosshairs are replaced with a rectangular box that has one corner anchored at the point just selected and the other corner at the current cursor position.
3. Position the second box corner and press ENTER. The box is erased and a crosshairs cursor appears to position the next box.
4. When you are finished, press ESC to return to the DRAW menu.

PEAKS/POSTER/SAVE

PEAKS/POSTER/SAVE saves all poster annotations in a PLOTSO file on disk. It can later be retrieved with PEAKS/FILE. Enter the PLOTSO filename and choose whether to APPEND.

PEAKS/POSTER/TEXT

Text can be positioned and sized interactively with PEAKS/POSTER/TEXT. To use TEXT:

1. Select TEXT from the PEAKS/POSTER submenu and press ENTER. You are prompted to enter the text string to be displayed.
2. Enter the text string to be displayed and press ENTER. All trailing spaces are removed from the text string, but leading spaces are retained. A box cursor appears that reflects the size of the text string.
3. Press ESC to return to the DRAW menu.
4. Move the cursor left (or right) to increase (or decrease) the size of the text string in the “x” direction. Move the cursor up and down to change the height of the text.
5. Press ENTER to anchor the text size.
6. Use the mouse to position the box cursor and press ENTER. The box disappears and the text is drawn. You are then prompted to enter the next text string to draw.

PEAKS/POSTER/LABEL

Spots or peaks can be labeled interactively with PEAKS/POSTER/LABEL. To use LABEL:

1. Select LABEL from the PEAKS/POSTER submenu. A pop-up menu appears.

2. Choose what type of data to retrieve (Data type): θs, 2θs, ds, Is, or HKLs.
3. Choose where to retrieve the data from (LABEL option): the frame, raw trace, or peaks table.
4. Choose what marker character to use to highlight the data. A crosshairs cursor appears and the selected label appears in the message window.
5. Press ENTER to draw the marker at the current cursor position and automatically display the TEXT option; when you have finished, press ESC to return to the POSTER menu without drawing the label.
6. Edit, position and size the label to be drawn (see *GRAPH/POSTER/TEXT*).

12.4.6 PEAKS/PROFILE

PEAKS/PROFILE has four subcommands:

EXIT	Close PROFILE submenu and return to PEAKS menu
NEW	Create a new profile lineshape file
ADD	Add a profile to existing lineshape file
DELETE	Delete a profile from an existing lineshape file

When you choose PEAKS/PROFILE from the PEAKS menu, GADDS displays a pop-up submenu containing these subcommands. When you start PEAKS/PROFILE from the command line, you need to specify one of these subcommands as a qualifier (if not, the submenu appears and GADDS waits until you have made a selection). To select one of the options, highlight it with the arrows or mouse to highlight the desired selection. A help message appears on the bottom status line describing the action taken by the selected item. To begin the highlighted action, press ENTER. When you are finished, select EXIT or press ESC to return to the menu bar.

Representative profile lineshapes can be either collected data, or simulated data using mathematical functions. SIMULATE allows you to use a Cauchy (Lorentian), Gaussian, modified Cauchy, asymmetrical Cauchy, Pseudo-Voight, Pearson VII, or a split Pearson VII function to model the profile shape.

PROFILE creates the profile lineshape file by allowing you to select one or more representative lineshapes at various 2θ positions. Each lineshape should be an isolated peak and the profile fitting algorithm works best with lineshapes taken at low, medium, and high 2θ angles. The α_2 contribution must be either consistently present or consistently absent from all peak profiles.

Profile lineshape is selected by specifying a 2θ background range on both sides of a peak. The average intensity within the low and high background regions is used to subtract a linear background from beneath the Bragg peak. The resulting peak function is rescaled and stored with the FWHM and 2T position in a profile parameter file, which is a special format of a DIFFRAC-AT v1 raw data file. Individual profile functions can be displayed with PEAKS/LOAD.

PEAKS/PROFILE/NEW

When started from the command line, PEAKS/PROFILE/NEW takes the following arguments:

```
PEAKS /PROFILE /NEW $1 $2 $3 $4 $5
```

where the arguments are:

$1	(CALIBRATON FILE) Filename for profile file (deletes existing file).
$2,$3	(START LOW BKGD) Low background start and end 2θ.
$4,$5	(START HIGH BKGD) High background start and end 2θ.

PEAKS/PROFILE/ADD

When started from the command line, PEAKS/PROFILE/ADD takes the following arguments:

```
PEAKS /PROFILE /ADD $1 $2 $3 $4 $5
```

where the arguments are:

$1	(CALIBRATON FILE) Filename for profile file to append or insert new profile.
$2,$3	(START LOW BKGD) Low background start and end 2θ.
$4,$5	(START HIGH BKGD) High background start and end 2θ.

PEAKS/PROFILE/DELETE

When started from the command line, PEAKS/PROFILE/DELETE takes the following arguments:

```
PEAKS /PROFILE /DELETE $1 $2
```

where the arguments are:

$1	Filename of profile file.
$2	Profile number to delete (profiles stored in ascending 2T order).

12.4.7 PEAKS/REFINE

PEAKS/REFINE performs a least squares fit of all variable parameters. Very accurate results can be obtained from user-specified peaks.

When started from the command line, PEAKS/REFINE takes the following arguments:

```
PEAKS /REFINE $1 /VERBOSE /GRAPH /
SPLIT=[n] /FLAG=[n] /RATIO=[n] $2 $3
```

where the arguments are:

$1	(CALIBRATION FILE) Calibration file containing representative profile lineshapes.
VERBOSE	(VERBOSE OUTPUT Y/N) Non-verbose output lists the resulting peak parameters. Verbose output lists regions, refinements with standard deviations, as well as the final peak parameter table.
GRAPH	(GRAPH PROFILE Y/N) Check the box to draw the resulting fitted peak profiles.
FLAG=[n]	(NO. OF WAVELENGTHS) [Default: 1] Flag = 1 or 2. Determines the number of wavelengths present.
	NOTE: If the profile shapes contain a1 and a2 lines, FLAG must be set to 1.
SPLIT=[n]	(ALPHA1/ALPHA2 SPLIT) [Default: 0.0] a1 to a2 split at true zero. May be non-zero for incident beam monochromator systems.
RATIO=[n]	(ALPHA2/ALPHA1 RATIO) [Default: 0.5] a1/a2 intensity ratio.
$2	(2THETA START) Starting 2θ for peak fitting.
$3	(2THETA END) Ending 2θ for peak fitting.

12.4.8 PEAKS/SAVE

SAVE copies the peak parameter table from memory to a specified disk file for retention. The peak file is ASCII and can easily be printed on any printer or read by any screen editor. The ASCII peak parameter files consist of three sections:

- General header with file, date, title, wavelengths, and range.
- Peak data table with ds, 2Ts, Is, Irel, and FWHMs.
- Background data table with 2T start and end of each region and background.

The peak parameter table is created with either AUTO or MANUAL. It is modified with MANUAL and REFINE and can be destroyed with CLEAR.

When started from the command line, PEAKS/SAVE takes the following arguments:

```
PEAKS /SAVE $1 /APPEND
```

Each argument is listed below by its command line name, followed by its input panel prompt in parentheses:

$1	(PEAKS FILE) Filename to create or append another peak table.
APPEND	(APPEND Y/N) Check the box to append the new peak table at the end of any existing file. Leave it blank to overwrite any existing peak file.

12.4.9 PEAKS/SIMULATE

SIMULATE has nine subcommands. When you choose it from the menu bar, GADDS displays a submenu containing the subcommands. When you start PEAKS/SIMULATE from the command line, you need to specify one of the subcommands as a qualifier (if not, the submenu appears and GADDS waits until you have made a selection). The subcommands are:

EXIT	Close REFINE submenu and return to PEAKS menu
CAUCHY	Symmetric Cauchy function (Lorentzian)
GAUSSIAN	Symmetric Gaussian function
MODCAUCHY	Modified Cauchy function
ASYMCAUCHY	Asymmetric Cauchy function
PSEUDO	Pseudo-Voigt function
PEARSON	Pearson VII function
SPLIT	Split Pearson VII function
COSINE	Cosine function for c scans

To select one of the options, highlight it with the arrows or mouse. A help message appears on the bottom status line describing the action taken by the selected item. To begin the highlighted action, press ENTER. When you are finished, select EXIT or press ESC to return to the menu bar.

Profile lineshapes are used in the least squares refinement of all peak parameters. Representative profile lineshapes can be either collected data, or simulated data using mathematical functions. SIMULATE lets you use a Cauchy (Lorentzian), Gaussian, modified Cauchy, asymmetrical Cauchy, Pseudo-Voigt, Pearson VII or a split Pearson VII function to model the profile shape.

Profile lineshape functions used by SIMULATE are given below:

Gaussian	A exp ((x/k)2)
Cauchy (Lorentzian)	A (1 + k2 x2)-1
Modified Cauchy	A (1 + k2 x2)-N
Asymmetric Cauchy	above with different N for each side of peak
PSEUDO-Voigt	A [w(x) + (1-w) G (x)]
Pearson VII	A [1 + 4 (2-M -1) (x/k)2]-M
SPLIT Pearson VII	above with different M for each side of peak
Cosine	1+cos x

You must supply the 2θ value of the peak and any required exponents or weight fractions. PEAKS/SIMULATE/VIEW then calculates and displays the lineshape function.

PEAKS/SIMULATE/CAUCHY

When started from the command line, PEAKS/SIMULATE/CAUCHY takes the following argument:

```
PEAKS /SIMULATE /CAUCHY $1
```

where the argument is:

$1	(2THETA)

PEAKS/SIMULATE/GAUSSIAN

When started from the command line, PEAKS/SIMULATE/GAUSSIAN takes the following argument:

```
PEAKS /SIMULATE /GAUSSIAN $1
```

where the argument is:

$1	(2THETA)

PEAKS/SIMULATE/MODCAUCHY

When started from the command line, PEAKS/SIMULATE/MODCAUCHY takes the following arguments:

```
PEAKS /SIMULATE /MODCAUCHY $1
/EXPONENT=[n]
```

where the arguments are:

$1	(2THETA)
Exponent=[n]	(EXPONENT)

PEAKS/SIMULATE/ASYMCAUCHY

When started from the command line, PEAKS/SIMULATE/ASYMCAUCHY takes the following arguments:

```
PEAKS /SIMULATE /ASYMCAUCHY $1
/LOWEXP=[n] /HIGHEXP=[n]
```

where the arguments are:

$1	(2THETA)
LOWEXP=[N]	(EXPONENT)
HIGHEXP=[N]	(EXPONENT)

PEAKS/SIMULATE/PSEUDO

When started from the command line, PEAKS/SIMULATE/PSEUDO takes the following arguments:

```
PEAKS /SIMULATE /PSEUDO $1
/FRACTION=[n]
```

where the arguments are:

$1	(2THETA)
FRACTION=[n]	(CAUCHY FRACTION)

PEAKS/SIMULATE/PEARSON

When started from the command line, PEAKS/SIMULATE/PEARSON takes the following arguments:

```
PEAKS /SIMULATE /PEARSON $1
/EXPONENT=[n]
```

where the arguments are:

$1	(2THETA)
EXPONENT=[n]	(EXPONENT)

PEAKS/SIMULATE/SPLIT

When started from the command line, PEAKS/SIMULATE/SPLIT takes the following arguments:

```
PEAKS /SIMULATE /SPLIT $1 /LOWEXP=[n]
/HIGHEXP=[n]
```

where the arguments are:

$1	(2THETA)
LOWEXP=[n]	(EXPONENT)
HIGHEXP=[n	(EXPONENT

PEAKS/SIMULATE/COSINE

When started from the command line, PEAKS/SIMULATE/COSINE takes the following argument:

```
PEAKS /SIMULATE /COSINE $1
```

where the argument is:

$1	(2THETA)

12.4.10 PEAKS/VIEW

VIEW displays the current peak parameter table. The peak parameter table is created with either AUTO or MANUAL. It is modified with MANUAL and REFINE and may be destroyed with CLEAR. When started from the command line, VIEW takes no arguments:

```
PEAKS /VIEW
```

12.4.11 PEAKS/ZOOM

ZOOM lets you rescale the currently displayed raw data pattern with new axes. Both the upper left corner and lower right corner of the graph must be specified. Enter the new values or select them with the mouse. Interactively, press R to restore the graph to full axes.

When started from the command line, PEAKS/ ZOOM takes the following arguments:

```
PEAKS /ZOOM $1 $2 $3 $4 /RESTORE
```

Each argument is listed below by its command line name, followed by its input panel prompt in parentheses:

$1	(ZOOM 2T-LEFT)
$2	(ZOOM 2T-RIGHT)
$3	(ZOOM I-MIN)
$4	(ZOOM I-MAX)
RESTORE	(RESTORE Y/N)—overrides $1–$4 and restores to original axes.

12.5 Ratemeter

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: RATEMETER $1/RESET=<n> /SHUTTER

The ratemeter option of Collect > Goniometer > Manual command is available in command mode. See Collect > Goniometer > Manual, Section 5.11 for more details.

Each argument is listed below by its command line name.

$1 .....(max seconds) [9999]

Enter maximum number of seconds for exposure.

/RESET=<n>.....(Reset Interval) [0.5]

Enter number of seconds between read-outs.

/SHUTTER.....(Open & Close Shutter) [No]

Check to open shutter before and close after this command.

12.6 Spawn

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: SPAWN

SPAWN is available in command mode at the GADDS> prompt. Use this command to spawn another program, but unlike the SYSTEM command, GADDS is not suspended until the spawned command terminates.

Each argument is listed below by its command line name.

$1 ..... (Command) []

See system command.

12.7 Video/Live

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: VIDEO /LIVE

Use this command to place the VIDEO program into “live” video mode. This command executes immediately without any arguments.

12.8 Video/Freeze

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: VIDEO /FREEZE

Use this command to place the VIDEO program into “frozen” video mode. This command executes immediately without any arguments.

12.9 Wait

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: WAIT $1

WAIT is available only in command line mode, at the GADDS> prompt. WAIT suspends execution of the program for a specified time. If you press ENTER or the left mouse button during the wait period, the program aborts the wait and proceeds. This command is useful in scripts, where you want to display a frame or text and have it remain visible for some minimum length of time.

The valid value range is -1 to 1.0×10^{10} seconds. WAIT will wait indefinitely if you specify a time value of -1. Syntax is:

WAIT $1

where $1 is the wait time in seconds, as a real number.

12.10 ! (comment)

Menu Command: None

Accelerator: None

User Level: Command

SLAM Syntax: ! (any text string)

Use the ! command to add comment lines within a script file. Simply place the “!” character at the start of any line and follow it with your comment statement.

```
! myscript.slm: created 26Mar98 by KLS
! - - - - - - - - - - - - - - - - - - - -
!
! Load first frame in series
DISPLAY...
```

12.11 @ (execute script file)

Menu Command: None, but see UserTasks

Accelerator: None

User Level: Command

SLAM Syntax: @filename p1 p2 p3 p4 p5 p6 p7 p8 p9 p0

Use the @ command to execute commands from a script file while in GADDS's command line mode. You must specify the name of the script file immediately after the @ symbol. By convention, SLAM script files have the extension .slm, and a .slm extension is assumed if none is given in the @ command. The program looks for a script file in three places: current project directory, system data directory (see GADDS$SYSDATA:) or common script directory (see GADDS$SCRIPT:). Follow the filename with the optional replaceable parameters. Replaceable parameters are space deliminated. Any replaceable parameter with embedded spaces must be enclosed within double quotes.

A script file is simply an ASCII file containing a list of SLAM commands in which each line is an individual SLAM command that is executed in sequential order. It is very powerful, and provides a convenient means for automating the more mundane sequence of commands from within the GADDS environment. For more information on script files (creating, editing, nesting, replaceable parameters, and running scripts), see the GADDS User's Manual, Scripts section.

When the script is invoked, each of the lines executes in sequence as if it had been typed at the command line using the parameters and arguments included within the script. That is, GADDS simply starts at the beginning of the script file and proceeds one line at a time until it reaches the end, at which point it stops.

To interrupt a script while in use, press CTRL+BREAK. This will stop the script execution and exit from the script, returning the user to the program's command line prompt. (To return to menus, enter menu mode.)

Several example scripts are provided in your system. The scripts are stored in the GADDS$TEST: directory and are used as part of the demo loop. To execute this demo on the frame buffer, enter:

```
GADDS> @GADDS$TEST:gadds
```

13. Utility Programs

13.1 FrmFix (FRaMe header FIX-up utility)

The program FRMFIX is designed to correct all known problems with Bruker frame file headers. Specifically it can:

- convert frames taken by MICRODIF for DOS to version 8 frame headers. These frames can then be read under GADDS for NT (but not under MICRODIF for DOS).
- correct frames taken by GADDS for NT version 3.300 to 3.302. Under these “beta” NT release, the “AXES2:” and “ENDING2:” lines were incorrectly located at records 076 and 077 and the “FILENAM:” record contained garbage.
- correct frames taken with improper fixed angle settings.
- correct frames with negative scan time bug. These frames were taken for over 12 hours and overnight under programs for DOS.
- correct frames with 360 degree scan width bug. These frames were taken in “STEP” mode under GADDS for DOS or GADDS for NT prior to v3.310.
- correct CCD frames taken on large CCD with SMART v4.040 (requires the switch /BIGCCD).
- correct frames with the first LINEAR frame header parameter having a value that is below 1.0. This is incorrectly stored as the reciprocal of the true value. So far, this problem has only been seen on 2K CCD systems when using 512 frame size but, theoretically, could occur on any area detector system.

- correct CCD frames for bad OCTMASK frame header parameters (frame taken by SMART, to be used by GADDS).
- correct for unreasonable scan times when external trigger was used. ELAPSDA and CUMULAT values are less than 0.05 seconds. Just use ELAPSDR as the scan time.
- correct frames collected on systems where the phi axis was configured to rotate in the wrong direction (Phi should rotate clockwise).

The command frmfix runs the program. When you run frmfix, it starts an interactive dialog. Default values are displayed in square brackets after the prompt. Pressing the ENTER key is the same as entering this default.

FRAME FILENAME ?

Enter the name of the input Bruker format frame. You must give the full pathname. FRMFIX does not merge filenames with the current frame directory. However, FRMFIX does translate logical names under NT or UNIX, and wildcard characters (that is, “*”, “?”) are allowed.

AXIS NUMBER TO RESET ?

Enter 0=none, 1=2T, 2=Om, 3=Ph, 4=Ch, 5=X, 6=Y, 7=Z.

This feature is particularly useful for manually adjustable chi stages, where a scan series was collected while the program contained the wrong fixed chi setting.

VALUE TO SET AXIS ?

Enter new value for scan axis entered above.

As the program executes, Frmfix will display messages stating what was fixed or the message:

Frame.000: Frame header is OK; no fix-up was required.

Alternately all input may be given on the command line. Brackets “[ ]” signify optional parameters and are not typed. <n> signifies that a number is required.

FRMFIX filename [/AXIS=<n> /VALUE=<n>] [/BIGCCD]

/BIGCCD

Updates frame header of CCD frames collected under SMART v4.040 to specify large CCD detector instead of small CCD.

13.2 Frm2Frm (FRaMe to FRaMe file format conversion utility)

Frm2Frm is useful to import of export frame data files to other programs.

Frm2Frm converts to and/or from:

- Bruker frame format (ASCII header, BINARY counts, ASCII overflow table).
- Bruker ASCII frame format (ASCII header, ASCII counts).
- TIFF (CHESS format) (BINARY header, BINARY counts).

It can also convert to (but cannot read these file formats):

- Small Bruker frame format (half-size, that is, 1K -> 512).
- JPEG (courtesy of Larry Finger).

And finally, it can also convert from (but cannot write these file formats):

- Bruker new frame format (ASCII header, BINART counts, Overflow tables).
- APS frame format (ASCII header, BINARY counts)
- TIFF (MMX/MarCCD frame format) (BINARY header, BINARY counts).

FRM2FRM only requires the names of certain files as user input. The user has the option of entering all filenames on the command line or leaving the command line blank and having the program prompt the user for all filenames. Wildcards are permitted in filename inputs.

Syntax for command line (console version only):

FRM2FRM [/B] [/Z] [/#] [/FORMAT:#] filename[.tif] [/OUT:filename[.out]] [/PIXPERCM:##.##] [/CMTOGRID:##.##]

filename.ext1

Required. The name of the frame image file. The input file format is automatically determined.

filename.ext2

Optional. Defaults to “<filename>.out”.

#

Optional. Defaults to Bruker. Possible values are:

1 = Bruker frame file

2 = small Bruker frame file (half-size, that is 1K -> 512)

3 = Bruker ASCII file

4 = TIFF file

5 = JPEG (courtesy of Larry Finger)

6 = imageNCIF (n.y.i.)

[/B]

Batch mode: suppresses final “Hit <Return> to continue” message.

[/Z]

Allow frame dimensions in multiples of 512, instead of $512*2^n$ (512, 1024, 2048, 4096). (SAINT currently does NOT support these odd frame dimensions of 1536, 3072, and 6144).

[/#]

Force output frame file to be 1, 2 or 4 bytes per pixel. (file is saved without an overflow table).

[/P:##.##]

PIXPERCM for imported frames. Default is 0.0= ignore.

[/C:##.##]

CMTOGRID for imported frames. Default is 0.0=ignore.

NOTE: Brackets “[ ]” are not type. They are used to bracket optional or defaulted values.

NOTE: All command line switches may be abbreviated and the separator character may be “:”, “=”, or “-” (that is, “/F:1”, “/F=1”, and “/FORMAT-1” are equivalent).

NOTE: The command line arguments may be in any order.

Current limitations (ignored fields in file header of various frame formats):

- Bruker: Defaults to version 8 frame headers with 4096-byte overflow.
- Bruker ASCII: Cannot read this format, only writes this format.
- TIFF: Reading TIFF files has many limitations:

  TIFF must be a single, full-size, monochrome, and uncompressed image.

  File headers are defaulted to best guess values.

  CHESS: private tags are not translated. Numerous frame header items are defaulted to best guesses.

  MMX/MarCCD: handles only omega or phi scan series.

  - Assume angles are already in Bruker conventions, except for chi (CHImar + 90.0 = CHIbruker). This works for frame series collected at 2t=0, Om=0, phi, Ch=0, which convert to 0, 0, phi, 90 in Bruker angle conventions.
  - Frame number and Number of frames in series are not converted.

  - CCD temp is not converted.
  - Detector roll, pitch and yaw are not converted.
  - NEXP and CCDparms are not converted.
- imageNCIF: (n.y.i.)
- APS: Read only; FRM2FRM cannot write this frame file format.

  Angles in frame header are not converted to Bruker conventions.

NOTE: For compatibility with software requiring 512-byte overflow table, use the environment variable: “SET SAXI$512MAXOVF=1”.

13.3 GADDSMAP (GADDS MAPping program)

This utility program is automatically started when the Analyze > Mapping command starts to process the run series. As each map parameter (e.g., integrated area) is calculated, the X, Y, and map parameter value is sent to GADDS-MAP. The result is a map of a parameter versus XY sample position (or different samples if a sample library was used).

The mapping can be displayed by either a value scale or by a pass/fail criteria. Ratio between two map files can be displayed and saved. The *.gmap file format is documented in online help.

For more information, see online documentation for GADDSMAP.

13.4 Indxtl • NIST index generator

INDXTL builds a hard-disk resident index to a NIST CDF CD-ROM. GADDS uses this index to reduce the time required to perform a CDF search. Normally this index file will reside in GADDS$SYSTEM:cryidx.bin. You must use INDXTL to create this file before GADDS will perform a CDF search.

The NIST Crystal Data CD is available in two major forms:

1. NIST 1999 and later: The inorganic and organic databases reside in separate files, which are CR/LF terminated.
2. ICDD 1997 and earlier: One file contains the inorganic followed by the organic, which is not CR/LF terminated.

To run INDXTL, the following environment variables should be defined (and the NIST CDF CD-ROM must also be placed in the CD-ROM drive):

SAXI$CDF:

This variable defines the directory in which to write the Crystal Data Information File binary index files CRYIDXINO.BIN and CRYIDXORG.BIN (new) or CRYIDX.BIN (old).

SAXI$CDROM:

This variable defines the drive and directory for the Crystal Data Information Files

CRYSTI.DAT and CRYSTO.DAT (new) or CRYSTAL.DAT (old). This is usually a CDROM disk and directory of <drive>:\ORIGFMT\ (new) or drive>:\CRYSTAL\ (old).

SAXI$CDCODE:

This variable defines the drive and directory for the Crystal Data CODENS Files CODENINO.TXT and CODENORG.TXT (new) or CODENS.DAT (old). This is usually a CDROM disk and directory of <drive>:\ (new) or <drive>:\CRYSTAL\VAXIND\ (old).

When you run INDXTL, it starts an interactive dialog. Default values are displayed on the line before the prompt. Pressing a forward slash followed by the ENTER key is the same as entering this default. The program requests the following information and will then run for several minutes periodically printing the number of entries processed as a progress indicator:

OPTIONS

```
  9. Exit
  1. Create indexes for new format (1999
  or later)
  0. Create index for old format

DEFAULT OF CRYSTAL DATA FILE NAME =
<default name>
CHOOSE DEFAULT (/) OR INPUT NEW NAME:
```

Enter the pathname of the CRYSTAL.DAT file. Typically this will be on the CD-ROM in <cd-rom drive>:\CRYSTAL\CRYSTAL.DAT, where <cd-rom drive> represents the drive letter of the CD-ROM on your system.

DEFAULT OF CODENS FILE NAME = <default name>

CHOOSE DEFAULT (/) OR INPUT NEW NAME:

Enter the pathname of the CODENS.DAT file. Typically this will be on the CD-ROM in <cd-rom drive>:\CRYSTAL\VAXIND\CODENS.DAT, where <cd-rom drive> represents the drive letter of the CD-ROM on your system.

13.5 Merge • RAW file range merging utility

This utility program combines the specified ranges from up to ten RAW data files into a single range RAW data file. Mostly, Merge is used to combine the integrated 2T spectra from several area detector frames of differing swing angle into a single continuous range which is more suitable for most DIFFRAC*plus* routines such as phase characterization and identification.

The user has the option of entering ALL filenames on the command line, or to leave the command line blank and have the program prompt the user for all filenames, ranges and options. The resultant merged raw file is always written in DIFFRAC*plus* format; however, the inputted raw files may be of several and even different file formats:

- DIFFRAC-PLUS raw or sim file format.
- DIFFRAC-AT V2 (a.k.a. V3) raw or sim file format.
- DIFFRAC-AT V1 raw or sim file format.
- PLOTSO file format (ASCII).

Merge checks the file and range header records to ensure the mergibility of the ranges. Several checks produce fatal errors:

- Collected on different x-ray tubes (anode).
- Collected at different temperatures.
- Collected at different generator voltage.
- Collected at different generator current.
- Collected using different step widths.
- Collected using overlapping step widths.
- Collected using different scan axes.

Other checks only produce warnings and the user must decide if the ranges are compatible:

- Collected on different dates.
- Collected by different users.
- Collected on different goniometer models.
- Collected on different goniometer stages.
- Collected at different detector distances.
- Collected for different step times.
- Collected using different scan types.

Syntax for command line:

MERGE [/B] [/A] [/S] [/R#[:#]] filein[.raw] [/R#[:#]] [+filein[.raw] [/R#[:#]] [+...]] [merge[.out]]

[/B]

Batch mode: suppresses final “Hit <Return> to continue” message.

[/A]

Averages overlapped regions instead of using weighting factor.

[/S]

Scales merged ranges to first using intensity fit scale factor.

[/R#[:#]]

Merge specific ranges # to #, inclusive. Defaults to all ranges. If [:#] is missing, the ending range defaults to the first range and only one range is merged. The location of the switch is important. Placed after MERGE, /R specifies the default ranges for all input files. When placed after a filename, /R specified the ranges only for that file and will override the default range(s) settings.

filein[.raw]

First input filename. Must be entered, but extension will default to [.raw]. The input file format is automatically determined.

[+...]

Additional input filename(s) and their ranges to merge may be specified up to a maximum of 10 filenames.

[merge[.out]]

Output merged data file. Defaults to “merge.out”.

NOTE: Brackets “[ ]” are not type. They are used to bracket optional or defaulted values.

NOTE: All command line switches may be abbreviated and the separator character may be “:”, “=”, or “-” (that is, “/F:1”, “/F=1”, and “/FORMAT-1” are equivalent).

NOTE: The command line arguments are order specific.

Current limitations (ignored fields in file formats):

- RAW PLUS: supplemental range header records (osc, psd, com).
- RAW PLUS: reading RAW1.00 measuring electronics may be incorrect.
- RAW V2: diffractometer configuration word.
- RAW V2: oscillating drive, amplitude, speed.
- RAW V2: supplemental range header record for comment (4).

Other limitations:

- Cannot merge an additional range in between two other ranges. One must reorder the ranges such that the additional range is being added to the head or tail of the previously merged ranges.

Range	start	end	
1	10.0	40.0	
2	60.0	90.0	
3	35.0	65.0	<- Fails!

- Cannot merge a range when previous ranges are a subset of current range.

Range	start	end	
1	10.0	40.0	
2	05.0	90.0	<- Fails!

13.6 PDFnoind • PDF2 index generator

PDFnoind builds a hard-disk resident index to an ICDD PDF2 CD-ROM. It is required for ICDD PDF2 set 47 and higher. For set 46 and earlier, PDFnoind also works, but the index file is also distributed on the PDF2 CDROM. GADDS uses this index to reduce the time required to perform a PDF2 search. Normally this index file will reside in PDF2$IND:pdfno.ind. You must use PDFNOIND to create this file before GADDS will perform a PDF2 search.

To run PDFNOIND, the following environment variables should be defined (and the ICDD PDF2 CD-ROM must also be placed in the CD-ROM drive):

PDF2$PDF:

> This variable defines the drive and directory for the ICDD PDF2 Database File, PDF2.DAT. This is usually a CDROM disk, and directory of <drive>:\PDF2\.

PDF2$IND:

> This variable defines the drive and directory for the ICDD PDF2 Index File, PDFNO.IND, created by this utility. This must be a hard disk, usually C:\PC-PDF\.

When you run PDFNOIND, it starts immediately and will then run for several minutes, periodically printing the number of entries processed as a progress indicator.

13.7 Plotso

PLOTSO is a separate program for displaying X-Y graphs of data stored in simple ASCII text files. PLOTSO can be started by entering the name of the ASCII file to be plotted on the DOS command line as in the following example:

PLOTSO SAXI$TEST:PLOTSO.DAT

If the filename is not given, PLOTSO will prompt for it. You can print the plot to any supported printer (that is, HP-compatible printer) by pressing CTRL+P after the graph has been drawn. A PRINT SCREEN panel appears with default settings for both the printer device and printer type. The default print filename is SAXI$PRINTER. You can either define this name as a logical name or environment variable, or input a different filename on the panel; use PRN to write directly to a printer on the PC, or SYS$PRINT to write directly to the VAX print queue. The default printer type is PCL4 (HP LaserJet or compatible printer). PLOTSO can also create TIFF files, which can be imported into word processors. TIFF files produced on the PC will include the PLOTSO window border and title, while on other computer platforms only the plot is sent to the TIFF file.

PLOTSO data files are simple ASCII text files which contain X,Y pairs in (FORTRAN-compatible) free format, one pair per line. This results in a simple X-Y plot with automatic scaling of the axes to accommodate the data. The data file may optionally contain directives, which are lines starting with the special 3-character sequence (!@!) that allow you greater control over the appearance of the plot and also allow multiple plots to be defined in the same file. The directive prefix !@! must begin in the first column of a line, one directive per line. A line with the character “!” in the first column is taken as a comment and skipped, unless it starts with the directive prefix. Most of the directives need to be followed by a few parameters, again in free format. Some of the directives require you to specify X,Y fractional coordinates. The convention for these coordinates is that (X,Y) = (0.0, 0.0) corresponds to the lower left of the graph viewport and (X,Y) = (1.0, 1.0) corresponds to the upper right. When you use a directive, the directive remains in effect for all remaining lines in the file, unless superseded by another occurrence of the directive. The directives are:

!@!A

Writes a text string at specified X,Y fractional coordinates. Requires the fractional X, fractional Y, and text string as parameters. Example: “!@!A 0.5,0.5 Your line of text here”.

!@!C

Specifies X,Y character size for subsequent annotation text. Requires the X character size and Y character size as parameters. Each size is specified as an integer from 1

to 4. Example: “!@!C 1,2”. (By default, text is written in size 1,1.)

!@!G

Normally the plot is drawn with a dashed grid highlighting certain tic marks. This directive lets you specify whether or not the grid is to be drawn. Examples are: “!@!G1” (to enable drawing of the grid) or “!@!G0” (to disable drawing of the grid).

!@!L

Sets plot axis limits, overriding the auto-scaling normally performed. Requires four parameters, Xmin, Ymin, Xmax, Ymax corresponding to the lower X, lower Y, upper X, and upper Y axis limits, respectively. If both the lower and upper limit for an axis are specified as zero, autoscaling is restored for that axis. The default limits are 0,0,0,0, meaning that auto-scaling is performed on each axis. When an axis is auto-scaled, a “nice” interval for tic marks is determined. This interval is always 1, 2 or 5 times some power of 10. Limits are then chosen which are integer multiples of this interval and which contain the range of values input for the axis being auto-scaled. An example of this directive is: “!@!L0,0,100,0”. (This example specifies that the X-axis will range from 0 to 100, and the Y will be auto-scaled based on the range of the input Y-values.)

!@!M

Specifies the character to be used as a Marker. The Marker Character is plotted at each subsequent X,Y point. The marker character must immediately follow the directive (that is, it must be the fifth character on the line). Examples are: “!@!M+” (to plot a + at each input X,Y position) or “!@!M” (to disable plotting of a character at each X,Y position).

!@!N

Specifies that subsequent X,Y points should be drawn as a new plot, rather than added to the existing set of axes. This directive requires no parameters. If you use this directive, you'll want to make sure to specify separate “!@!V” viewport directives for each plot, so they don't overlap within the graphing window.

!@!P

Specifies that the X,Y points encountered so far are to be drawn and that subsequent points will be drawn as a separate curve. If you're drawing multiple plots, issue a “!@!P” after the X,Y pairs of the first plot to draw it, followed by a “!@!N” to begin the second. If you're drawing multiple curves in the same plot, issue “!@!P” after the X,Y pairs in each curve.

!@!S

Specifies a line style for a connecting line to be drawn between X,Y pairs. Supply one of the characters 0,N,S or D as a parameter. Line styles are: “!@!S0” or “!@!SN” (for no connecting line, for example, for scatter plots), “!@!SS” (for a solid connecting line), and “!@!SD” (for a dotted connecting line).

!@!V

Specifies the viewport to be used for the subsequent plot, in fractional coordinates representing the fraction of the entire area available for graphs. Requires the four parameters Xmin, Ymin, Xmax, and Ymax, which represent the lower X, lower Y, upper X, and upper Y viewport limits, respectively. By default, these limits are 0,0,1,1, meaning that the viewport occupies the entire graphing area. For example, if you wanted to confine the graph to the left half of the available area, you could issue the directive: “!@!V0,0,.5,1”.

!@!X

This directive specifies the X-axis label. Follow the directive with the text to be drawn along the X axis. By default, the text is “X-AXIS.” For example, if you're plotting a function versus time, you might issue the directive “!@!XTime (seconds)”.

!@!Y

This directive specifies the Y-axis label. Follow the directive with the text to be drawn along the Y axis. By default, the text is “Y-AXIS.” For example, if you’re plotting pixel values as a function of position, you might issue the directive “!@!YPixel Value”. Normally, Y-axis text is written vertically (but not rotated, since some graphic environments, most notably X-Windows, don't support rotated text); however, if the text contains hyphens or parentheses, it writes the text horizontally. In this latter case, you need to keep the axis label very short.

!@!DB

Draws a rectangular box at specified X,Y,W,H fractional coordinates. Requires the fractional X, fractional Y, fractional W, and fractional H as parameters. Example: “!@!DB 0.5,0.5,0.1,0.1”.

!@!DD

Draws a dot at specified X,Y fractional coordinates. Requires the fractional X and fractional Y as parameters. Example: “!@!DD 0.5,0.5”.

!@!DE

Draws an ellipse at specified X,Y,W,H fractional coordinates. Requires the fractional X, fractional Y, fractional W, and fractional H as

parameters. Example: “!@!DE 0.5,0.5,0.1,0.1”.

!@!DL

Draws a line segment between specified X1,Y1,X2,Y2 fractional coordinates. Requires the fractional X1, fractional Y1, fractional X2, and fractional Y2 as parameters. Example: “!@!DL 0.5,0.5,0.1,0.1”.

!@!E

Erases a rectangular box at specified X,Y,W,H fractional coordinates. Requires the fractional X, fractional Y, fractional W, and fractional H as parameters. Example: “!@!E 0.5,0.5,0.1,0.1”.

See SAXI$TEST:PLOTSO.DAT for an example of a PLOTSO data file.

The syntax for starting PLOTSO by:

- NT is: PLOTSO /X=<n> /Y=<n> /W=<n> /H=<n> DATA_FILE
- IRIX is: PLOTSO -X=<n> -Y=<n> -W=<n> -H=<n> DATA_FILE

When you start PLOTSO you can also specify the qualifiers /W=<n> and /H=<n> on the command line, where <n> represents a numeric value. The value given for /W is the desired window width in pixels and the one for /H is the desired window height (if you want the full screen but are not sure of the number of screen pixels, use /W=9999 /H=9999. Under NT or IRIX you can also specify the X and Y pixel numbers desired for the upper left corner of the graphics window with /X=<n> and /Y=<n>. If the /W and /H are not given, they default to 704 and 600 respectively (providing a screen dump which reasonably covers the full page width of both the LaserJet (at 100 dpi) and the PaintJet (at 90 dpi). The window width affects the print screen option. The program requests a dot-per-inch resolution from the printer that is equal to or higher than the screen width in pixels divided by 7.75 inches. The following screen widths fill the printed page reasonably well:

/W=704 (default)	LaserJet @ 100 dpi, PaintJet @ 90 dpi
/W=520	LaserJet @ 75 dpi, PaintJet @ 90 dpi
/W=1024	LaserJet @ 150 dpi, PaintJet @ 180 dpi

NOTE: The smaller widths result in faster screen dumps, especially when the printer is on a serial port.

13.8 Prbatch • Profile fitting in batch mode utility

Used internally by GADDS to perform profile fitting on raw spectra. For more information, see PROFILE*plus* manual.

13.9 PVWave • Precision Visual's Wave procedures

Bruker provides procedures for importing and exporting data in Bruker file formats from within Precision Visual's Wave software (version 3.0).

Directory: C:\SAXI\PVWAVE

SAXII_READ_D5000.PRO	PV-wave procedure to read a Bruker D5000 file.
SAXII_READ_FRAME.PRO	PV-wave procedure to read a Bruker frame file.
SAXII_READ_PLOTSO.PRO	PV-wave procedure to read a Bruker PlotSO file.
SAXII_SAVE_D5000.PRO	PV-wave procedure to save a Bruker D5000 file.
SAXII_SAVE_FRAME.PRO	PV-wave procedure to save a Bruker frame file.
SAXII_SAVE_PLOTSO.PRO	PV-wave procedure to save a Bruker PlotSO file.

13.9.1 SAXII_READ_D5000 (VAX only)

PV-Wave procedure to read a Bruker DIFFRAC-5000 raw data file. Up to ten ranges will be read and displayed.

Usage:

.run saxii_read_d5000

saxii_read_d5000, xarray, yarray [, filename]

where:

xarray (dimension (500,10)) returns the 2theta values of up to ten ranges.

yarray (dimension (500,10)) returns the intensity counts of up to ten ranges.

filename DIFFRAC-5000 *.RAW filename. If missing the procedure will ask for the file-name.

13.9.2 SAXII_READ_FRAME

PV-Wave procedure to read a Bruker area detector frame. Header is type to screen and the image is displayed, and the color table is stretch to fit. This version handles 8-, 16-, or 32-bit frames WITHOUT an overflow table.

PV-Wave's image color table works only on byte images. Values above 256 are clipped upon being displayed. Thus, the user may wish to use the HIST_EQUAL function to rescale 16- or 31-bit frames into byte images:

image = hist_equal (image)

tv, image

Usage:

.run saxii_read_frame

saxii_read_frame, image [, filename, header]

where:

image (dimension (512,512)) returns the byte/word/dword image data

filename Frame data filename. If missing the procedure will ask for it.

header (dimension (*,80)) returns the header information

13.9.3 SAXII_READ_PLOTSO

PV-wave procedure to read a Bruker PLOTSO file.

Usage:

.run saxii_read_plotso

saxii_read_plotso, xarray, yarray [, filename]

where:

xarray (dimension (500,10)) returns the 2theta values of up to ten ranges.

yarray (dimension (500,10)) returns the intensity counts of up to ten ranges.

filename PLOTSO filename. If missing the procedure will ask for it.

13.9.4 SAXII_SAVE_D5000 (VAX only)

PV-wave procedure to save an array as a Bruker d5000 file.

Usage:

.run saxii_save_d5000

saxii_save_d5000, xarray, yarray [, filename]

where:

xarray (dimension (500,10)) 2theta values of up to ten ranges.

yarray (dimension (500,10)) intensity counts of up to ten ranges.

filename DIFFRAC-5000 *.RAW filename. If missing the procedure will ask for the filename.

13.9.5 SAXII_SAVE_FRAME

PV-Wave function to save a Bruker area detector frame. Header is modified from the original frame header. This version handles 8-, 16-, or 32-bit frames WITHOUT an overflow table.

Usage:

.run saxii_save_frame

saxii_save_frame, image [, filename, header]

where:

image (dimension (512,512)) byte/word/dword image data

filename Frame data filename. If missing the procedure will ask for it.

header (dimension (*,80)) header information

13.9.6 SAXII_SAVE_PLOTSO

PV-wave procedure to save an array as a Bruker PLOTSO file.

Usage:

.run saxii_save_plotso

saxii_save_plotso, xarray, yarray [, filename]

where:

xarray (dimension (500,10)) 2theta values of up to ten ranges.

yarray (dimension (500,10)) intensity counts of up to ten ranges.

filename PLOTSO filename. If missing the procedure will ask for it.

13.10 Raw12Fix • Fixes file headers of DIFFRAC-5000 files ported from PC to VAX

After copying a Diffrac-5000 file from PC to a VAX over the network, the RECL in the file header on the VAX file may be incorrectly set at 512-bytes. This is the default for the Community DOS NETCOPY /V command and other network packages. RAW12FIX will change the RECL in the file header.

Syntax: RAW12FIX filename[.raw]

or

$ run saxi$system:RAW12FIX

Enter filename [ra:*.raw]: filename

NOTE: RAW12FIX.VMS must be copied to VMS computer and renamed to RAW12FIX.EXE.

13.11 Raw2Raw • RAW to RAW file format conversion utility

Use RAW2RAW to export or import RAW spectra in various data file formats.

Converts to and/or from:

- DIFFRAC-PLUS raw or sim file format.
- DIFFRAC-AT V2 (aka V3) raw or sim file format.
- DIFFRAC-AT V1 raw or sim file format.
- PLOTSO file format (ASCII).

Can also convert to (but cannot read these file formats):

- DBW and DBWS file formats (ASCII).
- GSAS file format (ASCII).
- UXD file format (ASCII).

Can also convert from (but cannot write these file formats):

- DIFFRAC-5000 V2 (VAX/VMS)
- DIFFRAC-5000 V1 (VAX/VMS)
- NACS (VAX/VMS)
- NACS (PDP-11/TSX|RT-11)
- DIFFRAC-11 (PDP-11/RSX)
- DIFFRAC-5 (PDP-11/RSX)
- Philips UDF format (may read only a subset of UDF files).

RAW2RAW only requires the names of certain files as user input. The user has the option of entering ALL filenames on the command line, or to leave the command line blank and have the program prompt the user for all filenames. Wild-cards are permitted in filename inputs.

Syntax for command line:

RAW2RAW [/B] [/FORMAT:#] filename[.raw] [/OUT:filename[.out]]

Additional switches for UXD output: [/C] [/I:#] [/N] [/Sc] [/W:#] [/2]

[/B]

Batch mode: suppresses final “Hit <Return> to continue” message.

filename[.raw]

Required. The name of the RAW data file containing ranges. The input file format is automatically determined.

filename[.out]

Optional. Defaults to “<filename>.out”.

#

Optional. Defaults to DIFFRAC-PLUS. Possible values are:

1 = DIFFRAC-AT V1

2 = DIFFRAC-AT V2/V3

3 = DIFFRAC-PLUS

4 = PLOTSO

5 = DBW

6 = DBWS

7 = GSAS

8 = UDX

[/C]

CPS mode: Outputs data points in CPS, default is intensity.

[/I:#]

Item number: Outputs data points

[/N]

Noheader mode: Suppress output of header information.

[/Sc]

Separator: ,=comma, ;=semi-colon, s=space, t=tab, n=none.

[/W:#]

Width: Width of each item in characters for default separator.

[/2]

2theta mode: Include 2T angle on each line of data points.

NOTE: "[]" are not typed. They are used to bracket optional or defaulted values.

NOTE: All command line switches may be abbreviated and the separator character may be ":", "=", or "-". (i.e., "/F:1", "/F=1", "/FORMAT-1" are equivalent).

NOTE: The command line arguments may be in any order.

Current limitations (ignored fields in file formats):

- RAW PLUS: supplemental range header records (osc, psd, com).
- RAW PLUS: reading RAW1.00 measuring electronics may be incorrect.
- RAW V2: diffractometer configuration word.
- RAW V2: oscillating drive, amplitude, speed.
- RAW V2: supplemental range header record for comment (4).
- DIFFRAC-5000 V2:

  scintillation detector parameters

  conversions of slit settings (mm to degrees)

  temperature parameters

  other angle settings (chi, phi, x, y)
- DIFFRAC-5000 V1: many fields are not converted.
- NACS VMS: temperature hold time.
- NACS TSX/RT-11: not yet implemented!
- DIFFRAC-11:variable slit settings, fixed theta angle/delay time.
- DIFFRAC-5: totally untested!
- UXD: Only minimal information is in header.

13.12 SAXAD.SYS • Bruker HISTAR NT Driver

SAXAD.SYS is the NT Driver to support and access the Bruker's Area Detector Fast Interface card. For normal configurations, the SETUP program will properly install and configure this driver.

SAXAD driver will allocate 4.25 Mbytes of NON-PAGED memory. This will greatly affect performance on low memory NT systems. A system with at least 20 Mbytes of memory is recommend. Increase virtual memory to at least 35 Mbytes; the WNT default of 21 Mbytes is insufficient. For users who do not collect large frames, set MaxFrameSize = 512 in the registry as this will free 3 Mbytes of unused non-paged memory.

During data collection and flood fields, the SAXAD driver executes at the level "LOW_REALTIME_PRIORITY". Only when the driver checks for an event and no event is in the queue, does the driver permit any time allocation to other processes.

For real-time display during data collection or flood field, the NT system must be equipped with a super fast video card such as a PCI local video card. An ISA bus video card will be excruciatingly slow.

Possible error messages during loading of driver:

"Not enough memory was available to allocate internal storage needed..."

> STATUS_INSUFFICIENT_ RESOURCES, if out of system memory. Reboot might work, else add memory. Or set MaxFrameSize = 512.

"The hardware locations for saxad0 could not be translated to something..."

> STATUS_NONE_MAPPED, if NT cannot map port. Hopefully this error never occurs.

"The hardware addresses for saxad0 are already in use by another device"

> STATUS_DEVICE_ CONFIGURATION_ERROR if IO port is already in use.
> Change IO port address on FAD interface card and in registry.

"Unable to detect Bruker's FAD interface board"

> STATUS_NO_SUCH_DEVICE if Bruker FAD interface fails to respond. Possibly bad board or jumper settings. Or PDC was off when computer was booted.

"Unable to create the symbolic link for saxad0"

> STATUS_NO_SYMBOLICLINK_ CREATED NT cannot create a link to driver. Hopefully this error never occurs.

“Unable to create the device map entry for saxad0”

STATUS_NO_DEVICEMAP_CREATED Driver could not update registry. Hopefully this error never occurs.

Possible error messages during execution of driver:

“Application program passed a buffer too small to device saxad0”

STATUS_BUFFER_TOO_SMALL Bug in GADDS.EXE - report it!

“Application program passed an invalid parameter to device saxad0”

STATUS_INVALID_PARAMETER Bug in GADDS.EXE - report it!

13.12.1 Registry Keys (Optional)

DebugLevel:

[0] Determines which additional debug messages are sent to the Event Log. Range is 0 to 5.

0. Normal warning and error messages only.

1. Above plus driver load and unload messages.

2. Above plus device I/O messages.

3. Above plus data collection messages.

4. Above plus dispatch control messages.

5. Above plus data collection polling messages. (May overflow queue).

PortIOAddress:

[340 hex] Port IO Address of SAXAD Interface Card.

MaxFrameSize:

[1024] Valid values are 512 or 1024.

Orientation:

[0] Defines the mounting orientation of the HISTAR detector.

0. +x, +y, The default.
1. +x, -y, Useless.
2. -x, +y, Useless.
3. -x,-y, Rotated 180 CW
4. +y, +x, Useless.
5. +y, -x, Rotated 270 CW.
6. -y, +x, Rotated 90 CW
7. -y, -x., Useless.

13.13 SaxHelp • Bruker help topic display utility

NOTE: This program is now obsolete. Bruker now supplies help files in either Windows help file format or Acrobat PDF file format.

SaxHelp is used to display the Bruker help topic files: *._tp.

13.14 ToSAXII • Convert PCS XENGEN format frames to new SAXII format

The new SAXII format for data frames addresses the issues of data portability, speed of image I/O and display, and storage of all the data acquisition conditions required to reduce the data. Header and overflow information are stored in portable ASCII rather than binary—critical data such as setting angles can thus be stored portably as floating point values. The pixel values themselves are necessarily binary, but are assured to start on a 512-byte boundary and are stored a a byte stream without delimiters of any kind. This format is completely transportable between a VAX and X-1000 frame buffer over the network.

Older PCS computers used a XENGEN format for data frames. These files can be converted to the newer SAXII format using TOSAXII. The user will be prompted for any missing header information. Example session follows:

```
=> TOSAXII
```

Under DOS, UNIX, or VMS, the command tosaxii runs the program, which prompts you for the following additional information. Default values are displayed in square brackets after the prompt. Pressing the <ENTER> key (<Return> key on VAX) is the same as entering this default.

```
INPUT FILENAME ?
```

Enter the name of the input XENGEN format frame. You must give the full pathname. TOSAXII does not merge filenames with GADDS's or VGADDS's current frame directory; however, TOSAXII does translate logical names under DOS, VMS or UNIX.

INPUT .UPR FILENAME (BLANK IF NONE) ?

If you want to insert orientation information determined by XENGEN's REFINE program into the output frame header, supply the full pathname of the XENGEN parameter file. See the discussion above for more information. Otherwise, press the <ENTER> key without supplying a filename (<Return> key on VAX). GADDS users will simply press <ENTER>.

INPUT .UCA FILENAME (BLANK IF NONE) ?

If you have a .uca (“spline”) spatial calibration file from XENGEN, TOSAXII will obtain the beam center coordinates from it. Supply the full pathname here, otherwise press <ENTER> without supplying a filename, and TOSAXII will explicitly prompt for the beam center coordinates with the prompts:

BEAM X CENTER (XENGEN COORDS) ?

BEAM Y CENTER (XENGEN COORDS) ?

Supply the coordinates of the direct beam at swing angle of zero, in the XENGEN convention (0,0 at upper right in a frame displayed with GADDS or VGADDS).

OUTPUT FILENAME ?

Enter the full pathname to give the output data frame.

OUTPUT FRAME TITLE ?

The text you supply here is written to the output SAXII frame header in the first title record, and will be shown (truncated to 20 characters) on the screen when you display the output frame.

SAMPLE-DETECTOR DISTANCE IN CM (.LE.0 TO USE CURRENT)

If you want to override the detector distance that exists in the input frame header, enter the new value here, otherwise just press <ENTER>.

SWING ANGLE, DEG (9999. TO USE CURRENT)

If you want to override the detector swing angle that exists in the input frame header, enter the new value here, otherwise just press <ENTER>.

A. Area Detector Frame Format

The Bruker format addresses issues of data portability, speed of image I/O and display, and storage of all the data acquisition conditions required to reduce the data. Header and overflow information are stored in portable ASCII, rather than binary. Critical data, such as setting angles, can thus be stored portably as formatted floating-point values. The pixel values themselves are binary, but they are assured to start on a 512-byte boundary for quick, easy access (using Byte IO routines), and they are stored as a byte stream without delimiters of any kind.This format is completely transportable between all computers and networks, including PCs, NT workstations, and SGI systems. The only coding difference on these systems is that big-endian systems such as SGI must byte-swap the pixel values in the (relatively rare) case where it encounters a 16-bit frame.

Up to 32 bits/pixel are supported, although frames are stored where possible as 8 or 16 bits per pixel with an overflow table like that on earlier systems (but this overflow table is ASCII, as described below). BYTE ORDER OF PIXEL VALUES IN FRAMES WHICH ARE STORED IN THIS FORMAT ON DISK, TAPE, ETC. IS ALWAYS “LITTLE-ENDIAN” (LSB first, even though the header contains a flag indicating the pixel byte ordering). Bruker does not support big-endian frames that otherwise look like this format. The 16-bit format is fully implemented. If more than 4096 overflows occur on attempted compression to 8 bits, the frame buffer will compress to 16 bits with an overflow table (the GADDS HI-STAR and SMART CCD frame buffers accumulate 32 bits/pixel internally).

At the top level, a frame in Bruker format can be represented as:

Header
Image data
Overflow table
Trailer 1
.
.
.
Trailer N

A.1 Header

The header is 1) typeable ASCII and 2) an even multiple of the 512-byte disk block size. Each entry in the header is an 80-byte unterminated ASCII line. Thus, the header size is always a multiple of 5 disk blocks to hold an integral number of lines. The first eight characters of each item contain the item name, with the remaining 72 characters for ASCII data. Thus, the organization of the header can be represented as:

HEADER
Item_name1 (8 char): Item_Data1 (72 chars)
Item_name2 (8 char): Item_Data2 (72 chars)
.
.
.
Item_nameN (8 char): Item_DataN (72 chars)

This organization has several advantages. First, fast random access can be performed on the header to pull out or rewrite an individual entry. During random access, the item names provide a method for checking for corruption of the header block.

Second, frames are actually TYPEable on both PCs and workstations if the screen wraps at 80 columns. The padding to a multiple of 5 disk blocks contains ASCII dot characters. The last characters of the padding are a CTRL+Z and a CTRL+D. This convention provides a “warning indicator” on a workstation during which a CTRL+S or CTRL+C can be issued, before the binary pixel values start to appear. On a PC, an

MS-DOS TYPE command stops when it hits the CTRL+Z. Presence of the item names makes the output easily interpretable.

Third, the format is highly portable, because different byte and word ordering conventions don't enter into the interpretation of ASCII data. Items currently contained in the header are listed below in positional order. The format is expandable. New information to be added to the header will always be added at the end. A version number is present at the start of the header so programs can deal with new header information.

The header items are:

Mnemonic	Offset	Version	Type	Description
FORMAT:	0	1	Int	Frame format. Always “86” for Bruker-format frames or 100 for New Bruker format frames.
VERSION:	1	1	Int	Header version #, such as 1, 2, 3, 4, 5, 7, 8, 9, 10, or 11.
HDRBLKS:	2	1	Int	Header size in 512-byte blocks, such as 10 or 15.
TYPE:	3	1	C	String indicating king of data in the frame. Valid primary types are: DEFAULT Add frame Rotation frame SCAN FRAME UNWARPED UNWARPED LINEAR FIDUCIAL PLATE FLOOD FRAMES FLOOD TABLE BACKGROUND <A> & <B> COMBINATION POLE FIGURE, [POLAR | STEREO | WULFF] STRESS, SCHEME Sometimes the primary type is appended with CALIBRATED FIBER LPA MULT_FF PLATE SMOOTHED Pole figure type may be appended with: INTERPOLATED INVERTED NORMED ROTATED SCHEME SYMMETRIZED TILTED

SITE:	4	1	C	Site name, from Edit > Configure > User settings
MODEL:	5	1	C	Diffractometer model, from SAXI$ADMODEL
USER:	6	1	C	Username, from Edit > Configure > User settings
SAMPLE:	7	1	C	Sample ID, from Project > New/Edit
SETNAME:	8	1	C	Basic data set name
RUN:	9	1	Int	Run number within the data set
SAMPNUM:	10	1	Int	Specimen number within the data set
TITLE:	11–18	1	C	User comments (8 lines)
NCOUNTS:	19	1,9	Int	Total frame counts (followed by reference counts in Ver 9). 9: Adds direct-beam monitor counts to NCOUNTS line
NOVERFL:	20	1	Int	Number of overflows
MINIMUM:	21	1	Int	Minimum counts in a pixel
MAXIMUM:	22	1	Int	Maximum counts in a pixel
NONTIME:	23	1	Int	Number of on-time events
NLATE:	24	1	Int	Number of late events.
FILENAM:	25	1	C	(Original) frame filename
CREATED:	26	1	C	Date and time of creation
CUMULAT:	27	1	R	Accumulated exposure time in seconds
ELAPSDR:	28	1	R	Requested time for last exposure in seconds
ELAPSDA:	29	1	R	Actual time for last exposure in seconds
OSCILLA:	30	1	Int	Nonzero if acquired by oscillation
NSTEPS:	31	1	Int	# steps or oscillations in this frame
RANGE:	32	1	R	Scan range in decimal degrees (unsigned)
START:	33	1	R	Starting scan angle value, decimal degrees
INCREME:	34	1	R	Scan angle increment between frames (signed)
NUMBER:	35	1	Int	Sequence number of this frame in series (@0)
NFRAMES:	36	1	Int	Total number of frames in the series
ANGLES:	37	1	4R	Diffractometer angles (2T, OM, PH, CH)
NOVER64:	38	1	Int	Number of pixels > 64K

NPIXELB:	39	1	Int	Number of bytes/pixel, such as 1, 2, or 4.
NROWS:	40	1	Int	Number of rasters in frame, such as 512, 1024, or 2048.
NCOLS:	41	1	Int	Number of pixels/raster, such as 512, 1024, or 2048
WORDORD:	42	1	Int	Order of bytes in word (0=LSB first)
LONGORD:	43	1	Int	Order of words in a longword (0=LSW first)
TARGET:	44	1	C	X-ray target material: Cu, Mo, Ag, Fe, Cr, Co, or other.
SOURCEK:	45	1	R	X-ray source kV
SOURCEM:	46	1	R	X-ray source milliamps
FILTER:	47	1	C	Filter/monochromator setting: Such as: Parallel, graphite Ni Filter C Filter Zr Filter Cross coupled Goebel Mirrors
CELL:	48–49	1	6R	Unit cell A,B,C,ALPHA,BETA,GAMMA
MATRIX:	50–51	1	9R	Orientation matrix (P3 conventions)
LOWTEMP:	52	1,8,9	1: Int 8: Int,3R 9: 3Int	Low temp flag. Note: Version 8 and 9 headers diverge. 8: Add sub-mnemonic TEMP: Adds set point K, ramp rate deg/min, hold time sec 9: Adds experimental temperature in hundredths C and CCD sensor temperature in hundredths C
ZOOM:	53	1	3R	Zoom: Xc, Yc, Mag
CENTER:	54	1	2R	X, Y of direct beam at 2-theta = 0
DISTANC:	55	1	R	Sample-detector distance, cm
TRAILER:	56	1	Int	Byte pointer to trailer info
COMPRES:	57	1	C	Compression scheme ID, if any. Such as: NONE
LINEAR:	58	1	C	Linear scale, offset for pixel values, typically 1.0, 0.0.
PHD:	59	1	2R	Discriminator: Pulse height settings
PREAMP:	60	1	R	Preamp gain setting
CORRECT:	61	1	C	Flood table correction filename
WARPFIL:	62	1	C	Brass plate correction filename

WAVELEN:	63	1, 8	3R 8+: 4R	Wavelengths (average, a1, a2) 8+: Adds beta wavelength.
MAXXY:	64	2	2R	X,Y pixel # of maximum counts
AXIS:	65	3	Int	Scan axis (1–4 for 2-theta, omega, phi, chi) Default is 2.
ENDING:	66	3	4R	Actual goniometer angles at end of frame
DETPAR:	67–68	4	6R	Detector position corrections (dX,dY,dDist,Pitch,Roll,Yaw)
LUT:	69	4	C	Recommended display lookup table
DISPLIM:	70	4	2R	Recommended display limits
PROGRAM:	71	4	C	Name and version of program writing frame, such as: GADDS for WNT V4.0.07
ROTATE:	72	5	Int	Nonzero if acquired by rotation of phi during scan
BITMASK:	73	5	C	File name of active pixel mask associated with this frame or $NULL
OCTMASK:	74–75	5	8Int	Octagon mask parameters to use if BITMASK=$null
ESDCELL:	76–77	7	6R	Unit cell parameter standard deviations

DETTYPE:	78	7 8	C 8+: C, 2R	Detector type MULTIWIRE (default) CCD-PXL (small CCD) CCD-PXL-2K (Large CCD) CCD-PXL-ARR (Mosaic) CCD-PXL-L6000 CCD-PXL-KAF1500 UNKNOWN (imported) OTHER (imported) Version 8+: Added sub-mnemonics PIXPERCM: and CMTO-GRID: which are needed for UNKNOWN or OTHER types. If these values are missing, the defaults are: DETTYPE:PIXPERCM:CMTOGRID: --- MULTIWIRE47.52.0 CCD-PXL-2K56.020.8 CCD-PXL-ARR32.000.4 CCD-PXL-KAF150051.20.8 CCD-PXL-L6000N56.020.8 CCD-PXL-L6000F56.020.8 CCD-PXL-L6500 32.001.5 CCD-PXL-KAF281.920.8 CCD-PXL-KAF 81.920.8 CCD-PXL-MSPD 81.920.8 CCD-PXL 81.920.8 CCD-PXL-LDI 83.3330.0 CCD-MMXImported frames must ask for settings. UNKNOWN Imported frames must ask for settings. OTHER Imported frames must ask for settings.
NEXP:	79	7,9,10	7: Int 9: 2Int 10:3Int	Number of exposures: 1=single, 2=correlated sum (followed by fixed bias ADU in Vers 9). 9: Adds per-exposure bias level in ADU to NEXP line 10: Adds baseline offset (normally 32), Adds Orientation (value of SAXI$INVERTCCD), Adds Overscan flag (1 if overscan used)
CCDPARM:	80	7	5R	CCD parameters: readnoise, e/ADU, e/photon, bias, full scale
CHEM:	81	7	C	Chemical formula in CIFTAB string, such as “?”
MORPH:	82	7	C	Crystal morphology in CIFTAB string, such as “?”

CCOLOR:	83	7	C	Crystal color in CIFTAB string, such as “?”
CSIZE:	84	7	C	Crystal dimensions (3 ea) in CIFTAB string, such as “?”
DNSMET:	85	7	C	Density measurement method in CIFTAB string, such as “?”
DARK:	86	7	C	Name of dark current correction
AUTORNG:	87	7	5R	Auto-ranging: gain, high-speed time, scale, offset, full scale
ZEROADJ:	88	7	4R	Goniometer zero corrections (refined in least squares)
XTRANS:	89	7	3R	Crystal XYZ translations (refined in least squares)
HKL&XY:	90	8	5R	HKL and pixel XY for reciprocal space scan
AXES2:	91	8	4R	Diffractometer setting linear axes (4 ea). (X, Y, Z, Aux)
ENDING2:	92	8	4R	Actual goniometer linear axes @ end of frame. (X, Y, Z, Aux)
	93			
	94			
	95			

NOTE: Items in version 6 headers are obsolete (MICRODIF). Use FRMFIX to convert these frame headers to version 8.

NOTE: Version 5 and 8 items are mainly for GADDS.

NOTE: Version 7 and 9 items are mainly for SMART.

NOTE: Version 9 and 10 items do not add additional lines to the header, but instead append additional values to a previously existing line.

A.2 Image Data

The image data is a simple byte stream (no record delimiters) with one, two, or four bytes per pixel, as defined in the header. If the data are two bytes per pixel, the least-significant byte is first.

The order of the pixels in the file corresponds to the display of pixels on a screen, like the raster-scan order of a CRT display. The first pixel in the file corresponds to the upper-left corner of the display, the 512th to the upper right, and the last pixel to the lower right. This data ordering convention is the one used by most display devices and by the X-Windows library. Frames display as if viewed from the source toward the detector.

A.3 Overflow Table

The overflow table is stored as ASCII values. Each overflow entry is 16 characters, comprising a 9-character intensity and a 7-character pixel # offset. The table is padded to a multiple of 512 bytes. In an 8-bit frame, any pixel with a value of 255 in the image needs to be looked up in the overflow table to determine its true value (even if the true value is 255, to allow overflow table validity checks, which could not otherwise be made). In a similar manner, any pixel in a 16-bit frame with a value of 65535 must be looked up in the overflow table to determine its true value. To look up a pixel value, compute its pixel displacement (for example, in a 512x512 frame, 512*j + k, where j is the zero-based row number and k is the zero-based column number), and compare the displacement with that of each overflow table entry until a match is found. While the overflow table is normally sorted on displacement, it is not guaranteed to be sorted, so we recommend that you search the whole table until you find a match.

A.4 Trailers

The header contains a byte pointer (item name “TRAILER,” set to zero if none) to the location in the file of any “trailer” data that has been tacked onto the image. This provision won't be used immediately, but provides later expansion capability. For example, if a frame is derived from processing some other (parent) frame, the header of the parent could be tacked onto the processed frame as a trailer to provide processing history. The format of a trailer is:

TRAILER

Trailer size in 512-byte blocks (1 byte)

3-byte pad

Trailer data

B. DIFFRAC*plus* Raw Data File Format

The general format of a RAW file is a general file header of 712-bytes, followed by a variable length range header, which in turn is followed by the range's data records. Range header and data records are repeated for all defined ranges.

RAW_HEADER: 712-bytes of information that starts every RAW file. This is identical to DIF_HEADER structure, except for the initial ID code.

Offset	Code	Description
0	C8	ASCIIZ: “RAW1.01” for the 2. release [@2]
		“RAW1.00” for the 1. release
		Note: “RAW2” and “RAW” are DIFFRAC-AT
8	I4	current file status:
		0 = unmeasured
		1 = measured
		2 = active
		3 = aborted
		4 = interrupted
		10 = simulated data [@2]
12	I4	total number of measured ranges
16	C10	ASCIIZ [@2], in mm/dd/yy format, e.g. “12/31/95”
26	C10	ASCIIZ [@2], in 24 hours format, e.g. “18:34:04”
36	C72	ASCIIZ [@2], username (operator) or “Unknown” or “\0”
108	C218	ASCIIZ [@2], company name, etc. or “Unknown” or “\0”
326	C60	ASCIIZ [@2], sample identification
386	C160	ASCIIZ [@2], comment
546	C2	2-bytes of padding for alignment
548	I4	goniometer model:
		0 = Theta/2-Theta D5000
		1 = Theta/Theta D5000
		2 = D5000-matic

		3 = AL/Theta-D5000
		4 = GADDS/FRAMBO [@2]
		5 = SAXS [@2]
		6 = SMART [@2]
		7,8,9 = reserved
		10 = Theta/2-Theta D5005
		11 = Theta/Theta D5005
		12 = reserved
		13 = AL/Theta D5005
		20 = Theta/2-Theta other
		21 = Theta/Theta other
		22 = Matic other
		23 = AL/Theta other
		9999 = unknown
552	I4	goniometer stage:
		0 = Standard
		1 = Synchron. rotation
		2 = Rotation reflection
		3 = Rotation transmission
		4 = Open cradle
		5 = Closed cradle
		6 = Phi
		7 = Chi
		8 = XYZ
		9 = Low temp.
		10 = High temp.
		11 = External temp.
		12 = Other
		16 = Phi stage at fixed chi [@2]
		17 = 4-circle [@2]
		18 = Small XYZ stage [@2]
		19 = Large XYZ stage [@2]
		20 = 1/4-circle [@2]
		9999 = unknown
556	I4	sample changer:
		0 = None
		1 = 40-position
		2 = Y-matic
		3 = X/Y-matic
		9999 = unknown
560	I4	goniometer controller
		0 = STD only
		1 = STD+TC
		2 = STD+FDC
		3 = STD+FDC+TC
		16 = GGCS [@2]
		9999 = unknown
564	R4	goniometer radius in mm.
		9999.0 = unknown, 0.0 = unknown [@2]
568	R4	diverg.slit fix incidence in degrees, 9999.0 = unknown
572	R4	sample slit fix incidence in degrees, 9999.0 = unknown
576	I4	primary soller slit:
		0 = not present
		1 = present
		1 = 2 deg (@2.1)
		2 = 4 deg (@2.1)

		3 = other (@2.1)
		9999 = unknown
580	I4	primary monochromator:
		0 = None
		1 = Transmission
		2 = Reflection
		3 = Ge220 2-bounce
		4 = Ge220 4-bounce
		5 = Ge440 4-bounce
		6 = Flat graphite (@2.1)
		7 = Single Goebel mirror (@2.1)
		8 = Crossed Goebel mirror (@2.1)
		9 = Flat Germanium 111 (@2.1)
		10 = Flat Silicon 111 (@2.1)
		9999 = unknown
584	R4	anti slit diffracted side in degrees, 9999.0 = unknown
588	R4	detector slit diffr. side in degrees, 9999.0 = unknown
592	I4	secondary soller slit:
		0 = not present
		1 = present
		1 = 2 deg (@2.1)
		2 = 4 deg (@2.1)
		3 = other (@2.1)
		9999 = unknown
596	I4	thin film:
		0 = not present
		1 = present
		1 = 0.4 deg (@2.1)
		2 = 0.15 deg (@2.1)
		3 = 0.08 deg (@2.1)
		9999 = unknown
600	I4	beta filter (Yes=1, No=0), 9999 = unknown
604	I4	secondary monochromator:
		0 = None
		1 = graphite
		2 = LiF
		3 = Ge220 channel cut
		4 = Goebel mirror
		9999 = unknown
608	C4	ASCIIZ [@2], Anode material e.g. “Cu”
612	C4	4-bytes of padding for alignment
616	R8	average wavelength in A (Obs. or nm) (i.e. (Ka1+Ka2+R21)/(1+R21))
624	R8	primary wavelength in A (Obs. or nm) (i.e. Ka1)
632	R8	secondary wavelength in A (Obs. or nm) (i.e. Ka2)
640	R8	tertiary wavelength in A (Obs. or nm) (i.e. KB)
648	R8	intensity ratio of secondary to primary wavelength
656	C4	wavelength unit name: [@2] now always “A”
		(obs) in “RAW1.00” files both “A” or “nm” were used.
660	R4	intensity ratio of tertiary to primary wavelength

664	R4	total sample run time:
		9999.0 = unknown (obs.)
		-1.0 = unknown [@2]
668	C44	reserved for expansion

RAW_RANGE_HEADER: 304-bytes of range header information that precedes every range in a RAW file. Similar to DIF_RANGE_HEADER, but DIFFERENT!

Offset	Code	Description
0	I4	always 304, length of primary range header in bytes
4	I4	number of measured data
8	R8	theta start in degrees
16	R8	two-theta start in degrees
24	R8	chi start in degrees, use 9999.0 if not present or unknown
32	R8	phi start in degrees, use 9999.0 if not present or unknown
40	R8	x start in mm., use 9999.0 if not present or unknown
48	R8	y start in mm., use 9999.0 if not present or unknown
56	R8	z start in mm., use 9999.0 if not present or unknown
		Note: may use actual values for fixed axes
64	R8	div.slit start in degrees if divslit_code == “fix”
		(9999.0 if not present)
72	C8	div.slit code ASCIIZ: “V20”, “V6”, “V4”, “V2”, “fix”
		“V#” where # = sample illumination in mm
		or “Unkn” for unknown
		or “fix” for fixed
80	R8	anti.slit start in degrees if antislit_code = “fix”
		(9999.0 if not present)
88	C8	anti.slit code ASCIIZ: “V20”, “V6”, “V4”, “V2”, “fix”
		“V#” where # = sample illumination in mm
		or “Unkn” for unknown
		or “fix” for fixed
96	I4	[@2] detector used for this range
		(obs.) detector code for detector #1
		0 = none (now invalid value [@2])
		1 = Scintillation
		2 = Proportional
		3 = Solid State
		4 = Other
		5 = PSD,
		16 = X-1000 [@2]
		17 = Hi-Star [@2]
		18 = CCD [@2]
		19 = Large CCD [@2]
		20 = Mosaic CCD [@2]
		9999 = unknown
100	R4	[@2] highvoltage used in V, 9999.0 for unknown
		(obs) highvoltage in V of detector #1, 9999.0 for unknown

104	R4	[@2] amplifier gain used in ??, 9999.0 for unknown
		(obs) amplifier gain in ?? of detector #1, 9999.0 for unknown
108	R4	[@2] lower level used in V, 9999.0 for unknown
		(obs) lower level in V of detector #1, 9999.0 for unknown
112	R4	[@2] upper level used in V, 9999.0 for unknown
		(obs) upper level in V of detector #1, 9999.0 for unknown
116	I4	[@2] measuring channel: 1 or 2
		(obs.) detector code for detector #2
120	R4	[@2] unused field
		(obs.) highvoltage in V of detector #2, 9999.0 for unknown
124	R4	[@2] unused field
		(obs.) amplifier gain in ? of detector #2, 9999.0 for unknown
128	R4	[@2] alternate LLD as fraction of channel full scale
		(obs.) Lower level in V of det. #2, 9999.0 for unknown
132	R4	[@2] alternate ULD as fraction of channel full scale
		(obs.) Upper level in V of det. #2, 9999.0 for unknown
136	C8	ASCIIZ: “IN” or “OUT”, (“nc” if not present), “Unkn” for unknown
144	R8	start of aux. axis 1 (up to now 0.0) (i.e. h of hkl scan)
152	R8	start of aux. axis 2 (up to now 0.0) (i.e. k of hkl scan)
160	R8	start of aux. axis 3 (up to now 0.0) (i.e. l of hkl scan)
		(i.e. psi of psi scans)
168	I4	scan mode: step “SS” = 0 or continuous “SC” = 1
172	C4	4-bytes of padding for alignment
176	R8	step size: increment of 1st scan axis in drive units
184	R8	step size: increment of 2nd scan axis in drive units: 0.0
192	R4	step time in seconds: 1.0 if unknown [@2]
196	I4	scan type
		0 = locked coupled
		1 = unlocked coupled
		2 = 2theta scan I detector scan
		3 = omega scan I rocking curve
		4 = chi scan
		5 = phi scan
		6 = x scan
		7 = y scan
		8 = z scan
		9 = aux1 scan [@2]
		10 = aux2 scan [@2]
		11 = aux3 scan [@2]
		12 = psi scan [@2]
		13 = hkl scan [@2]
		14 = reciprocal space scan [@2.1]

		129 = PSD fixed scan [@2]
		130 = PSD fast scan [@2]
		257 = pixel s can (SAXS v4.X) [@2]
200	R4	delay time before a measurement was started in seconds.
		(obs.) 9999.0 = unknown, [@2] -1.0 = unknown
204	R4	the time the range was started relative to the time when the
		sample was started in sec. (obs.) 9999.0 = unknown
		[@2] -1.0 = unknown
208	R4	rotation speed in rps (0.0 = no rotation)
212	R4	temperature in K (-1.0 for room)
216	R4	heating/cooling rate of the TC in K/s
220	R4	delay in sec. before measurement if TC, -1.0 for unknown [@2]
224	I4	generator voltage kV or 9999=unknown
228	I4	generator current mA or 9999=unknown
232	I4	display plane number, needed for 3D display
236	C4	4-bytes of padding for alignment
240	R8	actually selected wavelength in A
248	I4	currently 0, but reserved for varying multiple scan parameters
		during a single scan in a non-standard fashion:
		two_theta -> bit 0
		theta -> bit 1
		chi -> bit 2
		phi -> bit 3
		x -> bit 4
		y -> bit 5
		z -> bit 6
		aux1 -> bit 7
		aux2 -> bit 8
		aux3 -> bit 9
		time -> bit 10
		temp -> bit 11
		e.g. chi and phi = 2**2 + 2**3 = 12
252	I4	length of each data record in bytes: currently 4 (float);
		but if the varying parameters are not 0, the data record length
		is 4 + 8 * number of bits set in above varying parameter flag
		e.g. chi and phi vary ==> data record length = 8+8+4 = 20
256	I4	total size of all supplementary range header records.
		if there are no extra defined records, this value is 0.
260	R4	[@2] smoothing width in degrees 0.0 = not smoothed
264	I4	[@2] flagword for simulated meas. condition
		bit 0->simulate a different slit option
		bit 1->variable slits are simulated
		Thus the valid settings are:
		00=no data manipulation

		01=converted to fixed slits from var.
		10=no data manipulation
		11=converted to var. slits from fixed
268	C4	[@2] 4-bytes of padding for alignment
272	R4	[@2] step size: increment of 3rd scan axis: 0.0
280	C24	reserved for expansion

RAW SUPPLEMENTARY RANGE HEADERS: Each supplementary range header record is composed of a variable number of bytes. The total number of supplementary range header bytes is store in offset 256 of the range header. A value of 0 indicates that there are no supplementary range headers. The currently defined supplementary range header records are listed below:

Offset	Code	Description for Oscillation record
0	I4	record type: 100 = oscillation parameters
4	I4	record length: 40-bytes
8	I4	oscillation drive:
		0 = tube
		1 = sample
		2 = detector
		3 = chi
		4 = phi
		5 = x
		6 = y
		7 = z
12	C4	4-bytes of padding for alignment
16	R8	oscillation amplitude in degrees or mm
24	R4	oscillation speed in degrees or mm per sec.
28	C12	reserved for expansion

Offset	Code	Description for PSD record
0	I4	record type: 110 = PSD parameters
4	I4	record length: 40-bytes
8	R8	actual two theta of goniometer in deg
16	I4	first channel used
20	C20	reserved for expansion

Offset	Code	Description for Optimized Quantitative Measurement record
0	I4	record type: 120 = OQM parameters
4	I4	record length: 72-bytes
??		undefined at this time

Offset	Code	Description for Quantitative Compound Indicator record
0	I4	record type: 130 = QCI parameters (obsolete)
4	I4	record length: variable number of bytes
8	I4	variable type: 0=peak; 1= low background; 2= high background
12	C??	ASCII: compound name
16	C12	reserved for expansion

Offset	Code	Description for Comment record
0	I4	record type: 140 = comment
4	I4	record length: variable number of bytes
8	C??	ASCII: comment, stored without null termination

Offset	Code	Description for Removed Data record
0	I4	record type: 150 = removed data for search
4	I4	record length: 32-bytes
8	R4	excluded 2-theta start in degrees
12	R4	excluded 2-theta end in degrees
16	I4	(obs.) number of points in this part
20	C12	reserved for expansion

Offset	Code	Description for Offset Assigned by EVA record
0	I4	record type: 190 = offset assigned by EVA
4	I4	record length: 32-bytes
8	R4	2-theta offset in degrees
12	R4	intensity offset in % of max
16	C16	reserved for expansion

Offset	Code	Description for Area Detector Parameters record [@2]
0	I4	record type: 200 = area detector parameters
4	I4	record length: 72-bytes
8	C8	reserved
16	R4	integration range: 2T start
20	R4	integration range: 2T end
24	R4	integration range: chi start or chi angle
28	R4	integration range: chi end or height + 1000.0
32	I4	normalization method: 1=avg, 2=arc length, 3=solid angle, 4=bin
36	C20	program name: i.e. “GADDS-NT ver 3.301”
56	R4	actual 2theta of goniometer
60	R4	actual omega of goniometer
64	R4	actual phi of goniometer
68	R4	actual chi goniometer

RAW_DATA: The data records immediately follow the range header (and supplementary range headers, if any). The data is stored as counts in R4 format. Should non-standard varying parameters be used, then each data record is comprised of the counts in a R4 field, followed by several R8 fields.

Codes used are:

I2 = 16-bit integer, I4 = 32-bit integer

R4 = 32-bit real, R8 = 64-bit real

Cn = ASCII character string of n bytes, no null character.

Cn = ASCIIZ character string of n bytes, ends in null character.

[@2] = new field or value for “RAW1.01” version files.

(obs) = obsolete field or value for “RAW1.00” version files.

C. DIFFRAC-AT Raw Data File Format

Diffrac-AT V1 raw data files are stored in a direct access, binary file without any record delimina-tors.

Record	Format	Field description
1	A4	“RAW” File identification text
2	I4	Number of steps for this range (1–32767)
3	R4	Measurement time per step (.1–999.0)
4	R4	Step size for this range in degrees
5	I4	Flag word in DACO-MP format, meaningful bits are:
		1024 = theta fixed
		2048 = continuous scan
		8192 = 2theta fixed (rocking curve)
		16384 = chi range
		16384 + 8192 = phi range
6	I4	Sample number in sample changer, 0=manual insertion
7	R4	Two-theta start in degrees, -1E6=unknown
8	R4	Theta start, -1E6=unknown
9	R4	Chi start, -1E6=unknown
10	R4	Phi start, -1E6=unknown
11–18	8A4	Sample name (32 characters)
19	R4	K alpha 1 wavelength
20	R4	K alpha 2 wavelength, 0.0 if monochromator used
21–38	--	Unused
39	I4	Number of ranges following this range, 0=single range
40–39+x	xR4	Data in raw counts, not counts/ second.
where x = number of steps in range		

Additional ranges use this same format and are appended to the end of the first range.

NOTE: Early Diffrac-AT raw data files did not repeat the “RAW” on additional ranges.

Profile *.PRO File Format (identical to Diffrac-AT V1 with these changes).

Record	Format	Field description
1	A4	“PRO” instead of “RAW”
29	R4	Two-theta of Imax in profile
30	R4	FWHM of profile
31	R4	Offset of peak angle position from the Imax position in profile

Diffrac-AT V2/V3 raw data files are stored in a direct access, binary file without any record deliminators. The structure starts with a 256-byte file header block, followed by a range header and data block, which are repeated for each range in the file.

Offset	Format	Field description
0	A4	“RAW2” File identification text
4	I2	Number of ranges in this file
6	?2	Unused
8	A32	Sample base name
40	A128	Sample extended name /comments
168	A20	Date/time measured: 07-Jun-1995 18:20:00
188	A2	Chemical symbol for tube anode
190	3R4	Lambda1, Lambda2, Intensity ratio
202	I2	Diffractometer code (0=2th/th, -1=th/th)
204	I2	Diffractometer configuration word
206	R4	Lambda 3 or K beta wavelength
210	R4	Total sample run time in seconds
214	R8	Date/time measured in Lotus123 format
222	?34	Unused

Offset	Format	Field description
0	I2	Total number of bytes in range header
2	I2	Step count for this range
4	I2	Stepping drive ID: 1–6 drive 1 to 6
		8 = PSD fixed position; 9 = PSD fast scan; 10 = drives 1 and 2
6	I2	Step mode:
		bit 0 = step scan mode 1:continuous;
		bit 1 = calibration indicator
8	R4	Step time: time per step (in seconds)
12	R4	Step size for range
16	6R4	Starting axes position for range
40	I2	Slit I position: 32767=FA1, 32766=FA2
42	I2	Slit II position: 32767=FA1, 32766=FA2
44	I2	Detector slit: 0=fine, 1=coarse
46	I2	Temperature in Kelvin: -1=room

48	I2	Oscillating drive: 0 = none, 1–6 = drives 1 to 6, 7 = spinner
		10,11 = 1 and 2 coupled +,-
50	R4	Oscillation amplitude: 999=mechanically fixed
54	R4	Oscillation speed
58	I2	Rotation code: 0 = none, 1–4 = 15–120 rpm, 5 = sync, 6 = SC
60	...	Variable supplementary information records
60+x	nR4	Raw data, counts, 4 bytes per step

D. PLOTSO Raw Data File Format

The PLOTSO Raw Data File Format is a subset of the general PLOTSO data file format (see PLOTSO, Section 13.7). The general format is an ASCII header, followed by an ASCII table of data. Range and data records are repeated for all defined ranges.

!@!!GADDS PLOTSO FILE: [Chi | R.C. | 2th | Rect | Pixel | ????] integration type

Identified file as PLOTSO RAW file.

!@!!Title: string

Sample title.

!@!!Comment:: string

General comment such as original frame file name.

!@!!Wavelengths: Kavg, Ka1, Ka2, Beta

Wavelengths.

!@!!Integration range: 2Theta: X to X Gamma: X to X
!@!!Integration range: 2Theta: X to X Gamma: X Width: X

Area detector integration region.

!@!!Integration method: pixel summation | average pixel | normalized by arc length | normalized by solid angle | bin summation | bin normalized | interpolated | unknown

How data was converted from frame to spectra.

!@!N

Specifies that subsequent X,Y points should be drawn as a new plot, rather than added to the existing set of axes.

!@!SS

Specifies a line style for a connecting line to be drawn between X,Y pairs. Supply one of the characters 0,N,S or D as a parameter. Line styles are: “!@!S0” or “!@!SN” (for no connecting line, for example, for scatter plots), “!@!SS” (for a solid connecting line), and “!@!SD” (for a dotted connecting line).

!@!M

Specifies the character to be used as a Marker. The Marker Character is plotted at each subsequent X,Y point. The marker character must immediately follow the directive (that is, it must be the fifth character on the line). Examples are: “!@!M+” (to plot a + at each input X,Y position) or “!@!M” (to disable plotting of a character at each X,Y position).

!@!L 0.0 0.0 0.0 0.0

Sets plot axis limits, overriding the auto-scaling normally performed. Requires four parameters, Xmin, Ymin, Xmax, Ymax corresponding to the lower X, lower Y, upper X, and upper Y axis limits, respectively. If both the lower and upper limit for an axis are specified as zero, autoscaling is restored for that axis. The default limits are 0,0,0,0, meaning that auto-scaling is performed on each axis. When an axis is auto-scaled, a “nice” interval for tic marks is determined. This interval is always 1, 2 or 5 times some power of 10. Limits are then chosen which are integer multiples of this interval and which contain the range of values input for the axis being auto-scaled. An example of this directive is: “!@!L0,0,100,0”. (This example specifies that the X-axis will range from 0 to 100, and the Y will be auto-scaled based on the range of the input Y-values.)

!@!XDegrees

This directive specifies the X-axis label. Follow the directive with the text to be drawn along the X axis. By default, the text is “X-AXIS”. For example, if you're plotting a function versus time, you might issue the directive “!@!XTime (seconds)”.

!@!YCounts

This directive specifies the Y-axis label. Follow the directive with the text to be drawn along the Y axis. By default, the text is “Y-AXIS”. For example, if you're plotting pixel values as a function of position, you might issue the directive “!@!YPixel Value”. Normally, Y-axis text is written vertically (but not rotated, since some graphic environments, most notably X-Windows, don't support rotated text); however, if the text contains hyphens or parentheses, it writes the text horizontally. In this latter case, you need to keep the axis label very short.

2theta, Intensity data pairs or 2theta, Intensity, Q, stderr table.

The actual data spectra.

E. TEXTURE-AT Raw Data File Format

Texture-AT raw data files are stored in a byte stream, binary file without any record delimina-tors. File extensions are *.rrw for reflection or *.trw for transmission.

Table E.1 – Range Header Block

Offset	Format	Field description
+0	A4	“RAW” File identification text
+4	I4	Number of steps for this range (1–32767)
+8	R4	Measurement time per step (.1–999.0)
+12	R4	Step size for this range in degrees
+16	I4	Flag word in DACO-MP format, meaningful bits are:
		1024 = theta fixed
		2048 = continuous scan
		8192 = 2theta fixed (rocking curve)
		16384 = chi range
		16384 + 8192 = phi range
+20	I4	Sample number in sample changer, 0=manual insertion
+24	R4	Two-theta in degrees
+28	R4	Theta for reflection, 2theta + alpha for transmission
+32	R4	Alpha for reflection, Beta start for transmission
+36	R4	Beta start for reflection, 0.0 for transmission
+40	A32	Sample name (32 characters)
+72	R4	K alpha 1 wavelength
+76	R4	K alpha 2 wavelength, 0.0 if monochromator used
+80	4R4	Background information for this range
		2theta for low background measurement, -1 = none
		2theta for high background measurement, -1 = none

		intensity at low 2theta rescaled to measuring time per circle
		intensity at high 2theta, 0.0 = none
+96	A32	Sample name extension (characters 33-64 of sample name)
+128	R4	Linear absorption coefficient * thickness
+132	I4	Pointer to measuring parameters block in this file
+136	I2	Measurement code
		1 = texture-less standard with background
		2 = texture-less standard without background
		3 = unknown sample without background
		4 = unknown sample, background measured for first chi only
		5 = unknown sample, background measured at phi=0 for all chi's
		6 = unknown sample with full background measurements
+138	14X	Reserved for future use. Must be 0
+152	I4	Number of data ranges after this one

Table E.2 – Data Range Block

Offset	Format	Field description
		+156 #R4 Counts, not counts/sec

Additional ranges use this same format and are appended to the end of the first range.

Table E.3 – Measuring Parameters Block (placed as trailer block)

Offset	Format	Field description
+0	8A8	hkl parameters in ASCII for up to 8 pole figures. Blank=unused.
+64	8R4	2theta values for up to 8 pole figures. -1E31=unused.
+96	8R4	low background 2theta for up to 8 pole figures. -1E31=unused.
+128	8R4	high background 2theta for up to 8 pole figures. -1E31=unused.
+160	R4	alpha start for reflection, -1E6=unused.
+164	R4	alpha end for reflection, -1E6=unused.
+168	R4	alpha step
+172	R4	beta start
+176	R4	beta end
+180	R4	beta step size
+184	R4	measuring time per step for reflection, 0.0=unused
+188	R4	alpha start for transmission, -1E6=unused.
+192	R4	alph end for transmission, -1E6=unused.

+196	R4	measuring time per circle for background(s), -1=unused.
+200	4X	unused, reserved bytes
+204	R4	x-oscillation amplitude in mm
+208	R4	x-oscillation speed in mm/sec
+212	R4	measuring time per step for transmission, 0.0=unused.
+216	16R4	contour levels, 15 values maximum, -1=unused, #16 must be -1.
+280	16I2	display colors for contours
+312	16I2	plotter pen colors for contours
+344	R4	CRT aspect ratio, unused
+348	R4	x scale factor of printer, unused
+352	R4	y scale factor of printer, unused
+356	R4	linear absorption of sample
+360	X2	unused
+362	A64	axis label
+426	A64	site label
+490	A64	analytical program comments, i.e. ‘GADDS v2.0’
+554	A32	name of data file for texture-less sample, i.e. correction file
+586	L1	.true. = continuous step scan mode
+587	L1	.true. = inverted transmission mode
+588	L1	.true. = no reference sample available/used
+589	I2	actual number of alpha scans in file (ignore R and T repeats)
+591	I2	max number of alpha scans = 1 + 90 /alpha_step
+593	I2	max number of beta steps = 360 / beta_step
+595	R4	actual alpha start in the file
+599	R4	alpha start / 2 in radians = [+595]*PI/360
+603	R4	beta start in radians = [+172]*PI/180
+607	R4	delta alpha / 2 in radians = [+168]*PI/360
+611	R4	delta beta in radians = [+180]*PI/180
+615	I2	actual number of pole figures in the file
+617	I2	number of pole figures currently selected for display
+619	I2	current display mode
		1 = color 3D, 2 = BW 3D, 3 = contours, 4 = maxima, 5 = phi cut
+621	I2	pole figure rotation, degrees as integer, normally 0
+623	I2	inclination for 3D view, degrees as integer
+625	3I2	3 values of chi for 3 phi-cuts as integers
+631	2X	unused
+633	8A8	hkl of pole figures, same as [+0]
+697	I2	maxima search option
		1 = 8 points, 2 = 12 points, 3 = 20 points, 4 = 32 points

+699	R4	absolute minimum of normalized data, computed by TEXD5
+703	R4	absolute maximum of normalized data, computed by TEXD5
+707	I2	diameter of pole figures for plotter in cm
+709	I2	number of copies for plotter
+711	L1	must be 0, .true. = data collection still in progress
+712	8R4	x-values for 8 pole figures in mm
+744	8R4	y-values for 8 pole figures in mm
+776	14X	unused
+790	A64	sample name (repeated)
+854	A32	data file name
+886	R4	sample thickness
+890	L1	.true. for a texture-less sample
+891	1X	unused
+892	R4	thichness of transmission sample
+896	124X	unused
+1020	A32	name of .TEX file used for measurement
+1052	I2	number of pole figures in the file, same as [+615]
+1054	I2	number of background positions in the file
+1056	I2	number of beta steps in the file
+1058	I2	number of beta steps in reflection mode
+1060	I2	number of beta steps in transmission mode
+1062	8R4	2theta of pole figures, same as [+64] and [+24] in range header
+1094	130X	reserved

F. POPLA Data File Format

REF: Kocks, Kallend, Wenk, Rollett, and Wright “popLA: Preferred Orientation Package - Los Alamos,” LA-CC-89-18, GTDA. Oct. 1995.

popLA data files are stored in ASCII format. Valid extensions are:

- *.epf experimental pole figure
- *.npf normalized pole figure
- *.rpf rotated pole figure
- *.tpf tilted pole figure

line 1: specimen, date, and title

A8	specimen name / filename (no central spaces allowed, trailing OK)
A72	popLA suggests that date is first part of title

line 2: parameter line

A5	hkl or other identification for pole image
F5.1	alpha step, usually 5.0 (currently only 5.0 is supported)
F5.1	alpha max, range 5.0–80.0 (GADDS always writes 80.0)
F5.1	beta step, usually 5.0 (currently only 5.0 is supported)
F5.1	beta max, usually 360.0 or 90.0 (GADDS always uses 360.0)
I2	alpha offset start: 0 = 0.0, 1 = 2.5 (GADDS always uses 1)
I2	beta offset start: 0 = 0.0, 1 = 2.5 (GADDS always uses 1)
3I2	choice of axes labels. (GADDS always assumes 1,2,3)
I5	scaling factor times 100.0. Default is 100 (scaling factor of 1).
I5	scaled background counts, usually 0 (GADDS always writes 0)
A?	extra bytes are unknown and unnecessary

line 3+: data lines

1X,18I4	data in integers scaled by factor in line 2. Scaling factor is only used when Imax exceeds 9999; otherwise, one uses 1.0 scale factor. Data is outputted one beta scan at a time starting at alpha = 0.0 to alpha max. The start of each beta scan begins a new line.

line—last line must be blank to identify the end of a set. Then there may be either end of file or another set, starting with another first line.

G. SLAM Command Reference

The following are the GADDS SLAM Command syntax for all valid commands. <n> denotes numeric value. <s> denotes string value.

```
! (any text string)
@filename p1 p2 p3 p4 p5 p6 p7 p8 p9 p0
ADD $1 /CLEAR /PATTERN /COUNTS=<n> /DISPLAY=<n> /REALTIME /RESET=<n> /SHUTTER
BADPIXELS /PROCESS $1 $2 $3 $4 $5 $6 $7 /LOCAL
CALIBRATE $1 /MININT=<n> /DISTANCE=<n> $2 /ANGLE=<n> $3  /X=<n> /Y=<n> $4 /AUTO /NOERASE
       /DELAY=<n>
CLEAR  $1 /QUADRANT=<n> /GRAPHICS_SAVE /IMAGE_SAVE
CONFIGURE /EDIT /USER=<s> /SITE=<s> /CALIBDIR=<s> /MINCPS=<n> /TIMEOUT=<n> /NAMECHAR=<n>
       /RUNCHARS=<n> /RUNBASE=<n> /NUMCHARS=<n> /NUMBASE=<n> /LOWTEMP /TEMP=<n> /XBEAM=<n>
       /YBEAM=<n> /FRAMESIZE=<n> /DISTANCE=<n>
CONFIGURE /ADMIN /TARGET=<s> /WAVELENGTH=<n> /ALPHA1=<n> /ALPHA2=<n> /BETA=<n> /UNITS=<s>
       /KV=<n> /MA=<n> /STANDBYKV=<n> /STANDBYMA=<n> /MONOCHROMATOR=<s> /OFFSET=<n>
CONFIGURE /READ $1
CONFIGURE /WRITE $1
CONFIGURE /SHOWMODEL
CONFIGURE /COLORS $1 /WINBG=<n> /WINFG=<n> /CURSOR=<n> /HIGHLIGHT=<n> /BORDER=<n> /GRAPH=<n>
       /OVERLAY=<n> /MATCH1=<n>
CONTRAST /LO=<n> /HI=<n>
CORRECTIONS /LPA  $1  $2  $3  /MONOCHROMATOR=<n>  /AIRMU=<n>  /NOREVERSE
CORRECTIONS /FIBER  $1  $2  $3  /X=<n>  /Y=<n>  /Z=<n>  /NSTEPS=<n>  /MU=<n>  /RADIUS=<n>
CORRECTIONS /PLATE  $1  $2  $3  /X=<n>  /Y=<n>  /Z=<n>  /MU=<n>  /THICKNESS=<n>
```

```
CURSORS /BOX  $1 $2 $3 $4 /DELAY=<n> /NOERASE
CURSORS /CIRCLE $1 $2 $3 /DELAY=<n> /NOERASE
CURSORS /PIXEL $1 $2 /DELAY=<n> /NOERASE /DUMP
CURSORS /VECTOR  $1 $2 $3 $4 /DELAY=<n> /NOERASE
CURSORS /CONIC  $1 $2 /DELAY=<n> /NOERASE
CURSORS /RBOX  $1 $2 $3 $4 /DELAY=<n> /NOERASE
DETECTOR /CU
DETECTOR /FE
DETECTOR /YVSX
DETECTOR /EVSE
DETECTOR /ADD  $1  /CLEAR  /PATTERN  /COUNTS=<n>  /DISPLAY=<n>  /REALTIME  /RESET=<n>
        /SHUTTER
DETECTOR /DETRESET
DETECTOR /XEVSX
DETECTOR /YEVSX
DETECTOR /PDCCUSTOM  $1  $2  $3
DISPLAY /NEW $1 /QUADRANT=<n> /LO=<n> /HI=<n> /X=<n> /Y=<n> /MAG=<n> /AUTOINCREMENT
       /GRAPHICS_SAVE /ORIENTATION /VIDEO /OVERLAY
DISPLAY /NEXT
DISPLAY /PREVIOUS
DISPLAY /MOVIE+
DISPLAY /MOVIE-
DISPLAY /RMOVIE+
DISPLAY /RMOVIE-
DISPLAY /RNEXT
DISPLAY /RPREVIOUS
DISPLAY /HKL $1 $2 $3
ECHO /OUT=<s> /APPEND /WAIT=<n> $1 $2 $3 .... $8 $9 $0
EXIT
LOOD /NEW  $1  /COUNTS=<n>  /DISPLAY=<n>  /REALTIME  /FILE=<s>  /XMIN=<n>  /YMIN=<n>
       /MAG=<n>  /SHUTTER
FLOOD /LOAD  $1
FLOOD /REPROCESS  $1  $2  /XMIN=<n> /YMIN=<n>   /MAG=<n>
FLOOD  /LINEAR
FRAME_INFO $1
GONIOMETER /MANUAL  $1  $2  $3  $4  $5  $6  $7  $8
       Or GONIOMETER /MANUAL  $1  $2  $3  $4  $5
RATEMETER  $1  /RESET=<n>  /SHUTTER
GONIOMETER /OPTICAL  [$1  $2  $3  $4  $5  $6  $7  $8 | $1  $2  $3  $4  $5]
GONIOMETER /FLATSAMPLE /X1=<n> /Y1=<n> /Z1=<n> /X2=<n> /Y2=<n> /Z2=<n> /X3=<n> /Y3=<n> /Z3=<n>
```

```
GONIOMETER /UPDATE  [$1  $2  $3  $4  $5  $6  $7  $8  $9 |  $1  $2  $3  $4]
GONIOMETER /LIMITS [$1 $2  $3  $4  $5  $6  $7  $8  $9  $0 | $1 $2  $3  $4  $5  $6  $7  $8  $9
       $0  /XMAX=<n>  /XMIN=<n>  /YMAX=<n>  /YMIN=<n>  /ZMAX=<n>  /ZMIN=<n>  /AMAX=<n>
       /AMIN=<n>  /DMIN=<n>  /DMAX=<n>]
GONIOMETER /EXTLIMITS
GONIOMETER /SPEEDS  [$1  $2  $3  $4  $5  $6  $7  $8  $9 | $1  $2  $3 | $1  $2]
GONIOMETER /ZERO
GONIOMETER /ATTENUATOR
GONIOMETER /SHUTTER
GONIOMETER /LASER
GONIOMETER /GENERATOR  $1  $2  /WAIT
GONIOMETER /FIXEDAXES  $1  $2  $3  $4  $5  $6  $7  $8
GONIOMETER /HOME  $1  $2
GONIOMETER /PARK
GONIOMETER /XYZ  $1  $2  $3  $4
GONIOMETER /TEMP  $1  /RAMP=<n>  /HOLD=<n>  /WAIT
GONIOMETER /ENCODERS  [$1  $2  $3  $4 | $1  $2  $3  $4 $5 $6 $7 $8 $9]
GRAPH /FILE $1 /QUADRANT=<n> /PRECLEAR  /NOCLEAR
GRAPH /VECTOR $1 $2 $3 $4 /QUADRANT=<n> /DELAY=<n> /NOERASE
GRAPH /ROCKING $1 $2 $3 $4 /QUADRANT=<n> /FRAME_HALFWIDTH=<n> /DELAY=<n> /NOERASE
GRAPH  /POSTER
GRAPH /HKL $1 /QUADRANT=<n> $2 $3 /DELAY=<n> /NOERASE
GRAPH /PSI $1 /QUADRANT=<n> $2 $3  /DELAY=<n>  /NOERASE
HELP
HELP /REFERENCE
HELP /USERGUIDE
HELP /ERRATA
HELP /MAP
HELP /RELNOTES
INTEGRATE /CHI $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n>
INTEGRATE /2THETA $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n>
INTEGRATE /AREA  $1  $2  $3  $4
INTEGRATE /SLICE $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n>
INTEGRATE /WRITE $1 /FILENAME=<n> /FORMAT=<n> /APPEND
INTEGRATE /CLEAR
INTEGRATE /RECTANGLE  $1  $2  $3  $4  /VERTICAL
INTEGRATE  /WRITE  $1  /FILENAME=<s>  /FORMAT=<s>  /APPEND  /SCALE=<n>
LEVEL1
LEVEL2
```

```
LEVEL3
LOAD  $1  $2  /DISPLAY=<n> /SCALE=<n> /OFFSET=<n> /LOGSCALE /USE_CONFIG
LOGFILE /NEW $1 /APPEND
LOGFILE [/ON | /OFF]
LOGFILE /SCRNEW $1 /APPEND
LOGFILE [/SCRON | SCROFF]
MAPPING  $1  /FRAME=<s>  /RUN=<s>  $2  /SLAM=<s>
MASK /CREATE $1 /FILTER /BORDER=<n>
MASK /SAVE $1
MASK /READ $1
MASK /VIEW $1
MASK /EDIT (interactive)
MASK /OCTAGON $1 $2 $3 $4 $5 $6 $7 $8
MENUMODE
PDF2 /VIEW $1 /NBS*AIDS /TYPE=<n>
PDF2 /PRINT $1 $2 /NBS*AIDS /TYPE=<n> /CARD
PDF2 /DISPLAY $1 /DASHED
PDF2 /SEARCH $1 /MINERAL /INORGANIC /ORGANIC
PDF2  /CLEAR
PER_CRYSTAL /EXTERNAL $1 $2 $3 $4 $5 $6 $7 $8 /COMPTON
PER_CRYSTAL /INTERNAL $1 $2 $3 $4 $5 $6 $7 $8 /LINEAR /COMPTON
PER_CRYSTAL /COMPTON $1 /SCALE=<n> /XSCALE=<n>
PER_CRYSTAL /FULL  $1  /DISPLAY=<n>  $2  /RADIUS=<n>
POLE_FIG /SCHEME $1 /POLE=<n> /DISTANCE=<n> $2 [/2THETA=<n> |/THETA1=<n>]  [/OMEGA=<n> |
       /THETA2=<n>] /PHI=<n> /CHI=<n> /AXIS=<n> /WIDTH=<n> /CLEAR $3 /MAPPING=<s> /REFLECTION
       /X=<n> /Y=<n> /Z=<n>
POLE_FIG /PROCESS $1 $2 $3 $4 $5 /POLE=<n> /MAPPING=<s> /BACKGROUND $6 $7 $8 $9 /FIBERGEOM
       /ABSORPTION=<s> /X=<n> /Y=<n> /Z=<n> /MU=<n> /RADIUS=<n> /NSTEPS=<n> /REFLECTION
POLE_FIG /INTERPOLATE $1 /DISPLAY=<n> /WIDTH=<n> $2
POLE_FIG /TILT $1 /DISPLAY=<n> /X=<n> /Y=<n> $2
POLE_FIG /ROTATE $1 /DISPLAY=<n> $2
POLE_FIG /SYMMETRIZE $1 /DISPLAY=<n> $2 /LAUE=<s>
POLE_FIG /INVERT $1 /DISPLAY=<n> $2
POLE_FIG /TEXTUREAT $1 /TITLE=<n> /HKL=<n> /APPEND /ALPHAINC=<n> /BETAINC=<n> /REFLECTION
POLE_FIG /POPLA $1 /TITLE=<n> /HKL=<n> /APPEND
POLE_FIG /ORIENT $1 /DISPLAY=<n> $2 /APPEND /FILM /HKL=<s>
POLE_FIG /STEIN $1 $2 /APPEND
POLE_FIG /NORMALIZE $1 /DISPLAY=<n> /NVAL=<n> $2
POLE_FIG /CONTOURS $1 /INTERVAL=<n>
POLE_FIG /SURFACE $1 /ROTATION=<n> /ELEVATION=<n> /COARSENESS=<n>  /LOGSCALE
```

```
POLE_FIG /FIBERPLOT  $1  $2  $3  $4  /NORMAL=<n>  /STEPSIZE=<n>
PRINT  $1 /FORMAT=<n> /THRESHOLD=<n> /GREYSCALE
PROJECT /SWITCH $1
PROJECT /LOAD $1 (not recommended to use in SLAM mode)
PROJECT /NEW /CNAME=<s> $1 /TITLE=<s> /WORKDIR=<s> /FORMULA=<s> /MORPH=<s> /CCOL=<s>
       /DENSITY=<s> /DENSMETH=<s>
PROJECT /COPY /CNAME=<s> $1 /TITLE=<s> /WORKDIR=<s> /FORMULA=<s> /MORPH=<s> /CCOL=<s>
       /DENSITY=<s> /DENSMETH=<s> /CLEAR /RESET
PROJECT /EDIT /TITLE=<s> /FORMULA=<s> /MORPH=<s> /CCOL=<s> /DENSITY=<s> /DENSMETH=<s> /CLEAR
       /RESET
PROJECT /BACKUP $1 $2 $3 /NOCALIB /NOWORK
PROJECT /REMOVE $1
PROJECT /DELETE $1
PROJECT /MAKEDEF
QUIT
RATEMETER $1/RESET=<n> /SHUTTER
REDRAW
REFL_ARRAY /THRESHOLD $1 $2 /CONTIG=<n> /COUNTS=<n> /SIGMA=<NN> /XEXMIN=<n> /XEXMAX=<n>
       /RMAX=<n> /DMIN=<n> /DMAX=<n> /DBIAS=<n> [$3 $4 $5 $6 $7 $8]
REFL_ARRAY /PICK $1 $2 $3 $4 /START=<n> /QUADRANT=<n> /FRAME_HALFWIDTH=<n>
REFL_ARRAY /INDEX $1 /AAX=<n> /BAX=<n> /CAX=<n> /U1=<n> /U2=<n> /U3=<n> /FCELL=<n> /SIGA=<n>
       /NOREDUCE /VERBOSE /FGROUP=<n> /HKLTOL=<n> /FFIT=<n>
REFL_ARRAY /BRAVAIS $1 $2 $3 $4 $5 $6 $7 /SIGA=<n> /SIGB=<n> /SIGC=<n> /SIGMA=<n> /SIGBEST=<n>
REFL_ARRAY /LEASTSQ $1 $2 $3 $4 $5 $6 $7 /DXC=<n> /DYC=<n> /DISTANCE=<n> /ROLL=<n> /YAW=<n>
       /U1=<n> /U2=<n>  /U3=<n> /HKLTOL=<n> /HALFWIDTH=<n> /MASK=<n> /PARNAME=<n>
REFL_ARRAY  /EDIT
REFL_ARRAY /MODIFY $1 $2 /FIELD=<n> /VALUE=<s>
REFL_ARRAY /SORT $1 $2 /FIELD=N /DESCENDING
REFL_ARRAY /TRANSFORM $1 $2 $3 $4 $5 $6 $7 $8 $9
REFL_ARRAY /MATRIX $1 $2 $3 $4 $5 $6 $7 $8 $9
REFL_ARRAY /HCALC $1 $2 $3 $4 $5 $6 $7 $8 $9
REFL_ARRAY  /CLEAR
REFL_ARRAY /LOAD $1
REFL_ARRAY  /RSPACE
REFL_ARRAY /CDF $1 $2 $3 $4 $5 $6 $7 $8 /FORMULA=<s> /TYPE=<s> /FILE=<s> /VERBOSE
REFL_ARRAY  /SAVE   $1  $2  $3
SAVE $1 /TITLE=<s> /XENGEN /DISPLAY=<n>
SCAN /SINGLERUN  $1  [/2THETA=<n> | /THETA1=<n>]  [/OMEGA=<n> | /THETA2=<n>>]  /PHI=<n>
       /CHI=<n>  /X=<n.  /Y=<n>  /Z=<n>  /AUX=<n>  /AXIS=<n>  /WIDTH=<n>  /SCANTIME=<n>
```

```
       /TITLE=<s>  /SAMPLE=<s>  /NUMSAMPLE=<n>  NAME=<s>  /RUN=<s>   /FRAMENO=<s>
       /DISPLAY=<n> /REALTIME  /CLEAR  /OLDXENGEN  /MODE=<n>  /ROTATE  /VIDEO
       /OSCILLATE=<s> /AMPLITUDE=<n> [/SNAME=<s>  /SRUN=<n>  /SFRAME=<s>]
SCAN /EDITRUNS (interactive command only)
SCAN /MULTIRUN $1 /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n> /DISPLAY=<n> /REALTIME /CLEAR
       /OLDXENGEN /STARTRUN=<n> ENDRUN=<n> /MODE=<n> /ROTATE /VIDEO /OSCILLATE=<s>
       /AMPLITUDE=<n> [/SNAME=<s>]
SCAN /RESUMERUNS  $1  /TITLE=<s>  /SAMPLE=<s> /NUMSAMPLE=<s>/DISPLAY=<n> /REALTIME /CLEAR
       /OLDXENGEN /STARTRUN=<n> /ENDRUN=<n> /MODE=<n> /ROTATE /VIDEO $2 /SNAME=<s>
       [/2THETA=<n> | /THETA1=<n>] [/OMEGA=<n> | /THETA2=<n>] /PHI=<n> /CHI=<n> /X=<n> /Y=<n>
       /Z=<n> /AUX=<n> /AXIS=<n> /WIDTH=<n> /SCANTIME=<n> /RUN=<s> /FRAMENO=<s> $3
SCAN /ROTATION $1 /TTZERO /PHI=<n> /CHI=<n> /DISPLAY=<n> /REALTIME /RESET=<n>
SCAN /HKL $1 $2 $3 /SCANTIME=<n> /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n> /NAME=<s> /RUN=<s>
       /FRAMENO=<s> /DISPLAY=<n> /REALTIME
SCAN /PSI $1 $2 /SCANTIME=<n> /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n> /NAME=<s> /RUN=<s>
       /FRAMENO=<s> /DISPLAY=<n> /REALTIME
SCAN /COUPLED $1 $2 $3 /WIDTH=<n> /SCANTIME=<n> /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<n>
       /NAME=<s> /RUN=<s> /ROTATE /X=<n> /Y=<n> /REALTIME
SCAN /ZONE $1 /WIDTH=<n> /SCANTIME=<n> /DISPLAY=<n>
SCAN /AXIAL $1 /WIDTH=<n> /SCANTIME=<n> /DISPLAY=<n>
SCAN /SELECTTARGETS
SCAN /GRIDTARGETS /XBEG=<n> /XEND=<n> /XINC=<n> /YBEG=<n> /YEND=<n> /YINC=<n> /TRANSMISSION
SCAN /EDITTARGETS
SCAN /MULTITARGETS $1 [/2THETA=<n> | /THETA1=<n>] [/OMEGA=<n> | /THETA2=<n>] /PHI=<n> /CHI=<n>
       /AXIS=<n> /WIDTH=<n> /SCANTIME=<n> $2 /TITLE=<s> /SAMPLE=<s> /NUMSAMPLE=<s>
       /DISPLAY=<n> /REALTIME /CLEAR /STARTRUN=<n> /ENDRUN=<n> /MODE=<n> /ROTATE /VIDEO
SCAN /MASTER  $1  /SEND_CONFIG
SCAN /SLAVE
SHUTTER
SMOOTH  /AVERAGE
SMOOTH  /MEDIAN
SMOOTH  /CONVOLVE  $1
SPATIAL /NEW $1 /COUNTS=<n> /DISPLAY=<n> /REALTIME /FILE=<s> /XENGEN /THRESHOLD=<n> /SHUTTER
SPATIAL /LOAD  $1
SPATIAL /LINEAR
SPATIAL  /PROCESS $1 /THRESHOLD=<n>
SPATIAL /UNWARP $1 $2 $3 /NONORMALIZATION /DISPLAY=<n> /XENGEN  /NOBEAMCENTER
SPAWN
STRESS /CONVENTIONAL $1 $2 $3 $4 /NORMAL=<n> /STEPSIZE=<n> /2THETA=<n> $5 /FILENAME=<s>
STRESS /SCHEME2D  $1  /PEAK=<n>  /DISTANCE=<n>  $2  [/2THETA=<n> | /THETA1=<n>]
```

```
        [/OMEGA=<n> | /THETA2=<n>]  /PHI=<n>  /CHI=<n>  /AXIS=<n>  /WIDTH=<n>  /CLEAR
STRESS  /BIAXIAL2D  $1  $2  $3  $4  /NORMAL=<n>  /STEPSIZE=<n>  /NUMBER=<n>  /2THETA=<n>  $5
        /FILENAME=<s>  /HKL=<s>  /YOUNG=<n>  /POISSON=<n>  /ARX=<n>  /LINESHAPE=<n>
        /CUTOFF=<n>  /BKGFIT=<s> /KALPHA2 /PHI=<n> /PSI=<n> /REPROCESS
STRESS /SHEAR2D …(same as biaxial2d)
STRESS /TRIAXIAL …(same as biaxial2d)
STRESS  /VIEW2D  $1  /DISPLAY=<n>  /DATA  /LINE  /DELAY=<n>  /DIRECTION=<s>
SYSTEM  $1
VIDEO /LIVE
VIDEO /FREEZE
WAIT $1
ZOOM  $1  $2  $3
```

H. Remote Operations (SMARTservice)

Online GADDS now supports remote operation from another program when GADDS is in command mode and another package called SMARTservice is loaded and started. SMARTservice operates as an NT Service, which is always running as part of the operating system. From any networked computer, you can connect to SMARTservice using winsockets. You can either use TELNET or write your own winsocket program to communicate with SMARTservice.

Remotely you can send to GADDS:

- Any SLAM command
- Hard abort (CTRL+C or CTRL+BREAK)
- Soft abort (ESC)
- Pause (CTRL+S)
- Resume (CTRL+Q)

Remotely you can receive from GADDS:

- Log file as it's generated
- Informational messages
- Error messages
- Angle, Drive, Shutter, Laser, Attenuator statuses

Remotely you can send to NT:

- Command to start a program (such as GADDS)
- Command to kill a program
- Command to reboot frame buffer

Typically, you can use TELNET to remotely and efficiently monitor data collection status. Simply connect via winsockets (modem or network) to SMARTservice. Then connect to the GADDS log file (when you are just monitoring the log file, GADDS may be running in either menu or com-

mand mode). You will see the last ten lines of the log file, enough to easily determine whether GADDS is still running or stopped with an error condition. New lines will display as they are received.

For more elaborate remote control of GADDS, you must either write your own winsocket-enabled program or modify a third party package such as EPICS, LABVIEW, or SPECS to send commands over winsockets. Bruker does not supply any such winsocket-enabled program.

See the SMARTservice Software Manual for more details.

NOTE: Bruker supplies PCAnywhere32 on our frame buffers for remote diagnostics by our service department using either modems or a network. PCAnywhere32 allows the entire desktop of the frame buffer to be remotely controlled from another computer running PCAnywhere32. You can install the client version of PCAnywhere32 on another NT workstation to remotely control the frame buffer (see PCAnywhere license agreement). Use PCAnywhere32 when you wish to run the GADDS program but are sitting in front of a different computer. Use SMARTservice when you wish to control the GADDS program from another program, such as EPICS, LABVIEW, SPECS, or TELNET.

I. Electronic Tracking of Instrument Configuration Changes (Bruker Log Service)

GADDS now supports electronic tracking of instrument configuration changes. GADDS only logs the Bruker Instrument Administrator changes such as:

- Calibrate: New detector parameters.
- Collect > Goniometer > Encoders: New encoder offset(s).
- Edit > Configure > User/Admin: New calibration direction, New detector parameters, and New wavelength parameters.
- Flood > New: New flood correction.
- Project > Overwrite defaults: New system defaults.
- Spatial > New: New spatial correction.

NOTE: Currently goniometer controller configuration changes other than encoder offsets are not logged, such as direct editing of device.ini when changing stages.

These changes are converted to a two-line ASCII string containing information for program and version, date, time, user, and log string. For example:

```
GADDS 4.1.02:  Date: Thu 12-Oct-2000
Time: 14:54:17  User: SmitKL
Log: Configure > Edit: New wavelen
parms: Cu 1.54184 1.54056 1.54439
1.39222
```

This informational string is sent to two places:

- ..\BrukerInstrumentLog.txt
- Bruker_FDA_GLP_LogService

The BrukerInstrumentLog.txt is typically located in the directory C:\saxi. You can use notepad to view this file.

The Bruker_FDA_GLP_LogService is a Windows 2000/NT Service that can be written to accept these electronic signatures and send it anywhere on your network. Essentially, Bruker provides a hook for easy customization so you can provide electronic tracking of the Bruker instrument in a means compatible with your special laboratory requirements, regulations, and company policy. Bruker does not write this Bruker_FDA_GLP_LogService. Interested parties should contact Bruker to obtain the document: “Integrating Bruker Instruments into an FDA 21 CFR part 11 compliant laboratory.”

NOTE: VIDEO 1.3.02 also supports electronic tracking of instrument configuration changes.