ID16 Beamline

HORIZONTAL and VERTICAL SPECTROMETERS USER MANUAL

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Computers

Inel6: This is the experiment control computer. It runs the experiment control programs FOURC and HORIZONTAL. The first workspace is dedicated to the control of the main mono, mirror, primary and secondary slits (the users are not concerned). In the second workspace should run the Control Program (Horizontal or Fourc). The third workspace is utilised to prepare macros to run a suite of IXS scans. The last workspace should have two panels open. One for editing the routine output CPLOT macro, and the second window to execute the macro.
You should not attempt to start more applications or do whatsoever what is the scope of this computer in order to avoid any potential overloading of this most crucial computer.

Inelsun: This is the data analysis computer. An image of the data files on *inel6* are automatically created on *inelsun*. This serves as a back-up, and allows to work on-line with the data. Here *newplot* and *sqwadd* are running as well as the relevant fitting programs.

Experiment control computer: **inel6**
login: opid16
password: tonic16
working directory: /data/runN_YY/HS_ABCD

Data analysis computer: **inelsun**
login: opid16
password: tonic16
working directory: /experiments/hsabcd

Inel2: This computer runs the beamline control applications such as the Front-End application and the Vacuum application. Nothing else should be running on this computer!!!

Pacifico: This PC is dedicated to the recording and diagnostics of focal spot images and the *SensiCam* images for crystal alignment purposes (see separate manual).

Pc2id16: This PC is utilised for further data display such as stacks of IXS scans, dispersion curves etc.

Id16pc1: same as **Pc2id16** but located in CC3.

The most important motors

On the ID16 beamline for the collective excitations studies are operating two different spectrometers with different characteristics. The two spectrometers can not be utilized simultaneously, consequently one of the two have to be taken apart. The HORIZONTAL Control Program controls the horizontal spectrometer and the FOURC Control Program controls the vertical spectrometers. The two Control Programs share some motors that can have different names. In the following list it will be specified when the name change or when a motor appear in one program only

General control motors (HORIZONTAL + FOURC):

mono [degree]; main theta axis of Kohzu premonochromator. Make the rotation of the two Si(111) crystals and the translation of the second crystal. This is usually set, and needs only to be tweaked, if the ratio *monocur/vdlacur* is not ok (see further below).

R2Th [degree]; Rotation of the second Si(111) crystal. This has to be adjusted from time to time (see monochk macro).

roty [mrad]; mirror angle. This needs to be tweaked, if the intensity ratio *ione/vdlacur* (or *ione/i10*) is not ok (see further below).

y [mm]; movement of the mirror perpendicular to beam direction. This has to be adjusted when there is a consistent horizontal movement of the beam.

Specific motors:

HORIZONTAL Control Program	FOURC Control Program	
sth [mm]	**tth** [deg]	2-theta arm of spectrometer; operates only towards positive values
sth [deg]	**th** [deg]	sample rotation around the y axis (perpendicular to incident beam axis); + acw looking towards ring wall
ax [mm]	**esse** [mm]	Move in and out of the beam the *S(Q)* detector;

Sample motors (HORIZONTAL + FOURC):

chi [deg]; sample rotation around incident beam axis; + cw looking towards undulator source.

phi [deg]; sample rotation around the z axis (perpendicular to incident beam axis); + acw (birds view).

sax [mm]; sample translation along beam direction (x axis) for sth = 0 (or th = 0); + towards the spectrometer.

say [mm]; sample translation along the y axis; + towards ring wall.

saz [mm]; sample translation along the z axis for sth =0 (or th = 0); + downwards.

Additional necessary motors (HORIZONTAL + FOURC):

i1hof	[mm]; horizontal offset of slit system defining beam size on sample
i1hgap	[mm]; horizontal gap of slit system defining beam size on sample
i1vof	[mm]; vertical offset of slit system defining beam size on sample
i1vgap	[mm]; vertical gap of slit system defining beam size on sample
wheel	[deg]; Attenuation wheel, increasing attenuation with increasing motor position: 45, 90, 135, 180, 225, 270 315. No attenuation: wheel 0.
ssy	[mm]; + towards experimental hall. Horizontal translation of entrance pinhole. It has to be aligned carefully before each experiment
ssz	[mm]; vertical translation of entrance pinhole; + upwards.

Additional necessary motors (HORIZONTAL only)

a2hof	[mm]; horizontal offset of analyser slits for ana#2
a2hgap	[mm]; horizontal gap of analyser slits for ana#2
a2vof	[mm]; vertical offset of analyser slits for ana#2
a2vgap	[mm]; vertical gap of analyser slits for ana#2
a1vgap	[mm]; vertical gap of analyser slits for ana#1
a1hgap	[mm]; horizontal gap of analyser slits for ana#1

Additional necessary motors (FOURC only)

hof	[mm]; horizontal offset of analyser slits
hgap	[mm]; horizontal gap of analyser slits
vof	[mm]; vertical offset of analyser slits
vgap	[mm]; vertical gap of analyser slits

Starting your experiment

Your local contact will set the name of the experiment directory and the name of the experimental file. This is usually only one file, where each scan has an increasing number within this datafile. Example: filename *exp102*, scan *#S 5*

Motor status, moving motors, and counting

N.B. The same commands are valid also in `fourc>`

```
horizontal> wa                  (shows all the motor positions)
horizontal> wm (motor name)     (shows the position of the particular motor)
horizontal> ct (n)              (counts for n seconds)
horizontal> umvr (motor name)   (change of actual position)
```

(relative movement with respect to actual value, motor moves back to initial position afterwards)
Example: umvr tth 0.5

```
horizontal> dscan (motor name) (-rel. change) (+rel. change)
(number of points) (counting time)
```
(scan around actual position, motor remains at end position)
Example: dscan say 1 -1 20 1

```
horizontal> ascan (motor name) (start value) (end value)
(number of points) (counting time)
```
(scan from actual position to end value)
Example: ascan say 2 5 30 1

For **sth** (or **th**) and **tth**, the scans should be done from large to small angles, in order to avoid the backlash movement for each point. Be careful when moving these motors over large distances. Pieces of equipment or the sample chamber might be in the way and might get damaged!

Position of alignment pin diode and S(Q) detector

Horizontal Control Program:

Pin Diode: Detector *diodo* in direct beam at **tth = 48** (07.3.2003)

```
horizontal> umv tth 48
```

This value may vary. For the exact position ask your local contact.
N.B. be sure that the *S(Q)* detector is out of the beam

```
horizontal> umv ax 5
```

S(Q) Detector: *S(Q)* Detector in direct beam at **tth = 0**

```
horizontal> umv tth 0
horizontal> umv ax 46   (S(Q) detector in)
horizontal> umv ax 5    (S(Q) detector out)
```

This value may vary. For the exact position ask your local contact.

Fourc Control Program:

Pin Diode alignment is not installed.

S(Q) Detector: *S(Q)* Detector in direct beam at **tth = 0**

```
horizontal> umv tth 0
horizontal> umv esse 29 (S(Q) detector in)
horizontal> umv esse 2  (S(Q) detector out)
```

This value may vary. For the exact position ask your local contact.

Make sure that the premonochromator and the mirror are optimised

Before starting an inelastic scan, you have to make sure that the premono angle **mono** (or **R2Th**) is optimised with respect to the backscattering monochromator (correct value of *monocur/vdlacur*). Furthermore, the mirror angle **roty** might need an optimisation so that the focussed beam is properly centred through the *ione*-slit unit (correct value of *monocur/vdlacur* or *ione/mon*). To scan these motors for optimisation the *monochk* and *mirrorchk* routines have to be deactivated, if there were active, or alternatively be set up properly.

Set-up of mono check routine

```
horizontal> offmonochk
horizontal> monochksetup
```

A menu appears on the screen:

MONOCHK SETUP

mono monitor counter mnemonic:	monocur
high threshold:	90
type:	integrating
machine current counter mnemonic:	vdlacur
low threshold:	10
type:	integrating
sleep time after beam is back:	300

lineup R2Th –0.002 0.002 20 3

mono motor mnemonic:	R2Th
tweak value:	0.0002
scan magnitude:	0.002
scan intervals:	20
scan integration time:	1
line up at :	PK
plot filter:	1

lineup R2Th –0.01 0.01 40 1

pre-scan magnitude magnitude after beam loss:	0.01
pre-scan magnitude intervals after beam loss:	40

The lowest level of check is associated with the presence of the x-ray beam on the premono. If the beam is gone, the spectrum stops automatically, detects when the beam is back, and waits the predefined sleep time after the beam is back. It then performs a pre-scan of the premono, followed by the line-up scan, after which the intensity ratio *monocur/vdlacur* should be optimised.

If during a scan the ratio *monocur/vdlacur* drops below 90% of the initially optimised value, the mono performs a small correction to both sides in order to improve the *monocur/vdlacur* ratio.

Set-up of mirror check routine

```
horizontal> offmirrorchk
horizontal> mirrorchksetup
```

A menu appears on the screen:

MIRRORCHECKSETUP SETUP

mirror monitor mnemonic:	i10
threshold:	90
type:	analog
roty scan counter mnemonic:	ione
lineup roty –0.02 0.02 20 1	
mirror motor mnemonic:	roty
roty tweak value:	-0.002
scan magnitude:	0.02
scan intervals:	20
scan integration time:	1
line up at :	CEN

This check routine makes sure that the beam is always properly steered through the *ione*-slit unit. This unit accommodates the last set of slits before the sample. For small samples and high pressure experiments, the vertical slit (**i1vgap**) is put to 100 µm typically, and during an IXS scan, the mirror needs to be adjusted from time to time. If the intensity ratio *ione/vdlacur* (or *ione/mon*) drops below 90% of the initially optimised value, a small angular correction (defined by the tweak value) is performed.

If the beam is lost, first the monocheck routine is executed, then the mirrorcheck routine. It consists of a line-up scan, after which the mirror is positioned at the maxiumum of the *ione/vdlacur* signal.

Activation of the check routines for the premono and the mirror

```
horizontal> kozon
horizontal> plotselect mon
horizontal> dscan mono -0.002 0.002 20 2
horizontal> umv mono pl_xMAX

horizontal> plotselect vdla
horizontal> dscan R2Th -0.0015 0.0015 20 2
horizontal> umv mono pl_xMAX
```

Before setting the *monochk* routine you have to continue with the optimisation of the mirror (**roty** and **y**) (otherwise the mirror optimisation will be hindered by the running *monochk*).

```
horizontal> hexaon
horizontal> plotselect ione
```

```
horizontal> umv i1hgap 0.1
horizontal> dscan y -0.5 0.5 30 1
horizontal> umv y pl_xMAX
horizontal> umv i1hgap .8


horizontal> umv i1vgap 0.1
horizontal> dscan roty -0.008 0.008 30 1
horizontal> umv roty pl_xMAX
horizontal> umv i1vgap 0.6
```

You have to check whether the mirror has really reached the optimum positions. If this is not the case, you have to try to optimise it by hand, using small corrections of the order of the defined tweak value.

Now after the complete optimisation set first the *monochk* routine:

```
horizontal> onmonochk 3
```

This activates the premonochromator (**mono**) control, as well as the beam control.
Then set the *mirrorchk* routine:

```
horizontal> onmirrorchk 3
```

This activates the mirror control.

Put the horizontal (or vertical) spectrometer arm to the correct scattering angle

```
horizontal> umv tth 658
```
the units are in mm. Look at the table 1b at the end of the document for the conversion a mm→Q(nm^{-1}).

```
fourc> umv tth 10
```
the units are in degrees. Look at the table 1a at the end of the document for the conversion a degrees→Q(nm^{-1}).

Put the Monochromator to the start temperature

Put a set point for the monochromator temperature by giving the values in degrees °C to the *pseudo*-motor **monot** as a normal motor positioning (umv monot *your_set_point*) *e.g.:*

```
horizontal> umv monot 22.00
```

You have to wait typically 5 to 10 minutes until the setpoint is reached.

You can also give the values in meV using the *pseudo*-motor **deltae**, for doing this you have to enter the zero-energy temperature setpoint:

```
horizontal> T0=actual_average_zero_Temp
```

and the wavelength you're using *(e.g. for the (999) reflection. A complete list of the reflection orders and the corresponding wavelengths are given at the end of the document):*

```
horizontal> LAMBDA=0.6968 (UPPER CASE for the variables, it is
        case sensitive)
```

otherwise your **deltae** value (see below) does not make any sense.

Doing a temperature scan

```
horizontal> ascan  monot  init_val  final_val  number_of_step
          integration time
```

or

```
horizontal>  rscan monot init_val1 final_val1 number_of_step1
                        init_val2  final_val2  number_of_step2
                        ..................................
                        init_valn  final_valn  number_of_stepn
                        integration time
```

alternatively you can use the **deltae** motor:

```
horizontal> ascan  deltae  init_val  final_val  number_of_step
          integration time
```

or

```
horizontal>  rscan deltae init_val1 final_val1 number_of_step1
                        init_val2  final_val2  number_of_step2
                        ..................................
                        init_valn  final_valn  number_of_stepn
                        integration time
```

Example: scan from -80 to 80 meV, with 0.5 meV step, 1mn int. time, at the (999) reflection (λ = 0.6968 Å), with T0=21.71, looks like:

```
horizontal> T0=21.71
horizontal> LAMBDA=0.69680026
          (just  once,  after  you  have  selected  the  mono-
          reflection and determined the elastic temperature)
horizontal> ascan monot 23.6 20.08 320 60
```

or

```
horizontal> ascan deltae -80 80 320 60
```

You can also type:

```
horizontal> ascan monot T0-1.76 T0+1.76 320 60
```

Stopping a scan

```
horizontal> [CTRL-C]
```

Scanning or counting will be stopped. If a *dscan* was running, the motor will return to its initial position.

Running a Macro

This is frequently utilised, if a sequence of scans shall be performed, once the measurement strategy has been defined.

1) Edit/modify the macro with the editor you like (*vi*, *emacs*, *nedit* etc.) in the working directory. The name of the macro (first line) must be the one of the macro file (example: name of the macro *macfilename*, name of the file *macfilename.mac*).

   Example:

```
def res'

#Si (11 11 11)
# file: res230603

# ANA2 & ANA1
umv tth 581
umv ssy -0.5
ascan monot 21.65 20.57 216 50
umv monot 21.65
sleep(400)

# ANA4 & ANA3
umv tth 276
umv ssy -0.30
ascan monot 21.65 20.57 216 50
umv monot 21.65
sleep(400)

# ANA5
umv wheel 45
umv tth 48.5
umv ssy 2.4
umv wheel 0
ascan monot 21.65 20.57 216 50
umv monot 21.11
'
```

2) Macro compilation:

```
horizontal> qdo macfilename.mac
```

   You can check the content of the compiled macro by

```
horizontal> prdef macfilename
```

3) Macro execution:

```
horizontal> macfilename
```

Plotting data file (in CPLOT)

This operation generates the standard output for the log book, and it is highly recommended. It makes it a lot easier to detect any potential bug in the spectrum and identify the problem, if the key characteristics are printed out.

Start Cplot in the fourth window of the X-Terminal: *cplot*
The Cplot-macros are called *rec1.do* and *quadro.do* for HORIZONTAL and *vertical.do* for FOURC.

Output on printer for HORIZONTAL:

```
PLOT-> do rec1.do $1 $2 $3 $4

$1 = filename; $2 = scan number; $3 = integration time;
$4 = momentum transfer Ana#1 in nm-1


PLOT-> do quadro.do $1 $2 $3 $4 $5 $6

$1 = filename; $2 = scan number; $3 = momentum transfer;
Ana#2 in nm-1; $4 = momentum transfer Ana#3 in nm-1; $5 =
momentum transfer Ana#4 in nm-1; $5 = momentum transfer
Ana#5 in nm-1
```

Output on printer for FOURC:

```
PLOT-> do vertical.do $1 $2 $3 $4

$1 = filename; $2 = scan number; $3 = integration time;
$4 = momentum transfer in nm-1
```

THINGS NOT TO DO

1) Move the spectrometer arm to small Q-values, where either analysers #1, #2 or the S(Q) detector are close or in the direct beam (or an intense Bragg reflection).
If this is necessary put by all means the absorber wheel in:

```
horizontal> umv wheel 315 (270)
```

but not less than 270, this will saturate the detector.

2) Move the sample angle theta (**th** or **sth**) to high angles or spectrometer arm to large scattering angles (**tth**), since you might hit into the sample vacuum can. Visual inspection is indispensable!!!!
Be as well careful when moving sample tilt angles (**phi**, **chi**) by larger amount; there is very little space available around the sample position! The sample chamber may run into surrounding equipment or parts of the instrument (detector chamber)!
For any problems phone your local contact, or the Experimental Hall Operators (***25-25***).

SAVE DATA OF YOUR EXPERIMENT!!!!!!!!!!!!!

Put your data on your user account (1-month lifetime). Connect on NICE (Solaris or Linux system) using the name of your experiment (typically HSXXX), and your password (initial of the name of the first applicant followed by the family name *e.g.* experiment HS123, first applicant Mr. H. Gbhkds:

telnet (or ftp) nice
login: hs123 (this is case sensitive)
password: hghs123.

Then transfer the data home using ftp out or telnet out (literally type *ftp out* or *telnet out* then follow the instructions).
For any computing problem phone to the ***24-24*** (computing hot line, 7 a.m.-8 p.m.).

Data conversion and analysis

On the data treatment/analysis computer **inelsun**, the data directory of **inel6** is mounted directly (read only) with all your data in real time. In this way you can analyse the data on-line, without interfering with the data acquisition. Your local contact will create a directory where all the treated data as well as the results of the fits will be stored.

```
inelsun:~% cd experiments
inelsun:~/experiments% mkdir hsnnn
inelsun:~/experiments% cd hsnnn
```

Data extraction

```
inelsun:~/experiments/hsnnn% newplot
```

1. Using the file menu in *newplot*, go into the corresponding data directory of your experiment.
   data/id16/inhouse/data/runN_yy/hsnnn/expNN.

2. Open the file which contains all the spectra.

You have a list of all your scans, you can visualise them, and make some basic analysis.

3. Set extraction script

Depending on the type of scan (horizontal or vertical spectrometer) you have to choose the corresponding extraction script which extracts the relevant columns out of the data file, and performs the conversion of resistance (of the temperature sensors) into temperature.

- Click on the button "Standard" on the bottom right part of the left panel and choose "Set Script".
- Go to the */users/opid16/Swadd_script* and choose the appropriate script:
  Horizontal: for standard IXS scans with the horizontal spectrometer.
  Vertical: for standard IXS scans with the vertical spectrometer.

4. Selection of the scans to be extracted

When you have chosen which scans you are interested in, select them by clicking (left button) on the little arrow on the left of the scan name (or select them and click on the select button). Then push the extract button on the bottom. *newplot* then extracts the chosen scans into separate files *expN.nscan* (*nscan*= number of the scan), with the following columns:

If you use *Horizontal*:

Monitor, Ione, Tmono, ΔT_1(ana1-mono), ΔT_2(ana2-mono), ..., ΔT_5, deta1, deta2, deta3, deta4, deta5, S(Q)-det

If you use *Vertical*:

Monitor, Ione, Setpoint, ΔT(ana-mono), Tana, Tmono, ΔT(ana-mono), ΔT(ana-mono), Signal/Ione, Signal, Signal, Signal, Signal, Signal.

Further raw data treatment and summing of spectra

sqwadd is a tool to prepare IXS-spectra for further fitting after they have been extracted from the standard SPEC-data file (extraction done via ***newplot***). It allows to display and inspect the individual spectra of each scan and each analyser, e.g. to compare repeated spectra, centre the individual spectra (by pre-fitting them), sum together several spectra (repetitions or extensions of spectra) and save the spectra or sums of spectra converted from a temperature-axis to an energy axis.

sqwadd has to be started in the directory, where you have saved the extracted file; the tool will save the results in this same directory (e.g. on inelsun.esrf.fr: ~/experiments/HS2000.) The tool opens in a window offering pull-down menus as well as click-buttons for the tasks to do.

Load data files: menu FILE – OPEN and load the data to be treated together.

Choice of reflection order: Choose the correct incident photon energy by selecting the corresponding correct backscattering reflection ("*Bragg Reflection*", e.g. *999*).

Output file names: Filenames have to be given for each analyser individually, either under "*SCANS*" or under "*OUTPUT*".

Selection of the analyser: The analyser whose spectrum shall be treated, has to be chosen by clicking on the corresponding button on the main panel.

The data-treatment is done in 3 steps. The described procedures have to be repeated for every spectrum and every analyser of interest. Note that this procedure is indispensable, even if you have only a single file. In order to fit the data with ***minuit*** (see below) you need a file with a constant step in temperature (energy).

1. Determination of the elastic line: The first step consists of determining the position of the elastic line, corresponding to zero energy-transfer. The fitting is started by clicking on the taskbar-button with two Gaussian-like profiles, which opens an additional window to first "estimate" the values of the fitting parameters and "start" the fitting itself. By default the fits are done with Lorentzian function plus some background, but other functions can be chosen from the menu. The number of peaks is "found" automatically and cannot be changed, even not by changing the type of fit-function. Note, that only the Lorentzian-fit results are taken into account automatically for the further treatment; if the fits are done using other fit-functions (Gaussian, PseudoVoigt etc.) the values have to be entered manually. If the number of peaks offered is not at all convenient, the zero-energy-transfer can also be estimated with help of crosshairs (to be found in the "*GRAPH*"-pull-down menu), and the value found can then be entered manually. At the end of the procedure, the column “SHIFT” in the sheet “SCANS” should contain the correct value by which the spectrum has to be shifted in order to have the elastic line centred at zero.

2. Centring of the spectrum: The centring of the spectrum is done by clicking on the taskbar-button showing a profile with crosshairs (or by choosing the "*CENTER*"-item in the pull-down menu). The procedure consists to shift the spectrum by the chosen amount, and interpolate the

spectrum in order to obtain an equally spaced grid on the x-axis. This is necessary, if the data shall be fitted with ***minuit***.

3. Summing the spectra: The third taskbar-button, displaying a profile with a "+"-symbol, then sums the highlighted spectra together, converts them into an energy (meV-) scale and saves the results under the filename given ("*OUTPUT*" or "*Output File Name*"). If you have prepared as described above the spectra for all analysers and have defined all filenames for the results, you can do the summing-up by only clicking on the "*SUM ALL*"-button, instead of doing the summing-up for each analyser individually.

sqwadd itself will not display whether or not it performed the tasks, but the window, where you started the tool will display comments on the tasks (for the centring, summing-up, saving into the file etc.).

To be able to use other software to continue to treat these summed-up data, here the description of the columns in the squadd-output (ASCII-) file:

1st col.:	energy tranfer
2nd col.:	counts (normalised to the average monoitor)
3rd col.:	error bar for col. 2
4th col.:	unknown porpose
5th col.:	original counts (as summed up)
6th col.:	summed-up monitor (from the *ione*-monitor in the SPEC-datafile)
7th col.:	error bar for col.5

On-line fitting with minuit

The fitting is done in your analysis directory (users/opid16/experiments/hsNNN). For fitting with the minuit library, called by the program ***minuit*** (n excitations: Lorentzians or damped harmonic oscillators), you need a file with a constant step in temperature (energy), so you have to use ***sqwadd*** beforehand, even for one single scan. You need the summed data and the actual resolution function files (ask the local contact), and to prepare an input file for each scan you want to analyse.

1. Preparation of the input file:

Copy the standard input file min.inp (for ***minuit***) on **inelsun** in *users/opid16/usermacros* to your directory: users/opid16/experiments/hsnnnn. Copy the resolution file (ask to the local contact the names of the resolution files) in the resolution directory *users/opid16/resolutions* to your directory: *users/opid16/experiments/hsnnn*. The format of the input file is as follows:

```
g-03.003      ! data input file
g-03f.003     ! fitted output file
out03g.do     ! file do for c-plotting
a1res11.dat   ! resolution file
DHO           ! fitting model
80            ! temperature
3             ! momentum transfer
MINUIT :
         1  BG      .12       .01       .000001   50.
         2  SL      -.000     .0001     -0.2      0.2
         3  ZR      0.008     .001      -2.       2.
         4  GR      1.        .1        .000001   10.
         5  PC      21.       .10       10.       220000.
         6  GC      0.28      .01       .001      10.
         7  PL      .10       0.01      .000001   2000.
         8  OL      6.07      0.01      .001      9.0
         9  GL      1.04      0.10      .000001   10.

SET PRInt  2.
SET ERRdef 1.
FIX        4.
SEEK       200.
SIMPLEX
MIGRAD
HESSE
EXIT
```

1. line: name of data file (input data)
2. line: name of output file, containing the experimental data and the fit
3. line: name of the C-PLOT do-file with which one can visualise and print the results
4. line: file of the experimental resolution function with which the model function is convoluted
5. line: fit (main) model used: dho: Damped Harmonic Oscillator
   lor: Lorentzian functions
6. line: temperature in degree Kelvin (real number)
7. line: momentum transfer in nm^{-1}

The meaning of the fitting parameters is as follows:

BG	background
SL	linear slope of the background
ZR	energy position of the elastic line
GR	only used if one convolutes with a Lorentzian function, otherwise has to be kept fixed
PC	central line intensity
GC	central line width
PL	1st. phonon line intensity
OL	1st. phonon line energy
GL	1st. phonon line width

The following lines are standard commands to execute the minuit libraries minimisation, the only ones you need to specify is the FIX line: put 1 FIX line for each parameters you want to minimise, with the number of the parameter (1 for BG, 3 for ZR and so on).

If you need to fit your data file with other models (see visco-elastic) or fit your data file with more than one excitations ask directly to your local contact.

2. Running the fitting program:

```
> minuit < name_file.inp  (example: minuit < min.inp)
```

3. Plotting the result of the fit:

The results of the fit can be visualised and printed using CPLOT with the CPLOT macro generated by minuit (with the name you put on line 5 of the input file *e.g.* on CPLOT:

```
PLOT>do cpfilename.do
```

To print, modify the CPLOT macro, putting the zi x11 statement in comment (#zi x11), and run the macro again.

To be able to use any other software to visulize the fit-curves, here the description of the columns in the fit-output (ASCII-)file (the filename is defined in the 2nd line of the input –file):

1st col.:	Energy transfer
2nd col.:	data
3rd col.:	error bar of data
4th col.	total fit (sum of all contributions)
5th col.:	fit of the exitations (DHO model or lorentzians)

Horizontal Control Program Column list
from TEMPERATURE SCANS as of Jan. 30,2003

Col#	Counter name	Counter meaning	Inv.#
1	Monot	monot setpoint in °C	-32
2	Epoch		-31
3	S(q)-Det		-30
4	S(k)	Alignment Diode end of the arm	-29
5	IONE	Ione Detector	-28
6	Det-CH1	Detector Sig1	-27
7	Det-CH2	Detector Sig2	-26
8	Det-CH3	Detector Sig3	-25
9	Det-CH4	Detector Sig4	-24
10	Det-CH5	Detector Sig5	-23
11	Mono	NTC n.1 mono in Ω	-22
12	Tc(mV)	NTC n.2 mono in Ω	-21
13	ana_1	NTC analyser #1 in Ω	-20
14	ana_2	NTC analyser #2 in Ω	-19
15	ana_3	NTC analyser #3 in Ω	-18
16	ana_4	NTC analyser #4 in Ω	-17
17	ana_5	NTC analyser #5 in Ω	-16
18	VDL ANAL	Vdl	-15
19	Det Check		-14
20	VDL CORR		-13
21	Srcur		-12
22	Counter 21		-11
23	Counter 22		-10
24	Ione/mon		-9
25	Diodo		-8
26	temp_euro		-7
27	Moncur		-6
28	asl 10	Pt100 mono in °C	-5
29	ntc1	NTC n.1 mono in °C	-4
30	Ntc2	NTC n.2 mono in °C	-3
31	Monitor	Monitor Detector	-2
32	Seconds	Integration Time	-1

Fourc Control Program Column list
from TEMPERATURE SCANS as of June 20,2003

Col#	Counter name	Counter meaning	Inv.#
1	monot	monot setpoint in °C	-26
2	H		-25
3	K		-24
4	L		-23
5	Epoch		-22
6	Signal	Signal Back. Detector	-21
7	Tmono	NTC mono in Ω	-20
8	Tana	NTC analyzer in Ω	-19
9	VDL ANAL	Vdl	-18
10	Det Check		-17
11	VDL CORR		-16
12	IONE	Ione Detector	-15
13	Ione/mon		-14
14	S(k)	S(Q) detector	-13
15	Diodo	Alignment diode	-12
16	Cryo T2	Si diode inside ST15	-11
17	srcur		-10
18	moncur		-9
19	p_wika		-8
20	volto		-7
21	ampo		-6
22	NTC_m	NTC mono in °C	-5
23	NTC_a	NTC analyzer in °C	-4
24	aslmono	Pt100 mono in °C	-3
25	Monitor	Monitor Detector	-2
26	Seconds	Integration Time	-1

Scattering angle – Q relation and angular spacing of analysers:

$Q\ [nm^{-1}] = 4\pi/\lambda * \sin(2\theta/2)$

Table 1a – Conversion factor (angle → nm^{-1}), wavelength and Energy for each reflections. To use with the FOURC program.

Reflection	Momentun Transfer Q	Lambda λ [Å]	Energy [keV]
Si(7 7 7)	140.26 nm^{-1} *sin(2θ/2)	0.8959	13.840
Si(8 8 8)	160.3 nm^{-1} *sin(2θ/2)	0.7839	15.816
Si(9 9 9)	180.35 nm^{-1} *sin(2θ/2)	0.6968	17.794
Si(11 11 11)	220.414 nm^{-1} *sin(2θ/2)	0.5701	21.7477
Si(12 12 12)	240.45 nm^{-1} *sin(2θ/2)	0.5226	23.7246
Si(13 13 13)	260.49 nm^{-1} *sin(2θ/2)	0.4824	25.7017

Table 1b – Conversion factor (mm → nm^{-1}) and Energy for each reflections. To use with the HORIZONTAL program.

Reflection	Momentun Transfer Q [nm^{-1}]	Energy [keV]
Si(7 7 7)	140.26 nm^{-1} *sin((arctg(x/5555))/2)	13.840
Si(8 8 8)	160.3 nm^{-1} * sin((arctg(x/5555))/2)	15.816
Si(9 9 9)	180.35 nm^{-1} * sin((arctg(x/5555))/2)	17.794
Si(11 11 11)	220.414 nm^{-1} * sin((arctg(x/5555))/2)	21.7477
Si(12 12 12)	240.45 nm^{-1} * sin((arctg(x/5555))/2)	23.7246
Si(13 13 13)	260.49 nm^{-1} * sin((arctg(x/5555))/2)	25.7017

Table 2 – tth values corresponding at a Momentum Transfer Q = 10 nm^{-1} for each analyzers and each reflections

Analyzer No°	**Si(7 7 7)**	**Si(8 8 8)**	**Si(9 9 9)**	**Si(11 11 11)**	**Si(12 12 12)**	**Si(13 13 13)**
1	9.754°	8.730°	7.934°	6.777°	6.3441°	5.977
2	8.177°	7.153°	6.357°	5.200°	4.7671°	4.40°
3	6.669°	5.645°	4.849°	3.692°	3.2591	2.892
4	5.119°	4.095°	3.299°	2.142°	1.7091	1.342
5	3.551°	2.527°	1.731°	0.574°	0.1411	-

Table 3 - Relative tth angle between analyzers

	#1	#2	#3	#4	#5
#1	-	1.577°	3.085°	4.635°	6.203°
#2	1.577°	-	1.508°	3.058°	4.626°
#3	3.085°	1.508°	-	1.550°	3.118°
#4	4.635°	3.058°	1.550°	-	1.568°
#5	6.203°	4.626°	3.118°	1.568°	-

Table 4- Maximum momentum transfer, Q_{max}, for the Horizontal and Vertical Spectrometer. ΔQ indicates the Q-spacing between adjacent analysers.

Energy [keV]	Reflection order n	Horizontal Spectrometer		Vertical Spectrometer
		Q_{max} [nm^{-1}]	ΔQ [nm^{-1}]	Q_{max} [nm^{-1}]
13.840	7	21.3	1.89	124
15.817	8	24.4	2.16	142
17.794	9	27.4	2.43	160
21.747	11	33.5	3.0	-
23.725	12	36.5	3.24	-
25.704	13	39.6	3.5	-

Table 5. High Resolution Si(h h h) monochromator and useful conversions

Reflection	**(7 7 7)**	**(8 8 8)**	**(9 9 9)**	**(11 11 11)**	**(12 12 12)**	**(13 13 13)**
Wavelength [$Å^{-1}$]	**0.895886**	**0.7839003**	**0.6968003**	**0.5701093**	**0.52260096**	**0.48240018**
Energy [eV]	**13839.35**	**15816.40**	**17793.45**	**21747.56**	**23724.57**	**25701.66**
Conversion meV → K	**0.02822**	**0.02470**	**0.02195**	**0.01796**	**0.01646**	**0.01520**
$(\Delta E)_M$ [meV]	**5.3**	**4.4**	**2.2**	**1.02**	**0.73**	**0.5**
$(\Delta E/E)_M$	**3.8×10^{-7}**	**2.8×10^{-7}**	**1.2×10^{-7}**	**4.7×10^{-8}**	**3.0×10^{-8}**	**2.0×10^{-8}**
Conversion angles→nm^{-1}	**140.26**	**160.31**	**180.34**	**220.42**	**240.46**	**260.50**
Flux [ph/s 200 mA]	**7×10^{10}**	**6×10^{10}**	**1.8×10^{10}**	**4.4×10^{9}**	**3.9×10^{9}**	**9.8×10^{8}**