

INITIALIZE

The **INITIALIZE** statement sets up the initial structure for a simulation.

INITIALIZE

```
{ ( IN.FILE=<c> { ( [SCALE=<n>] [FLIP.Y] ) | TIF } )
  | ( [WIDTH=<n> [DX=<n>]] [ {<111> | <110> | <100> | ORIENTAT=<n>} ]
    [ {ROT.SUB=<n> | X.ORIENT=<n>} ] [RATIO=<n>] [LINE.DAT]
  )
}
[ IMPURITY=<c> { I.CONC=<n> | I.RESIST=<n> } ]
[ MATERIAL=<c> ] [ANTIMONY=<n>] [ARSENIC=<n>] [BORON=<n>] [PHOSPHOR=<n>]
[ {CONCENTR | RESISTIV} ]
```

Parameter	Type	Definition
IN . FILE	character	Name of a saved structure file. If this parameter is omitted, a rectangular grid is generated, using previously specified LINE , ELIMINATE , REGION , and BOUNDARY statements. Default: none Synonyms: INFILE
SCALE	number	The mesh read in from IN . FILE is scaled by this factor. Units: none Default: 1.0
FLIP . Y	logical	Specifies that the input structure is to be reflected about y=0. Default: false
TIF	logical	Specifies that the input file is a TIF (Technology Interchange Format) file. Default: false
WIDTH	number	The width of the initial structure. (Only used if no LINE X statements are specified.) Units: microns Default: the width of the MASK information, if any, or 1.0
DX	number	The grid spacing to use in the x direction. Units: microns Default: the current value of DX . MAX from the MESH statement
<111>	logical	Specifies that the crystalline orientation of the silicon substrate is <111>. Default: false
<110>	logical	Specifies that the crystalline orientation of the silicon substrate is <110>. Default: false
<100>	logical	Specifies that the crystalline orientation of the silicon substrate is <100>. Default: True, if no other orientation is specified.

Parameter	Type	Definition
ORIENTAT	number	The crystalline orientation of the silicon substrate. Only 100, 110, and 111 are recognized. Units: none Default: 100 Synonyms: Y . ORIENT
ROT . SUB	number	The rotation of the substrate about the y axis. The reference orientation (ROT . SUB =0) is defined such that the x axis points in a <110> direction. Units: degrees Default: 0.0
X . ORIENT	number	The crystalline orientation of the x axis. This must be a 3-digit integer value. Units: none Default: 110
RATIO	number	The maximum ratio of adjacent grid spacings to be used in generating a grid. Units: none Default: 1.5 Synonyms: INTERVAL
LINE . DAT	logical	Specifies that the location of each x and y grid line be listed on the standard output and in the output listing file. Default: false
IMPURITY	character	The name of the impurity with which the initial structure is doped. Default: none
I . CONC	number	The concentration of the specified IMPURITY in the initial structure. Units: atoms/cm ³ Default: none
I . RESIST	number	The resistivity of the initial structure. Units: ohm-cm Default: none
MATERIAL	character	Specifies the material of the initial structure. Default: SILICON
ANTIMONY	number	The uniform concentration or resistivity of antimony in the initial structure. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: SB
ARSENIC	number	The uniform concentration or resistivity of arsenic in the initial structure. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: AS
BORON	number	The uniform concentration or resistivity of boron in the initial structure. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: B

Parameter	Type	Definition
PHOSPHOR	number	The uniform concentration or resistivity of phosphorus in the initial structure. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: P
CONCENTR	logical	Specifies that the impurity concentration in the initial structure is given. Default: true
RESISTIV	logical	Specifies that the impurity resistivity in the initial structure is given. Default: false

Description

The **INITIALIZE** statement sets up the mesh from either a rectangular specification or from a previously saved structure file. This statement also initializes the background doping concentrations of the impurities specified.

Mesh Generation

If **IN.FILE** is not specified, a rectangular mesh is generated. If **LINE** statements have been specified for the x or y direction, they are used along with any **ELIMINATE**, **BOUNDARY**, and **REGION** statements and the value of the **RATIO** parameter to generate the mesh in that direction. If no **LINE** statements are specified for the y direction, a default y mesh is generated. If no **LINE** statements are specified for the x direction, and **WIDTH** is specified, a mesh of the requested width is generated, with spacing given by **DX**. If no **LINE X** statements are given and **WIDTH** is not specified, the width is taken from mask information read with a preceding **MASK** statement, if any. Otherwise, a one-micron wide structure with a grid spacing of one micron (i.e., one grid space wide) is generated. See [Chapter 2, “Grid Structure” on page 2-2](#) for a complete description of the mesh generation process. The locations of the generated grid lines are listed if **LINE.DAT** is true.

Previously Saved Structure Files

A mesh read from a file must be in either TSUPREM-4 format or TIF (Technology Interchange Format). Meshes read from TSUPREM-4 files can be scaled or flipped about y=0 by specifying the **SCALE** or **FLIP.Y** parameters, respectively.

When a structure is read from a file, the last processing temperature as well as the choice of silicon substrate orientation, oxidation model, and point defect model are automatically set through information stored in the file. You need not respecify these parameters after reading in a structure file at the start of a simulation.

Crystalline Orientation

The crystalline orientation of any silicon regions in a generated structure can be specified by <100>, <110>, or <111> parameters. The **ORIENTAT** parameter is also accepted, for compatibility with older versions of the program. The specified

orientation is used for all single-crystal silicon regions in the simulation, whether present in the initial structure or deposited later. By default, the x axis points in a <110> direction. This can be changed by specifying a rotation about the y axis (**ROT . SUB**) or the crystal orientation of the x axis (**X . ORIENT**).

The orientation parameters do not apply when reading a structure from a file; the orientation of the saved structure is used instead.

Specifying Initial Doping

The **ANTIMONY**, **ARSENIC**, **BORON**, and **PHOSPHOR** parameters can be used to specify the initial resistivity or impurity concentrations in the structure. Any combination of these parameters can be specified if impurity concentrations are given (**CONCENTR** true), but only one impurity can be specified if the resistivity is given (**RESISTIV** true). An impurity can also be specified by name with the **IMPURITY** parameter; **I . CONC** or **I . RESIST** are used to specify the concentration or resistivity, respectively, associated with the named impurity.

The resistivity is calculated from tables of mobility as a function of doping concentration. These tables are described in [Chapter 2, “Initial Impurity Concentration” on page 2-10](#).

Although the source of the grid (read or generated) and the specification of doping are independent, the doping specification is normally used when a grid is generated but not when a grid is read from a file.

Examples

1. The following statement reads in a previously saved structure in file *oldstr*:

INITIALIZE IN.FILE=oldstr

2. The following statement generates a rectangular mesh and initializes the structure with a boron doping of $10^{15}/\text{cm}^3$:

INIT <111> X.ORIENT=211 BORON=1e15

The orientation of single-crystal silicon regions are <111>, while the x axis points in a <211> direction.

3. The following statement generates a mesh and initializes the structure to contain arsenic with resistivity of 20 ohm-cm:

INIT IMPURITY=arsenic I.RESIST=20



Note:

*The conversion from a resistivity to a concentration is based on Masetti's mobility table, while the calculation of electrical characteristics in the **ELECTRICAL** statement uses the same mobility table as in Medici. Thus, the sheet resistances of the initial structure given by the **EXTRACT** statement do not correspond exactly to the resistivity specified on the **INITIALIZE** statement.*

LOADFILE

The **LOADFILE** statement reads mesh and solution information from a file.

LOADFILE

```

      IN.FILE=<c>
      { ( [SCALE=<n>] [FLIP.Y] ) | TIF |
DEPICT }

```

Parameter	Type	Definition
IN.FILE	character	The identifier of a structure file to be read. Default: none Synonyms: INFILE
SCALE	number	A scaling factor to be applied to the mesh when reading TSUPREM-4 structure files. All coordinate values are multiplied by this factor as they are read. Units: none Default: 1.0
FLIP.Y	logical	Specifies that the structure should be reflected about $y=0$ when reading TSUPREM-4 structure files. All y coordinates are multiplied by -1 as they are read. Default: false
TIF	logical	Specifies that the input file is a TIF (Technology Interchange Format) file. Default: false
DEPICT	logical	Specifies that the input file is a formatted file written by <i>Avant!</i> TCAD's Taurus-Lithography (formerly Depict). Default: false

Description

The **LOADFILE** statement reads a mesh and solution from a file. Either TSUPREM-4 or TIF structure files (created with the **SAVEFILE** statement) or Taurus-Lithography structure files can be read. TSUPREM-4 structure files can be scaled or flipped about the x axis ($y=0$) during reading.

TSUPREM-4 Files

The silicon substrate orientation, last processing temperature, current oxidation model, and current point defect model are saved in TSUPREM-4 structure files, and are automatically restored when the file is read. There is no need to respecify these parameters after reading in a structure. (This does not apply to versions of TSUPREM-4 prior to version 9035; versions older than 9035 only saved the substrate orientation.)

Older Versions

Files saved with older versions of TSUPREM-4 can be loaded by newer versions of the program. Files saved with version 5.1 and newer of TSUPREM-4 cannot be read by older versions of the program.

In versions of TSUPREM-4 prior to version 5.1, the **STRUCTURE** statement is used to load structure files. Starting with version 5.1, the **LOADFILE** statement should be used instead. The **IN.FILE**, **SCALE**, **FLIP.Y**, and **DEPICT** parameters are still accepted on the **STRUCTURE** statement, however, for compatibility with older TSUPREM-4 input files.

User-Defined Materials and Impurities

Any user-defined materials and impurities referenced in a structure file should be defined before the file is loaded. If a file containing undefined materials or impurities is loaded, a warning is issued for each undefined material or impurity encountered. The material or impurity is defined, but its properties are not set. Further simulation using the material or impurity may fail unless the properties are set.

Taurus-Lithography Files

Files produced by Taurus-Lithography do not contain the complete mesh and solution information required by TSUPREM-4. Rather, they are used to update an existing structure with the results of a Taurus-Lithography simulation. Thus, the usual sequence for interfacing with Taurus-Lithography is:

1. Generate a structure in TSUPREM-4, either from an initial mesh definition or by reading a saved structure.
2. Save the structure in both TSUPREM-4 and Taurus-Lithography formats. This requires two **SAVEFILE** statements and two output files.
3. Use Taurus-Lithography to process the structure, starting with the saved Taurus-Lithography-format file. Save the results in a new Taurus-Lithography-format file.
4. Read the saved TSUPREM-4-format file into TSUPREM-4 (with an **INITIALIZE** or **LOADFILE** statement).
5. Read the new Taurus-Lithography-format file into TSUPREM-4 (with a **LOADFILE** statement).

Examples

1. The following statement reads in a previously saved structure from file *savestr*:

```
LOADFILE IN.FILE=savestr
```

2. The following statements save a structure to be processed further with Taurus-Lithography:

```
SAVEFILE OUT.FILE=STRTS4  
SAVEFILE OUT.FILE=STRTOSEP DEPICT
```

Taurus-Lithography can read the file *STRTOSEP*. The structure file *STRTS4* is needed when reading the results produced by Taurus-Lithography. If Taurus-Lithography stored its results in file *STRFRDEP*, they could be read into TSUPREM-4 with the statements

```
INITIALIZE IN.FILE=STRTS4  
LOADFILE IN.FILE=STRFRDEP DEPICT
```

3. The statements

```
LOADFILE IN.FILE=savestr
```

and

```
INITIALIZE IN.FILE=savestr
```

are equivalent, except that the program recognizes that an initial structure has been set up in the second case. (An **INITIALIZE** statement must be given before any processing or output statement can be processed.)

SAVEFILE

The **SAVEFILE** statement writes mesh and solution information to a file.

SAVEFILE

```

OUT.FILE=<c> [TEMPERAT=<n>]
{ ( [SCALE=<n>] [FLIP.Y] [ACTIVE] )
  | (TIF [TIF.VERS=<c>]) | DEPICT
  | ( MEDICI [POLY.ELE] [ELEC.BOT] ) )
  | ( MINIMOS5 X.MASK.S=<n>
    { HALF.DEV | ( FULL.DEV X.MASK.D=<n> [X.CHANNE=<n>]
      [X.MIN=<n>] [X.MAX=<n>] [Y.MIN=<n>] [Y.MAX=<n>]
      [DX.MIN=<n>] [DY.MIN=<n>]
    )
  | ( WAVE [ACTIVE] [CHEMICAL] [DEFECT] [OXID] [MISC] )
}

```

Parameter	Type	Definition
OUT.FILE	character	The identifier of the structure file to be written. Default: none Synonyms: OUTFILE
TEMPERAT	number	The temperature used for evaluating active impurity concentrations. Units: °Celsius Default: the last processing temperature specified or 800°C
SCALE	number	A scaling factor to be applied to the mesh when writing TSUPREM-4 structure files. All coordinate values saved in the file are multiplied by this value. The SCALE parameter does not affect the structure used by subsequent simulation steps. Units: none Default: 1.0
FLIP.Y	logical	Specifies that the structure should be reflected about y=0 when writing TSUPREM-4 structure files. All y coordinates are multiplied by -1 as they are written to the file. FLIP.Y does not affect the structure used by subsequent simulation steps. Default: false
TIF	logical	Specifies that the output file be saved as a TIF (Technology Interchange Format) file. Default: false
TIF.VERS	character	The version of TIF to be used for saving the file. The default is to use the latest version of TIF; a value of 0 produces files compatible with version 6.0 of TSUPREM-4. Units: none Default: 1.2.0

Parameter	Type	Definition
DEPICT	logical	Specifies that the output file is a formatted file that can be read by <i>Avant!</i> TCAD's Taurus-Lithography programs. Default: false
MEDICI	logical	Specifies that the saved output file is a formatted file that can be read by the Medici device simulator. The output file can also be read by older versions of TMA PISCES-2B and by other versions of PISCES. Default: false Synonyms: PISCES
POLY.ELE	logical	Specifies that polysilicon regions should be converted to electrodes in the Medici output file. Default: false
ELEC.BOT	logical	Specifies that an electrode should be placed along the backside of the structure in the Medici output file. Default: false
MINIMOS5	logical	Specifies that the saved output file contains a two-dimensional doping profile that can be read by MINIMOS 5. Default: false
X.MASK.S	number	The x coordinate of the mask edge in the source area of the MINIMOS 5 simulation region. MINIMOS 5 interprets this coordinate as the left edge of the gate electrode. Units: microns Default: none
HALF.DEV	logical	Specifies that the MINIMOS 5 simulation region includes only the source area of the device. Either FULL.DEV or HALF.DEV must be specified if MINIMOS5 is specified. Default: false
FULL.DEV	logical	Specifies that the MINIMOS 5 simulation region includes both the source and drain areas of the device. Either FULL.DEV or HALF.DEV must be specified if MINIMOS5 is specified. Default: false
X.MASK.D	number	The x coordinate of the mask edge in the drain area of the MINIMOS 5 simulation region. MINIMOS 5 interprets this coordinate as the right edge of the gate electrode. X.MASK.D must be specified if FULL.DEV is specified; it must not be specified if HALF.DEV is specified. Units: microns Default: none
X.CHANNE	number	The x coordinate of the center of the channel of the MINIMOS 5 simulation region. Units: microns Default: $(X.MIN + X.MAX)/2$ if FULL.DEV is specified; not applicable if HALF.DEV is specified
X.MIN	number	The x coordinate of the left edge of the MINIMOS 5 simulation region. Units: microns Default: left edge of the TSUPREM-4 simulation region

Parameter	Type	Definition
X.MAX	number	The x coordinate of the right edge of the MINIMOS 5 simulation region. Units: microns Default: right edge of the TSUPREM-4 simulation region
Y.MIN	number	The y coordinate of the top edge of the MINIMOS 5 simulation region. MINIMOS 5 interprets this coordinate as the gate oxide/silicon interface. Units: microns Default: 0.0
Y.MAX	number	The y coordinate of the bottom edge of the MINIMOS 5 simulation region. Units: microns Default: bottom edge of the TSUPREM-4 simulation region
DX.MIN	number	The minimum spacing in the x direction used to specify the doping profiles in the output file. Units: microns Default: $\min((X.MAX - X.MIN)/80, 0.01)$
DY.MIN	number	The minimum spacing in the y direction used to specify the doping profiles in the output file. Units: microns Default: $\min((Y.MAX - Y.MIN)/80, 0.01)$
WAVE	logical	Specifies that the output file is a formatted file in Wavefront Technologies' wave file format. These files can be read by Wavefront Technologies' Data Visualizer program. Default: false
ACTIVE	logical	Specifies that active impurity concentrations are to be saved in TSUPREM-4 and WAVE output files. Default: true
CHEMICAL	logical	Specifies that chemical impurity concentrations are to be included in the WAVE output file. Default: false
DEFECT	logical	Specifies that point defect concentrations are to be included in the WAVE output file. Default: false
OXID	logical	Specifies that oxidant concentrations, oxidation flow rates, and stresses (if available) are to be included in the WAVE output file. Default: false Synonyms: STRESS
MISC	logical	Specifies that miscellaneous solution values are to be included in the WAVE output file. At present, this includes diffusivities of impurities and point defects. Default: false

Description

The **SAVEFILE** statement writes mesh and solution information into a file, in one of several formats. If no format is specified, a TSUPREM-4 structure file is created. TSUPREM-4 structure files can be read with the **LOADFILE** or **INITIALIZE** statements. The mesh can be scaled or flipped about the x axis as the structure is written or when it is read. Scaling and flipping during writing only affect the saved structure, and do not affect the structure used by subsequent simulation steps.

TSUPREM-4 Files

The silicon substrate orientation, last processing temperature, current oxidation model, and current point defect model are saved in TSUPREM-4 structure files, and are automatically restored when the file is read. There is no need to respecify these parameters after reading in a structure. (This does not apply to versions of TSUPREM-4 prior to version 9035; versions older than 9035 only saved the substrate orientation.)

Older Versions

Files saved with older versions of TSUPREM-4 can be loaded by newer versions of the program. Files saved with version 5.1 and newer of TSUPREM-4 cannot be read by older versions of the program.

In versions of TSUPREM-4 prior to version 5.1, the **STRUCTURE** statement is used to load structure files. Starting with version 5.1, the **LOADFILE** statement should be used instead. The **IN . FILE**, **SCALE**, **FLIP . Y**, and **DEPICT** parameters are still accepted on the **STRUCTURE** statement, however, for compatibility with older TSUPREM-4 input files.

Effective in version 5.2 of TSUPREM-4, active impurity concentrations are saved by default in TSUPREM-4 structure files. Structure files without the active impurity concentrations can be produced by specifying **^ACTIVE** on the **SAVEFILE** statement. This is necessary if the structure files are to be read by older (prior to 5.2) versions of TSUPREM-4 or by other programs that cannot accept the active concentration information.

TIF Files

The **TIF** parameter specifies that the file should be saved as a TIF (Technology Interchange Format) file. The version of TIF can be specified with the **TIF . VERS** parameter; newer products use version 1.2.0, while older products (including version 6.0 of TSUPREM-4) use version 1.00 or version 0 (which are equivalent, as far as TSUPREM-4 is concerned).

Correct writing of a user-defined material or impurity to a TIF file requires that a **TIF . NAME** be specified when the material or impurity is defined; **MD . INDEX** must also be specified for materials. Before other programs can read the saved TIF

file, an entry corresponding to the TIF name must be added to the appropriate database (*mat.dbs* for materials, or *sol.dbs* for impurities).



Note:

*Versions 6.1 and later of TSUPREM-4 can read TIF files created by version 6.0, but version 6.0 cannot read TIF files created by versions 6.1 and later unless **TIF . VERS =0** is specified when the file is written.*

Medici Files

The **MEDICI** parameter creates an output file that can be read by the Medici device simulator. **MEDICI** structures can also be read by older versions of TMA PISCES-2B and by other versions of PISCES. The **POLY . ELE** and **ELEC . BOT** parameters are not needed when creating files for *Avant!* TCAD's device simulators, because these simulators allow the treatment of polysilicon and backside contacts to be specified in a **MESH** statement.

Correct writing of a user-defined material to a Medici file requires that **MD . INDEX** be specified when the material is defined (see "MATERIAL" on page 3-215).

Taurus-Lithography Files

The **DEPICT** parameter allows you to create files to be read by *Avant!* TCAD's Taurus-Lithography program.

Files produced by Taurus-Lithography do not contain the complete mesh and solution information required by TSUPREM-4. Rather, they are used to update an existing structure with the results of a Taurus-Lithography simulation. Thus, the usual sequence for interfacing with Taurus-Lithography is:

1. Generate a structure in TSUPREM-4, either from an initial mesh definition or by reading a saved structure.
2. Save the structure in both TSUPREM-4 and Taurus-Lithography formats. This requires two **SAVEFILE** statements and two output files.
3. Use Taurus-Lithography to process the structure, starting with the saved Taurus-Lithography-format file. Save the results in a new Taurus-Lithography-format file.
4. Read the saved TSUPREM-4-format file into TSUPREM-4 (with an **INITIALIZE** or **LOADFILE** statement).
5. Read the new Taurus-Lithography-format file into TSUPREM-4 (with a **LOADFILE** statement).

DEPOSITION

The **DEPOSITION** statement is used to deposit a specified material on the exposed surface of the current structure.

DEPOSITION

```
{ MATERIAL=<c> | SILICON | OXIDE | OXYNITRI | NITRIDE
  | POLYSILI | ALUMINUM
  | ( PHOTORES [ { POSITIVE | NEGATIVE } ] )
}
[ IMPURITY=<c> { I.CONC=<n> | I.RESIST=<n> } ]
[ANTIMONY=<n>] [ARSENIC=<n>] [BORON=<n>] [PHOSPHOR=<n>]
[ {CONCENTR | RESISTIV} ]
THICKNES=<n> [SPACES=<n>] [DY=<n>] [YDY=<n>] [ARC.SPAC=<n>]
[TEMPERAT=<n>] [GSZ.LIN]
TOPOGRAP=<c>
```

Parameter	Type	Definition
MATERIAL	character	The name of the material to be deposited. Default: none
SILICON	logical	Deposit silicon. Default: false
OXIDE	logical	Deposit oxide. Default: false
OXYNITRI	logical	Deposit oxynitride. Default: false
NITRIDE	logical	Deposit nitride. Default: false
POLYSILI	logical	Deposit polysilicon. Default: false
ALUMINUM	logical	Deposit aluminum. Default: false
PHOTORES	logical	Deposit photoresist. Default: false
POSITIVE	logical	Specifies that the deposited photoresist (and all other photoresist in the structure) is positive, i.e., that the DEVELOP statement removes exposed photoresist while leaving unexposed photoresist. Default: true, unless NEGATIVE is specified
NEGATIVE	logical	Specifies that the deposited photoresist (and all other photoresist in the structure) is negative, i.e., that the DEVELOP statement removes unexposed photoresist while leaving exposed photoresist. Default: false

Parameter	Type	Definition
IMPURITY	character	The name of the impurity with which the deposited layer is doped. Default: none
I . CONC	number	The concentration of the specified IMPURITY in the deposited layer. Units: atoms/cm ³ Default: none
I . RESIST	number	The resistivity of the deposited layer. Units: ohm-cm Default: none
ANTIMONY	number	The uniform concentration or resistivity of antimony in the deposited layer. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: SB
ARSENIC	number	The uniform concentration or resistivity of arsenic in the deposited layer. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: AS
BORON	number	The uniform concentration or resistivity of boron in the deposited layer. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: B
PHOSPHOR	number	The uniform concentration or resistivity of phosphorus in the deposited layer. Units: atoms/cm ³ or ohm-cm Default: 0.0 Synonyms: P
CONCENTR	logical	Specifies that the impurity concentration in the deposited layer is given. Default: true
RESISTIV	logical	Specifies that the resistivity in the deposited layer is given. Default: false
THICKNES	number	The thickness of the deposited layer. Units: microns Default: none
SPACES	number	The number of vertical grid spacings in the layer. This value is divided by the value of GRID . FAC (see "MESH" on page 3-44). Units: none Default: 1/ GRID . FAC Synonyms: DIVISION
DY	number	The nominal grid spacing to be used in the deposited material layer at the location specified by the YDY parameter. This value is multiplied by the value of GRID . FAC (see "MESH" on page 3-44). Units: microns Default: GRID . FAC*THICKNES/SPACES Synonyms: DX

Parameter	Type	Definition
YDY	number	The location of the nominal grid spacing specified by DY relative to the top of the deposited layer. Units: microns Default: 0.0 Synonyms: XDX
ARC . SPAC	number	The maximum spacing allowed along an arc on the new surface. This value is multiplied by the value of GRID . FAC (see “MESH” on page 3-44). Units: microns Default: $0.5 * \text{THICKNES} * \text{GRID . FAC}$
TEMPERAT	number	The deposition temperature; used to determine initial grain size when depositing polycrystalline materials. Units: degrees Default: 0.0 Kelvins
GSZ . LIN	logical	Specifies that the grain size increases linearly with depth from the bottom of the deposited layer. (If false, grain size is constant through the layer.) Default: true
TOPOGRAP	character	The name of a file containing Taurus-Topography input commands that define the deposition to be performed. Default: none Synonyms: TERRAIN

Description

This statement provides a basic deposition capability. Material is deposited on the exposed surface of the structure, with the upper surface of the deposited layer becoming the new exposed surface. The **ANTIMONY**, **ARSENIC**, **BORON**, and **PHOSPHOR** parameters specify the initial impurity concentrations or resistivity in the deposited layer, depending on whether **CONCENTR** or **RESISTIV** is true. Doping can also be specified with the **IMPURITY** and **I . CONC** or **I . RESIST** parameters.

The deposited material conforms to the contours of the original surface. Outside corners on the original surface produce arcs on the new surface, which are approximated by straight line segments. The maximum segment length is set by the **ARC . SPAC** parameter. The **SPACES**, **DY**, and **YDY** parameters used to control the grid spacing in the deposited layer are scaled by the value of the **GRID . FAC** parameter on the **MESH** statement (see [Chapter 2, “Changes to the Mesh During Processing” on page 2-7](#)).



Note:

It is not possible to deposit a layer on the bottom of a structure, even if it is exposed. Attempting to do so may cause the program to fail.

Polycrystalline Materials

The **TEMPERAT** and **GSZ . LIN** parameters are used only when depositing a polycrystalline material. If no temperature is specified, or if the temperature is less than the value of **TEMP . BRE** for the material, the deposited layer is amorphous; recrystallization occurs at the start of the next high-temperature step.

Photoresist

Photoresist can be positive or negative, but all photoresist in a structure must be of the same type. If photoresist of one type is deposited on a structure containing photoresist of the other type, a warning is issued and the type of the old photoresist is changed to that of the newly deposited photoresist.

Deposition with Taurus-Topography

The **TOPOGRAP** parameter invokes Taurus-Topography with the specified command input file. The command input file contains Taurus-Topography commands describing one or more processing steps to be simulated by Taurus-Topography. It should not contain the **INITIALIZE** or **STOP** statements.

The values of variables set with the **ASSIGN**, **DEFINE**, and **EXTRACT** statements are substituted in the Taurus-Topography command input file. In addition to variables set explicitly by you, if the **THICKNES** parameter is set on the **DEPOSITION** statement then its value is assigned to the variable **THICK** prior to substitution. (If the variable **THICK** is assigned in this way, it will be unset after the **DEPOSITION** statement, even if it was set by you previously.) This allows parameter values (such as deposition thickness) to be passed to Taurus-Topography. The most recent mask file specified in the TSUPREM-4 input file is passed to Taurus-Topography for use in masked etch steps.

By default, Taurus-Topography is called by requesting that the command **topography** be executed by the operating system, but if the environment variable **S4TERRAIN** is set, its value is used instead. It may be necessary for you to define other environment variables (e.g., **TERR_LIB**) for Taurus-Topography to run correctly. For additional details refer to the *Taurus-Topography Reference Manual*.

When Taurus-Topography is invoked with the **DEPOSITION** statement, the full set of parameters is used for any deposited layer of the specified material. Thus you have full control over grid spacing, doping, and polycrystalline grain size. Note that the parameters specified on the **DEPOSITION** statement only apply to the specified material. They are ignored for other materials deposited by Taurus-Topography.

Examples

1. The following statement deposits 200 angstroms of silicon dioxide:

DEPOSIT OXIDE THICK=0.02

2. The following statement deposits a one-micron thick layer of photoresist, using four grid spaces in the layer:

DEPOSIT PHOTO THICK=1.0 SPACES=4 ARC.SPAC=0.1

The maximum segment length used to approximate arcs is 0.1 micron. By default, the newly deposited photoresist (and any photoresist already present in the structure) is assumed to be positive.

3. The following statement deposits 0.1 micron of poly:

DEPOSIT MAT=POLY THICK=0.1 TEMPERAT=650 GSZ.LIN

The initial grain size is calculated at 650 °C and increases linearly over the thickness of the layer, with minimum value at the bottom of the layer.

4. The following statement calls Taurus-Topography with the input command file *PolyDep.inp*:

**DEPOSIT MAT=POLY THICK=0.1 TEMPERAT=650 GSZ.LIN +
TOPOGRAPHY=PolyDep.inp**

References to “@THICK” in the Taurus-Topography input file are replaced with the value “0.1”. If the call to Taurus-Topography causes the deposition of a polysilicon layer then the specified temperature and grain size model are used for that layer.

Additional DEPOSITION Notes

1. The calculation of doping concentration from resistivity uses mobility tables for silicon and polysilicon. If the resistivity is specified when depositing some other material, a warning is issued. The mobility tables used for calculating the doping concentration are not the same as the tables used by the **ELECTRICAL** statement. The extracted sheet resistance for the deposited layer does not correspond exactly to the resistivity specified during deposition.
2. Deposition of one material on top of another can cause a third material to be added between them. This happens when titanium is deposited on silicon, for example—a layer of TiSi₂ is inserted. Insertion of extra layers is specified with the **REACTION** statement (see [page 3-239](#)).
3. Diffusion of impurities during a deposition step is not simulated, even though a temperature may be specified.

ETCH

The **ETCH** statement is used to remove portions of the current structure.

ETCH

```
[ { MATERIAL=<c> | SILICON | OXIDE | OXYNITRI | NITRIDE
  | POLYSILI | PHOTORES | ALUMINUM
}
]
{ ( TRAPEZOI [THICKNES=<n>] [ANGLE=<n>] [UNDERCUT=<n>] )
  | ( {LEFT | RIGHT} [P1.X=<n>] [P1.Y=<n>] [P2.X=<n>] [P2.Y=<n>] )
  | ( {START | CONTINUE | DONE} X=<n> Y=<n> )
  | ISOTROPI
  | ( OLD.DRY THICKNES=<n> )
  | ALL
  | TOPOGRAP=<c>
}
```

Parameter	Type	Definition
MATERIAL	character	The name of the material to be etched. Default: none
SILICON	logical	Etch silicon only. Default: false
OXIDE	logical	Etch oxide only. Default: false
OXYNITRI	logical	Etch oxynitride only. Default: false
NITRIDE	logical	Etch nitride only. Default: false
POLYSILI	logical	Etch polysilicon only. Default: false
PHOTORES	logical	Etch photoresist only. Default: false
ALUMINUM	logical	Etch aluminum only. Default: false
TRAPEZOI	logical	Use an etch model that removes material from a trapezoidal region when applied to a planar surface. This is a generalization of the DRY model in older versions of TSUPREM-4. Default: true Synonyms: DRY

Parameter	Type	Definition
THICKNES	number	The thickness of the layer to be removed when the TRAPEZOI or OLD.DRY parameter is specified. Units: microns Default: $\text{UNDERCUT} * \tan(\text{ANGLE})$ for $\text{ANGLE} < 90$, infinite otherwise; no default if OLD.DRY is specified
ANGLE	number	The angle of the sidewalls produced when the TRAPEZOI parameter is specified. The angle is measured from the horizontal, so that vertical sidewalls have an angle of 90° . Units: degrees Default: $\arctan(\text{THICKNES}/\text{UNDERCUT})$ if THICKNES and undercut are both specified, 90 otherwise
UNDERCUT	number	The distance that the etch extends under masking layers when the TRAPEZOI parameter is specified. Units: microns Default: $\text{THICKNES}/\tan(\text{ANGLE})$ for $\text{ANGLE} < 90$, 0 otherwise
LEFT	logical	Etch material to the left of the specified position. Default: false
RIGHT	logical	Etch material to the right of the specified position. Default: false
P1.X	number	The x coordinate of the first point used when LEFT or RIGHT is specified. Units: microns Default: 0.0
P1.Y	number	The y coordinate of the first point used when LEFT or RIGHT is specified. Units: microns Default: a point above the top of the structure
P2.X	number	The x coordinate of the second point used when LEFT or RIGHT is specified. Units: microns Default: the value of P1.X
P2.Y	number	The y coordinate of the second point used when LEFT or RIGHT is specified. Units: microns Default: a point below the bottom of the structure
START	logical	The point (X,Y) is the first point in a series defining the region to be etched. Default: false
CONTINUE	logical	The point (X,Y) is the next point in a series defining the region to be etched. Default: false
DONE	logical	The point (X,Y) is the last point in a series defining the region to be etched. Default: false Synonyms: END
ISOTROPI	logical	Specifies removal of material that lies within THICKNES of an exposed surface. Default: false

Parameter	Type	Definition
X	number	The x coordinate used with the START , CONTINUE , or DONE parameter. Units: microns Default: none
Y	number	The y coordinate used with the START , CONTINUE , or DONE parameter. Units: microns Default: none
OLD.DRY	logical	The exposed surface is etched vertically by an amount given by the THICKNES parameter. Default: false
ALL	logical	The specified material is etched away entirely. Default: false
TOPOGRAP	character	The name of a file containing Taurus-Topography input commands that define the etch to be performed. Default: none Synonyms: TERRAIN

Description

This statement is used to remove a portion of the current structure. The user defines a region to be removed and may optionally specify a material to be removed; if no material is specified, all materials are considered to be etchable. Portions of the structure are removed provided that they are of an etchable material, lie within the defined etch region, and are exposed to the ambient. See [Chapter 2, “Etching” on page 2-101](#) for a more complete description. The surface under the etched portions of the structure is marked as exposed. The warning:

```
*** Warning: No material removed by ETCH statement.
```

is produced by an attempt to etch a material that is not exposed, or by specifying etch coordinates that do not include any etchable material.

Removing Regions

You can specify the region to be removed in one of the following ways:

1. If **TRAPEZOI** is specified, the etch region is found from a simple model of a primarily anisotropic (i.e., vertical, or directional) etch with a small isotropic component. This model can produce profiles with sloped sidewalls and undercutting of masking layers. See [Chapter 2, “The Trapezoidal Etch Model” on page 2-103](#).
2. If **LEFT** or **RIGHT** is specified, the etch region includes all material to the left or right of the line between (**P1.X,P1.Y**) and (**P2.X,P2.Y**).
3. The **START**, **CONTINUE**, and **DONE** parameters are used with the **X** and **Y** parameters to define arbitrarily complex etch regions. The boundary of the region is determined by a series of **ETCH** statements, each specifying a point on the boundary. The first statement of the series should contain the **START**

parameter, the last should contain the **DONE** parameter, and statements in between should use the **CONTINUE** parameter. The last point is connected to the first point to produce a closed region defining the portion of the structure to be removed.

4. If **ISOTROPI** is specified, the etch region includes all material within the distance **THICKNES** of the exposed surface. This produces a simple isotropic etch, without rounding of outside corners.
5. If the **OLD . DRY** parameter is specified, the etch region includes all material within a vertical distance **THICKNES** of the exposed surface. This model (the **DRY** model in previous versions of TSUPREM-4) has been replaced by the **TRAPEZOI** model.

The **OLD . DRY** model in version 5.1 of TSUPREM-4 is the same as the **DRY** model in older versions of the program. In version 5.1, **DRY** is a synonym for **TRAPEZOI**. The **TRAPEZOI** model with default values of **ANGLE** and **UNDERCUT** is equivalent to the **OLD . DRY** model, except that surface layers of nonetchable material blocks etching of underlying material, even if the surface layer is thinner than **THICKNES**. Specifying **DRY** in version 5.1 is equivalent to specifying **DRY** in previous versions in cases of practical interest.

6. If the **ALL** parameter is specified, the etch region includes the entire structure.
 - If no region specification is given, **TRAPEZOI** is assumed.
 - If a material is specified, only that material is etched; otherwise, the entire region specified is subject to removal.

It is possible to cut the structure into two or more pieces with an **ETCH** statement. In this case, all pieces except the one with the largest area are removed. A warning is issued for each piece removed.



Note:

*The **ETCH** statement (except when used with the **TERRAIN** parameter) is not intended to simulate a physical etching process; its purpose is to provide a means to generate the required structures for simulation of diffusion and oxidation. Note in particular that the statement “**ETCH OXIDE TRAP**” does not implement a selective etch of oxide, but rather defines a region geometrically in which all exposed oxide is removed.*

Etching with Taurus-Topography

The **TOPOGRAP** parameter invokes Taurus-Topography with the specified command input file. The command input file contains Taurus-Topography commands describing one or more processing steps to be simulated by Taurus-Topography. It should not contain the **INITIALIZE** or **STOP** statements.

The values of variables set with the **ASSIGN**, **DEFINE**, and **EXTRACT** statements are substituted in the Taurus-Topography command input file. In addition to variables set explicitly by you, if the **THICKNES** parameter is set on the **ETCH** statement then its value is assigned to the variable **THICK** prior to substitution. (If

the variable **THICK** is assigned in this way, it will be unset after the **ETCH** statement, even if it was set by you previously.) This allows parameter values (such as etch thickness) to be passed to Taurus-Topography. The most recent mask file specified in the TSUPREM-4 input file is passed to Taurus-Topography for use in masked etch steps.

By default, Taurus-Topography is called by requesting that the command **topography** be executed by the operating system, but if the environment variable *S4TERRAIN* is set, its value is used instead. It may be necessary for you to define other environment variables (e.g., *TERR_LIB*) for Taurus-Topography to run correctly. For additional details refer to the *Taurus-Topography Reference Manual*.

Examples

1. The following statement etches the nitride to the left of 0.5 μ to a depth of 1 micron:

```
ETCH NITRIDE LEFT P1.X=0.5 P2.Y=-1.0
```

Note that **P1.Y** defaults to a location above the top of the structure and **P2.X** defaults to the value of **P1.X** (i.e., 0.5).

2. This statement etches the oxide in the square defined by (0,0), (1,0), (1,1), (0,1):

```
ETCH OXIDE START X=0.0 Y=0.0  
ETCH      CONTINUE X=1.0 Y=0.0  
ETCH      CONTINUE X=1.0 Y=1.0  
ETCH      DONE X=0.0 Y=1.0
```

Material is removed only if there is an exposed oxide surface somewhere within the boundaries of the etch.

3. The following statement calls Taurus-Topography with the input command file *PolyDep.inp*:

```
ETCH THICK=0.1 TOPOGRAPHY=PolyDep.inp
```

References to “**@THICK**” in the Taurus-Topography input file are replaced with the value “0.1”.

DIFFUSION

The **DIFFUSION** statement is used to model high temperature diffusion in both oxidizing and nonoxidizing ambients. **DIFFUSE** is accepted as a synonym for the **DIFFUSION** statement.

DIFFUSION

```

TIME=<n> [CONTINUE]
TEMPERAT=<n> [ {T.RATE=<n> | T.FINAL=<n>} ]
[ { DRY02 | WET02 | STEAM | INERT
  | AMB.1 | AMB.2 | AMB.3 | AMB.4 | AMB.5
  | ( [F.O2=<n>] [F.H2O=<n>] [F.H2=<n>] [F.N2=<n>] [F.HCL=<n>] )
  }
]
[IMPURITY=<c> I.CONC=<n>]
[ANTIMONY=<n>] [ARSENIC=<n>] [BORON=<n>] [PHOSPHOR=<n>]
[PRESSURE=<n>] [ {P.RATE=<n> | P.FINAL=<n>} ] [HCL=<n>]
[D.RECOMB=<n>] [MOVIE=<c>] [DUMP=<n>]

```

Parameter	Type	Definition
TIME	number	The duration of the diffusion step. Units: minutes Default: none
CONTINUE	logical	Indicates that this step is a continuation of a previous diffusion step. No native oxide deposition occurs and the time step is not reset. No processing steps should be specified between the preceding DIFFUSION statement and the DIFFUSION CONTINUE statement. The starting temperature of the step should be the same as the final temperature of the preceding step, and the ambient must also be the same. Default: false
TEMPERAT	number	The ambient temperature at the beginning of the step. Units: degrees Celsius Default: none
T.RATE	number	The time rate of change of the ambient temperature. Units: degrees Celsius/minute Default: 0.0
T.FINAL	number	The ambient temperature at the end of the step. Units: degrees Celsius Default: TEMPERAT
DRY02	logical	Specifies that the ambient gas is dry oxygen. Default: false
WET02	logical	Specifies that the ambient gas is wet oxygen. Default: false

Parameter	Type	Definition
STEAM	logical	Specifies that the ambient gas is steam. Default: false
INERT	logical	Specifies that the ambient gas is inert. Default: true Synonyms: NEUTRAL, NITROGEN, ARGON
AMB . 1	logical	Specifies that the ambient gas is ambient number one. Ambient number one is defined by the user with the AMBIENT statement. Default: false
AMB . 2	logical	Specifies that the ambient gas is ambient number two. Ambient number two is defined by the user with the AMBIENT statement. Default: false
AMB . 3	logical	Specifies that the ambient gas is ambient number three. Ambient number three is defined by the user with the AMBIENT statement. Default: false
AMB . 4	logical	Specifies that the ambient gas is ambient number four. Ambient number four is defined by the user with the AMBIENT statement. Default: false
AMB . 5	logical	Specifies that the ambient gas is ambient number five. Ambient number five is defined by the user with the AMBIENT statement. Default: false
F . O2	number	The flow of O2 associated with the ambient gas. If H2 is also present, the O2 and H2 is assumed to react completely to form H2O. The flows of O2 and H2 are reduced and the flow of H2O is increased. Units: none Default: 0.0
F . H2O	number	The flow of H2O associated with the ambient gas. If O2 and H2 are also present, the O2 and H2 are assumed to react completely to form H2O. The flows of O2 and H2 are reduced and the flow of H2O is increased. Units: none Default: 0.0
F . H2	number	The flow of H2 associated with the ambient gas. If O2 is also present, the O2 and H2 are assumed to react completely to form H2O. The flows of O2 and H2 are reduced and the flow of H2O is increased. Units: none Default: 0.0
F . N2	number	The flow of N2 (and other inert components) associated with the ambient gas. Units: none Default: 0.0
F . HCL	number	The flow of chlorine associated with the ambient gas. Units: none Default: 0.0

Parameter	Type	Definition
IMPURITY	character	The name of an impurity present in the ambient gas at the surface of the structure. Default: none
I . CONC	number	The concentration of IMPURITY in the ambient gas at the surface of the wafer. Units: atoms/cm ³ Default: none
ANTIMONY	number	The concentration of antimony in the ambient gas at the surface of the structure. Units: atoms/cm ³ Default: 0.0 Synonyms: SB
ARSENIC	number	The concentration of arsenic in the ambient gas at the surface of the structure. Units: atoms/cm ³ Default: 0.0 Synonyms: AS
BORON	number	The concentration of boron in the ambient gas at the surface of the structure. Units: atoms/cm ³ Default: 0.0 Synonyms: B
PHOSPHOR	number	The concentration of phosphorus in the ambient gas at the surface of 116 the structure. Units: atoms/cm ³ Default: 0.0 Synonyms: P
PRESSURE	number	The total pressure of the ambient gas at the start of the step. Units: atmospheres Default: the pressure specified in the corresponding AMBIENT statement, or 1.0 if flows are specified
P . RATE	number	The time rate of change of the ambient gas pressure. Units: atmospheres/minute Default: 0.0
P . FINAL	number	The ambient gas pressure at the end of the step. Units: atmospheres Default: PRESSURE
HCL	number	The percentage of chlorine present in the ambient gas. Units: percent Default: value calculated from F . HCL or specified on AMBIENT statement
D . RECOMB	number	The fraction of Frenkel pair implant damage remaining after initial recombination. Units: none Default: 0.0

Parameter	Type	Definition
MOVIE	character	A string of TSUPREM-4 commands to be executed at the beginning of each time step. Multiple input statements can be given, separated by semicolons (;). Default: no commands executed
DUMP	number	Write a solution file after every DUMP time step. The files are readable with the LOADFILE and INITIALIZE statements. The names are of the form <i>s<time></i> , where <i><time></i> is the time in seconds from the start of the diffusion step. Units: none Default: no intermediate solutions saved

Description

This statement specifies a diffusion step, with or without oxidation. Any impurities present in the wafer are diffused. If the wafer is exposed to a gas, predeposition and/or oxidation can be performed. If an oxidizing ambient is specified and the **VISCOUS** oxidation model is in effect, reflow of surface layers occurs.

The duration of the step must be specified with the **TIME** parameter. The ambient temperature must be specified with the **TEMPERAT** keyword (unless **CONTINUE** is specified). For linear ramping of the temperature, specify either the ramp rate (with **T . RATE**) or the temperature at the end of the step (with **T . FINAL**).

Ambient Gas

The ambient gas used during the diffusion step can be specified in one of two ways:

1. Specify one of the **DRY02**, **WET02**, **STEAM**, **INERT**, or **AMB . 1** through **AMB . 5** parameters. These select an ambient that has been predefined with the **AMBIENT** statement. The **DRY02**, **WET02**, **STEAM**, and **INERT** ambients are defined by the standard initialization file; the **AMB . 1** through **AMB . 5** ambients must be defined by the user before they are used. The predefined ambients include a default pressure and HCl percentage, which can be overridden with the **PRESSURE** and **HCL** parameters, respectively, on the **DIFFUSION** statement.
2. Define the ambient by specifying the flows of oxidizing (O₂ and H₂O) and nonoxidizing (H₂, N₂, and HCl) species. The flows can be specified as flow rates, fractions, or percentages, but the units of all the flows in a single **DIFFUSION** statement are assumed to be the same.

Any O₂ and H₂ in the gas are assumed to react (two units of H₂ for each unit of O₂) to form H₂O. Thus, the effective flow contains zero units of O₂ or H₂ (or both). If the effective gas contains nonzero amounts of both O₂ and H₂O, the oxidation rate is based on the partial pressure of H₂O.

Ambient Gas Parameters

The amount of chlorine in the ambient can be specified either by the flow of HCl (**F . HCL** parameter) or by the percentage of HCl (**HCL** parameter), but not both. If

the specified ambient contains O_2 or H_2O , oxidation takes place at interfaces between silicon dioxide and silicon or polysilicon. A native oxide (with thickness given by the **INITIAL** parameter on the **AMBIENT** statement) is deposited on any exposed silicon or polysilicon surfaces before the start of the diffusion step. **ANTIMONY**, **ARSENIC**, **BORON**, and **PHOSPHOR** and the combination of **IMPURITY** and **I . CONC** specify the concentration of impurities at the wafer surface for predeposition. The total pressure for an oxidizing ambient is given by **PRESSURE**. To ramp the pressure, specify either the ramp rate (**P . RATE**) or the pressure at the end of the step (**P . FINAL**).

The parameters for oxidation are set by the **AMBIENT** statement. Diffusivities and segregation parameters are set on the various impurity statements (i.e., the **IMPURITY**, **ANTIMONY**, **ARSENIC**, **BORON**, and **PHOSPHORUS** statements). The oxidation and point defect models and the numerical methods to be used are specified on the **METHOD** statement. The default values for these parameters are normally set by the *s4init* file, which is read each time TSUPREM-4 is executed.

See [Chapter 2](#) for complete descriptions of the models used for diffusion and oxidation and [Appendix A](#) for a list of default model coefficients.

Oxidation Limitations

Oxidation of polysilicon is simulated only when the **COMPRESS**, **VISCOELA**, or **VISCOUS** model has been specified (with the **METHOD** statement).

The oxidation algorithms provide limited support for the case where silicon (or polysilicon), oxide, and a third material meet at a point. The results are reasonably accurate when only one of the materials in contact with oxide is oxidizing; results are less accurate if both materials in contact with oxide are oxidizing at a significant rate.

Impurities present in the ambient during an oxidation step are incorporated into the growing oxide. Note, however, that the program does not currently contain models for the changes in physical properties of heavily-doped glasses.

Reflow

Reflow of surface layers occur whenever oxidation with the **VISCOUS** model is specified. The amount of reflow is proportional to the ratio of the surface tension (specified by the **SURF . TEN** parameter on the **MATERIAL** statement) to the viscosity for each material. Reflow can occur in any material having a nonzero value of **SURF . TEN**. Only exposed layers flow due to surface tension, but underlying layers can deform due to stresses produced by reflow of the exposed layers.

Reflow in an inert ambient can be approximated by specifying an oxidizing ambient with a negligible partial pressure of oxidant, e.g., by setting **PRESSURE**=1e-6 or by a combination such as **F . N2**=1.0 and **F . O2**=1e-6. Note that a native oxide

is added whenever the partial pressure of the oxidizing species is nonzero; it may be necessary to do a shallow etch to remove this oxide following a reflow step.

Examples

1. The following statement specifies a 1000-degree, 30-minute boron predeposition:

```
DIFFUSION TIME=30 TEMP=1000 BORON=1E20
```

2. The following statement calls for a 30-minute diffusion in an inert ambient:

```
DIFFUSION TIME=30 TEMP=800 T.FINAL=1000 INERT
```

The temperature is ramped from 800°C to 1000°C during the step.

3. The following statement calls for a 60-minute dry oxidation at 900°C with an ambient containing 2 percent HCl:

```
DIFFUSION TIME=60 TEMP=900 DRYO2 HCL=2
```

4. The following statement performs a 30-minute, 1000°C diffusion:

```
DIFFUSION TIME=30 TEMP=1000 +  
  MOVIE="SELECT Z=log10(Boron)  
  PLOT.1D X.V=1.0"
```

The boron concentration is plotted before each time step.

SELECT

The **SELECT** statement evaluates a quantity to be printed or plotted. It is also used to specify plot titles and axis labels.

SELECT

[Z=<c>] [TEMPERAT=<n>] [LABEL=<c>] [TITLE=<c>]

Parameter	Type	Definition
Z	character	A mathematical expression defining the quantity to be printed or plotted. If the expression contains spaces, it must be enclosed in parentheses. Default: "0"
TEMPERAT	number	The temperature at which the solution is to be evaluated. Units: degrees Celsius Default: last specified temperature or 800
LABEL	character	The label to be used on the y axis of a one-dimensional plot, or the z axis of a three-dimensional plot. Default: the expression given by Z
TITLE	character	The title to be used on plots. Default: the name and version number of the program

Description

The **SELECT** statement evaluates the quantity to be displayed by the **CONTOUR**, **PLOT . 1D**, **PRINT . 1D**, **PLOT . 2D**, and **PLOT . 3D** statements or to be extracted by the **EXTRACT** statement. No solution data can be printed or plotted until this statement is specified. The values calculated by a **SELECT** statement are used until another **SELECT** statement is specified. If the solution changes, a new **SELECT** statement is given in order for the new values to be printed or plotted.

Solution Values

The **Z** parameter specifies a mathematical expression for the quantity to be plotted. The following solution values can be used in the expression, provided that the solution is available:

<i>antimony</i>	antimony concentration (atoms/cm ³)
<i>arsenic</i>	arsenic concentration (atoms/cm ³)
<i>boron</i>	boron concentration (atoms/cm ³)
<i>phosphorus</i>	phosphorus concentration (atoms/cm ³)

<i>doping</i>	net active concentration (atoms/cm ³)
<i>oxygen</i>	oxidant concentration (atoms/cm ³)
<i>silicon</i>	silicon concentration (in silicide) (atoms/cm ³)
<i>interstitial</i>	interstitial concentration (#/cm ³)
<i>vacancy</i>	vacancy concentration (#/cm ³)
<i>damage</i>	damage concentration (#/cm ³)
<i>ci.star</i>	equilibrium interstitial concentration (#/cm ³)
<i>cv.star</i>	equilibrium vacancy concentration (#/cm ³)
<i>trap</i>	concentration of filled interstitial traps (#/cm ³)
<i>cl_interst</i>	concentration of clustered interstitials (#/cm ³)
<i>dloop</i>	density of dislocation loops (#/cm ³)
<i>rloop</i>	radius of dislocation loops (cm)
<i>lgrain</i>	average polycrystalline grain size (um)
<i>electron</i>	concentration of electrons (#/cm ³)
<i>x.v</i>	x velocity (cm/sec)
<i>y.v</i>	y velocity (cm/sec)
<i>Sxx, Sxy, Syy</i>	components of the stress tensor (dynes/cm ²)
<i>x</i>	x coordinate (microns)
<i>y</i>	y coordinate (microns)

- The names of user-specified impurities can also be used, giving the concentration of the impurity in atoms/cm³.
- The chemical concentration is reported unless the active function is used, for example, *active(phosphorus)*.
- The net concentration is defined as the sum of the donor concentrations minus the sum of the acceptor concentrations.
- The electron concentration is calculated using the assumptions of local charge neutrality and complete ionization of impurities.

Mathematical Operations and Functions

The symbols “+”, “-”, “*”, “/”, and “^” are used for the mathematical operations of addition, subtraction, multiplication, division, and exponentiation, respectively. In addition, the following functions are available:

<i>active</i>	electrically active part of impurity concentration
<i>gb</i>	concentration of impurity in polycrystalline grain boundaries
<i>abs</i>	absolute value
<i>diffusivity</i>	diffusivity (in cm ² /sec) of an impurity or point defect species
<i>erf</i>	error function
<i>erfc</i>	complementary error function
<i>exp</i>	exponential
<i>log</i>	natural logarithm of the absolute value
<i>log10</i>	base-10 logarithm of the absolute value
<i>slog10</i>	base-10 logarithm of the absolute value times the sign of the value
<i>sqrt</i>	square root
<i>sin, cos, tan</i>	trigonometric functions (arguments in radians)
<i>asin, acos, atan</i>	inverse trigonometric functions (results in radians)
<i>sinh, asinh, cosh, acosh, tanh, atanh</i>	hyperbolic and inverse hyperbolic functions

The *log*, *log10*, and *slog10* functions return the value 0.0 if their argument is zero; the *log*, *log10*, *slog10*, and *sqrt* functions take absolute value of their arguments. The following constant is available:

Kb Boltzmann's constant (eV/°C)



Note:

The active and net concentrations depend on the temperature. If TEMPERAT is not specified, the last processing temperature is used. If the last process step ended with a ramp to a low temperature, you may need to specify a higher value of TEMPERAT in order to obtain realistic levels of dopant activation.

Examples

1. The logarithm (base 10) of the arsenic concentration is evaluated with

```
SELECT Z=log10(Arsenic)
```

2. The phosphorus concentration minus a constant profile of 5×10^{14} is evaluated with

```
SELECT Z=(Phosphorus - 5.0e14)
```

3. The difference between the phosphorus concentration and an analytic profile is evaluated with

```
SELECT Z=(phos - 1.0e18 * exp ( y * y ) )
```

4. The excess vacancy-interstitial product is evaluated with

```
SELECT Z=(inter * vacan - ci.star * cv.star)
```

5. The diffusivity (in cm^2/sec) of boron at each point in the structure is evaluated with

```
SELECT Z=diffusivity(Boron)
```

Note that when the **PD . TRANS** or **PD . FULL** model for point defects is used, the diffusivity can be different at each point in the structure and may vary with time.

6. The following statements print junction depths:

```
SELECT Z=doping  
PRINT LAYERS X.V=0
```

The **PRINT LAYERS** statement assumes that a new layer begins whenever the selected value (net doping in this case) changes sign.

7. The following statements print the thicknesses of material layers:

```
SELECT Z=1.0  
PRINT LAYERS X.V=0
```

The **SELECT** statement specifies a constant value of one, so the **PRINT** statement only uses material boundaries to define layers. Further, when the value "1.0" is integrated over each layer, the result is just the layer thickness.

8. The following statement specifies the title to be used on the next plot:

```
SELECT TITLE="Final N-Channel Structure"
```

Because no **Z** value is specified, **Z=0** is assumed, and any attempt to print or plot solution data uses the value zero.

PRINT .1D

The **PRINT .1D** statement prints the value of the selected expression along a line through the structure. It can also print layer thickness and integrated doping information.

PRINT .1D

```
{ X.VALUE=<n> | Y.VALUE=<n>
  | ( { MATERIAL=<c> | SILICON | OXIDE | OXYNITRI | NITRIDE
      | POLYSILI | PHOTORES | ALUMINUM
      }
      { /MATERIA=<c> | /SILICON | /OXIDE | /OXYNITR | /NITRIDE
      | /POLYSIL | /PHOTORE | /ALUMINU | /AMBIENT | /REFLECT
      }
    )
  }
[SPOT=<n>] [LAYERS]
[X.MIN=<n>] [X.MAX=<n>]
```

Parameter	Type	Definition
X.VALUE	number	The x coordinate of a vertical section along which values are to be printed. Units: microns Default: 0.0
Y.VALUE	number	The y coordinate of a horizontal section along which values are to be printed. Units: microns Default: none
MATERIAL	character	Print values in the named material, at the interface with the other specified material. Default: none
SILICON	logical	Print values in silicon, at the interface with the other specified material. Default: false
OXIDE	logical	Print values in oxide, at the interface with the other specified material. Default: false
OXYNITRI	logical	Print values in oxynitride, at the interface with the other specified material. Default: false
NITRIDE	logical	Print values in nitride, at the interface with the other specified material. Default: false
POLYSILI	logical	Print values in polysilicon, at the interface with the other specified material. Default: false
PHOTORES	logical	Print values in photoresist, at the interface with the other specified material. Default: false

Parameter	Type	Definition
ALUMINUM	logical	Print values in aluminum, at the interface with the other specified material. Default: false
/MATERIA	character	Print values in the other specified material, at the interface with the named material. Default: none
/SILICON	logical	Print values in the other specified material, at the interface with silicon. Default: false
/OXIDE	logical	Print values in the other specified material, at the interface with oxide. Default: false
/OXYNITR	logical	Print values in the other specified material, at the interface with oxynitride. Default: false
/NITRIDE	logical	Print values in the other specified material, at the interface with nitride. Default: false
/POLYSIL	logical	Print values in the other specified material, at the interface with polysilicon. Default: false
/PHOTORE	logical	Print values in the other specified material, at the interface with photoresist. Default: false
/ALUMINU	logical	Print values in the other specified material, at the interface with aluminum. Default: false
/AMBIENT	logical	Print values in the other specified material, at the interface with the exposed surface (if any). Default: false Synonyms: /EXPOSED, /GAS
/REFLECT	logical	Print values in the other specified material, at the interface with the reflecting boundary (if any). Default: false
SPOT	number	Print the coordinate along the cross-section at which the selected quantity equals the specified value. Units: units of the selected quantity Default: none
LAYERS	logical	Report the integral of the selected quantity over each layer of the device structure. Default: false
X.MIN	number	The minimum position along the cross-section to be printed. Units: microns Default: none
X.MAX	number	The maximum position along the cross-section to be printed. Units: microns Default: none

Description

The **PRINT . 1D** statement prints the values of the selected quantity along a cross-section through the device. cross-sections are defined as vertical or horizontal (by the **X . VALUE** and **Y . VALUE** parameters, respectively), along the interface between two materials, or along a boundary of the device structure. The quantity to be printed must be specified on a **SELECT** statement preceding the **PRINT . 1D** statement. The **SPOT** parameter finds all points along the specified path at which the selected quantity equals the specified value.

Layers

If **LAYERS** is specified, the integral of the selected quantity over each layer is printed. The integration is along the path defined by the **X . VALUE**, **Y . VALUE**, or interface specification. Layers are delimited by those points along the path where the material type changes or the sign of the selected quantity changes. If a cross-section passes out a structure into the ambient and then re-enters the structure, the ambient “layer” may be omitted from the **LAYERS** output.

Interface Values

The values along the interface between two materials depend on the order in which the materials are specified. Thus **SILICON /OXIDE** and **OXIDE /SILICON** print values at the same interface, but the first prints the values in the silicon, while the second prints the values in the oxide.

Values along an interface are sorted by their x coordinates. The values printed may not be in order if there are vertical or reentrant interfaces, or if the structure contains more than one interface between the specified materials.

Examples

1. The following statements print the boron concentration at x=1.0 micron between the top of the mesh and y=3.0 microns:

```
SELECT    Z=Boron
PRINT . 1D X . VAL=1 . 0 X . MAX=3 . 0
```

2. The following statements print the x and y coordinates of the interface between silicon and oxide:

```
SELECT    Z=y
PRINT . 1D SILICON /OXIDE
```

3. The following statements prints junction depths:

```
SELECT Z=doping
PRINT LAYERS X . V=0
```

The **PRINT** statement assumes that a new layer begins whenever the selected value (net doping in this case) changes sign.

4. The following statements print the thicknesses of material layers:

```
SELECT Z=1.0  
PRINT LAYERS X.V=0
```

The **SELECT** statement specifies a constant value of one, so the **PRINT** statement only uses material boundaries to define layers. Further, when the value “1.0” is integrated over each layer, the result is just the layer thickness.

PLOT.1D

The **PLOT.1D** statement plots the value of the selected expression along a line through the structure.

PLOT.1D

```
{ { [ { X.VALUE=<n> | Y.VALUE=<n> } ]
  | ( { MATERIAL=<c> | SILICON | OXIDE | OXYNITRI | NITRIDE
      | POLYSILI | PHOTORES | ALUMINUM
      }
    { /MATERIA=<c> | /SILICON | /OXIDE | /OXYNITR | /NITRIDE
      | /POLYSIL | /PHOTORE | /ALUMINU | /AMBIENT | /REFLECT
      }
    )
  }
| { IN.FILE=<c>
  { (TIF X.AXIS=<c> Y.AXIS=<c>)
    | ( { (COLUMN [X.COLUMN=<n>] [Y.COLUMN=<n>])
        | (ROW [X.ROW=<n>] [Y.ROW=<n>]) }
      [X.LABEL=<c>] [Y.LABEL=<c>] )
    }
    [X.SHIFT=<n>] [Y.SHIFT=<n>]
    [X.SCALE=<n>] [Y.SCALE=<n>]
    [Y.LOG] [X.LOG]
  }
| ELECTRIC
}
[BOUNDARY] [CLEAR] [AXES]
[SYMBOL=<n>] [CURVE] [LINE.TYP=<n>] [COLOR=<n>]
[LEFT=<n>] [RIGHT=<n>] [BOTTOM=<n>] [TOP=<n>]
[X.OFFSET=<n>] [X.LENGTH=<n>] [X.SIZE=<n>]
[Y.OFFSET=<n>] [Y.LENGTH=<n>] [Y.SIZE=<n>]
[T.SIZE=<n>]
```

Parameter	Type	Definition
X.VALUE	number	A vertical cross-section is to be plotted at this value of <i>x</i> . Units: microns Default: 0.0
Y.VALUE	number	A horizontal cross-section is to be plotted at this value of <i>y</i> . Units: microns Default: none
MATERIAL	character	Plot a cross-section through the named material, at the interface with the other specified material. Default: none

Parameter	Type	Definition
SILICON	logical	Plot a cross-section through silicon, at the interface with the other specified material. Default: false
OXIDE	logical	Plot a cross-section through oxide, at the interface with the other specified material. Default: false
OXYNITRI	logical	Plot a cross-section through oxynitride, at the interface with the other specified material. Default: false
NITRIDE	logical	Plot a cross-section through nitride, at the interface with the other specified material. Default: false
POLYSILI	logical	Plot a cross-section through polysilicon, at the interface with the other specified material. Default: false
PHOTORES	logical	Plot a cross-section through photoresist, at the interface with the other specified material. Default: false
ALUMINUM	logical	Plot a cross-section through aluminum, at the interface with the other specified material. Default: false
/MATERIA	character	Plot a cross-section through the other specified material, at the interface with the named material. Default: none
/SILICON	logical	Plot a cross-section through the other specified material, at the interface with silicon. Default: false
/OXIDE	logical	Plot a cross-section through the other specified material, at the interface with oxide. Default: false
/OXYNITR	logical	Plot a cross-section through the other specified material, at the interface with oxynitride. Default: false
/NITRIDE	logical	Plot a cross-section through the other specified material, at the interface with nitride. Default: false
/POLYSIL	logical	Plot a cross-section through the other specified material, at the interface with polysilicon. Default: false

Parameter	Type	Definition
/PHOTORE	logical	Plot a cross-section through the other specified material, at the interface with photoresist. Default: false
/ALUMINU	logical	Plot a cross-section through the other specified material, at the interface with aluminum. Default: false
/AMBIENT	logical	Plot a cross-section through the other specified material, at the interface with the exposed surface. Default: false Synonyms: /GAS , /EXPOSED
/REFLECT	logical	Plot a cross-section through the other specified material, at the interface with the reflecting boundary (if any). Default: false
IN.FILE	character	The identifier for the file containing the data to plot. This file may contain experimental data or data produced by the EXTRACT or ELECTRICAL statements. Default: none
TIF	logical	Specifies that the format of IN.FILE is TIF (.ivl file from Medici). Default: false
X.AXIS	character	The quantity used for the horizontal axis when plotting data stored in a TIF file. The label is automatically assigned with the string composite of the X.AXIS and the unit associated with X.AXIS in a TIF file. Default: none
Y.AXIS	character	The quantity used for the vertical axis when plotting data stored in a TIF file. The label is automatically assigned with the string composite of the Y.AXIS and the unit associated with Y.AXIS in a TIF file. Default: none
COLUMN	logical	Specifies that the format of IN.FILE is column-wise. Default: true
X.COLUMN	number	The index of the column in the file specified by the IN.FILE parameter that contains the horizontal coordinates of the plot. Units: none Default: 1
Y.COLUMN	number	The index of the column in the file specified by the IN.FILE parameter that contains the vertical coordinates of the plot. Units: none Default: 2
ROW	logical	Specifies that the format of IN.FILE is row-wise. Default: false
X.ROW	number	The index of the row(line) in the file specified by the IN.FILE parameter that contains the horizontal coordinates of the plot. Units: none Default: 1

Parameter	Type	Definition
Y.ROW	number	The index of the row(line) in the file specified by the IN.FILE parameter that contains the vertical coordinates of the plot. Units: none Default: 2
X.LABEL	character	The label of the horizontal axis for X.COLUMN data in the IN.FILE file. Default: "Distance (microns)"
Y.LABEL	character	The label of the vertical axis for Y.COLUMN data in the IN.FILE file. Default: if the SELECT statement is defined, LABEL in SELECT , otherwise, "Concentration ($\#/cm^3$)"
X.SHIFT	number	The offset by which X.COLUMN data are shifted when reading IN.FILE file. Units: the same as for the X.COLUMN data Default: 0.0
Y.SHIFT	number	The offset by which Y.COLUMN data are shifted when reading IN.FILE file. Units: the same as for the Y.COLUMN data Default: 0.0
X.SCALE	number	The scaling factor by which X.COLUMN data are multiplied when reading IN.FILE file. Units: none Default: 1.0
Y.SCALE	number	The scaling factor by which Y.COLUMN data are multiplied when reading IN.FILE file. Units: none Default: 1.0
Y.LOG	logical	Specifies that the vertical axis for Y.COLUMN data in the IN.FILE file is logarithmic. Default: the current value dependent on Z quantity in the SELECT statement Synonyms: LOG
X.LOG	logical	Specifies that the horizontal axis for X.COLUMN data in the IN.FILE file is logarithmic. Default: the current value in the previous specification. Otherwise, false.
ELECTRIC	logical	Specifies plotting of results from a preceding ELECTRICAL statement. Default: false
BOUNDARY	logical	If true, material boundaries that are crossed are indicated by dashed vertical lines on the plot. Default: true
CLEAR	logical	If true, the graphics screen is cleared before the graph is drawn. Default: true

Parameter	Type	Definition
AXES	logical	Specifies that axes should be drawn, using scaling information from this statement and/or the current structure. If AXES is false, no axes are drawn and scaling information from the previous plotting statement is used (i.e., LEFT, RIGHT, BOTTOM, and TOP are ignored). If AXES is false and no previous plotting statement has been given, an error is reported. Default: true Synonyms: AXIS
SYMBOL	number	The type of centered symbol to be drawn at each point where the cross-section intersects a mesh line. This value must be in the range 1 to 15. Values of this parameter are associated with the following symbols: 1 Square 2 Circle 3 Triangle 4 Plus 5 Upper case X 6 Diamond 7 Up-arrow 8 Roofed upper case X 9 Upper case Z 10 Upper case Y 11 Curved square 12 Asterisk 13 Hourglass 14 Bar 15 Star Units: none Default: no symbols drawn
CURVE	logical	Specifies that a line is to be drawn through the data points. Default: true
LINE . TYP	number	The dashed line type used for the plotted data. (The axes are always drawn with line type 1.) Units: none Default: 1
COLOR	number	The color of line used for the plotted data. (The axes are always drawn with color 1.) Units: none Default: 1
LEFT	number	The minimum value to be plotted on the x axis. Units: microns Default: minimum x or y coordinate of the structure Synonyms: X . MIN

Parameter	Type	Definition
RIGHT	number	The maximum value to be plotted on the x axis. Units: microns Default: maximum x or y coordinate of the structure Synonyms: X . MAX
BOTTOM	number	The minimum value of the selected expression to be plotted, in units of the plot variable. Units: units of the selected expression Default: minimum value of the selected expression Synonyms: Y . MIN
TOP	number	The maximum value of the selected expression to be plotted, in units of the plot variable. Units: units of the selected expression Default: maximum value of the selected expression Synonyms: Y . MAX
X . OFFSET	number	The distance by which the left end of the horizontal axis is offset from the left edge of the graphics viewport. Units: cm Default: 2.0
X . LENGTH	number	The length of the horizontal axis. Units: cm Default: viewport width - X . OFFSET - 1.25
X . SIZE	number	The height of the characters used to label the horizontal axis. Units: cm Default: 0.25
Y . OFFSET	number	The distance by which the bottom end of the vertical axis is offset from the bottom edge of the graphics viewport. Units: cm Default: 2.0
Y . LENGTH	number	The length of the vertical axis. Units: cm Default: viewport height - Y . OFFSET - 1.25
Y . SIZE	number	The height of the characters used to label the vertical axis. Units: cm Default: 0.25
T . SIZE	number	The height of the characters in the character string used as the plot title. Units: cm Default: 0.4

Description

The **PLOT . 1D** statement plots cross-sections vertically or horizontally through the device, or along an interface between two materials, or along a boundary of the device. The statement has options to provide for initialization of the graphics

device and plotting of axes. The statement can optionally draw vertical lines whenever a material boundary is crossed. The vertical axis corresponds to the variable selected with the **SELECT** statement.

Limits can be specified so that only a portion of the entire device is shown, or more than one variable can be conveniently plotted. By default the limits of the *x* axis extend to the edges of the structure, and the *y* axis is scaled according to the minimum and maximum values of the selected value over the entire structure.

The quantity to be plotted must be defined by a preceding **SELECT** statement. The type of graphics device must be set, either with an **OPTION** statement or through use of a suitable default. (See “OPTION” on page 3-33 and [Appendix B](#).)

If two materials are specified (e.g., **OXIDE /SILICON**), a cross-section is plotted in the first material (e.g., oxide) at the interface with the second material (e.g., silicon). Note that **OXIDE /SILICON** produces different results from **SILICON /OXIDE**. For interface plots, the points along the interface are sorted by their *x* coordinates; specifying interfaces containing vertical segments or reentrant angles may not produce useful plots.

Line Type and Color

The **LINE . TYP** parameter specifies the dashed line type for plotting the data. Line type 1 is solid, while types 2 through 7 are dashed lines with increasing dash sizes. Types 8 through 10 produce more complicated patterns of dashes.

The **COLOR** parameter specifies the color for plotting the data. Color 1 is the default, and produces a line that contrasts with the background color (e.g., black on white or white on black). The **COLOR** parameter has no effect on monochrome displays.

The colors produced by the **COLOR** parameter depend on the type of display being used. Where possible, the colors 2 through 7 have been set up to produce the colors red, green, blue, cyan (light blue), magenta (light purple), and yellow, in that order. Colors 8 and above produce a repeating series of 12 colors in rainbow order, from red to violet.

IN . FILE Parameter

The format of the file specified by the **IN . FILE** parameter can be either columnwise or TIF. In the case of a columnwise format, the file may contain the following two types of lines:

1. Lines that are blank or contain a slash (/) as the first nonblank character are ignored and can be used to document the file.
2. Other lines define the data at one point in the distribution. These lines must contain the following values:
 - a. Value number **X . COLUMN** is the horizontal coordinate of the point.

b. Value number **Y . COLUMN** is the vertical coordinate of the point.

If this line contains fewer than *N* numerical values in free-field format, where *N* is the maximum of indices (**X . COLUMN** and **Y . COLUMN**) for the values listed above, the line is ignored.

Since the .ivl log file of Medici is a TIF format file, the results of device simulation can be plotted if **TIF**, **X . AXIS** and **Y . AXIS** are specified. This capability makes it possible to easily compare the electrical calculations of TSUPREM-4 and Medici.

The transformation of data read by the **IN . FILE** parameter is as follows:

Data of X axis = **X . SCALE** × *Data of X . COLUMN* or **X . AXIS** + **X . SHIFT**

Data of Y axis = **Y . SCALE** × *Data of Y . COLUMN* or **Y . AXIS** + **Y . SHIFT**

Examples

1. The following statement clears the screen, draws a set of axes, and plots a (vertical) cross-section at *x*=1.0 micron:

PLOT . 1D X . V=1 . 0 SYMB=1 ^CURVE

Symbol 1 (a small square) is drawn at each data point; the line through the data points is suppressed.

2. The following statement plots a cross-section at *x*=2.0 microns on the previous set of axes, without clearing the screen:

PLOT . 1D X . V=2 . 0 ^AXES ^CLEAR LINE . TYP=2 COLOR=3

A line consisting of short dashes is used, and appears in color 3 on color displays.

LABEL

The **LABEL** statement is used to add a label to a plot.

LABEL

```
{ ( X=<n> Y=<n> [CM] ) | ( [X.CLICK=<c>] [Y.CLICK=<c>] ) }
[SIZE=<n>] [COLOR=<n>]
[ LABEL=<c> [ {LEFT | CENTER | RIGHT} ] ]
[LINE.TYP=<n>] [C.LINE=<n>] [LENGTH=<n>]
[ { ( [SYMBOL=<n>] [C.SYMBOL=<n>] )
  | ( [RECTANGL] [C.RECTAN=<n>] [W.RECTAN=<n>]
    [H.RECTAN=<n>] )
}
]
```

Parameter	Type	Definition
X	number	The horizontal location corresponding to the left end, center, or right end of the character string (depending on whether LEFT , CENTER , or RIGHT is specified). If the CM parameter is specified, then this parameter specifies a location in centimeters relative to the left edge of the graphics viewport. Otherwise, this parameter specifies the location in axis units along the horizontal axis. Units: cm or horizontal axis units Default: none
Y	number	The vertical location corresponding to the bottom of the character string. If the CM parameter is specified, then this parameter specifies a location in centimeters relative to the bottom edge of the graphics viewport. Otherwise, this parameter specifies the location in axis units along the vertical axis. Units: cm or vertical axis units Default: none
CM	logical	Specifies that the X and Y parameters are locations in centimeters relative to the lower left edge of the graphics viewport. Default: false
X.CLICK	character	The variable name to store the x-coordinate of the position at which a mouse is clicked. Units: horizontal axis units Default: none
Y.CLICK	character	The variable name to store the y-coordinate of the position at which a mouse is clicked. Units: cm or vertical axis units Default: none

Parameter	Type	Definition
SIZE	number	The height of the characters in the character string, and the default size to be used for rectangles and centered symbols. Units: cm Default: 0.25 Synonyms: C . SIZE
COLOR	number	The color of the label text, and the default color for rectangles, centered symbols, and line segments. Units: none Default: 1
LABEL	character	The character string to be used to label the plot. Default: none
LEFT	logical	Specifies that the character string is to start at the position given by X and Y . Default: true if neither CENTER or RIGHT is true
CENTER	logical	Specifies that the character string is to be centered horizontally about the position given by X and Y . Default: false
RIGHT	logical	Specifies that the character string is to end at the position given by X and Y . Default: false
LINE . TYP	number	The dashed type of a line segment to be plotted before the label. If LABEL is not specified, the line segment is centered at the point given by X and Y . Units: none Default: 1
C . LINE	number	The color of the line segment to be plotted before the label. Units: none Default: COLOR
LENGTH	number	The length of the line segment to be plotted before the label. Units: cm Default: 4* SIZE

Parameter	Type	Definition
SYMBOL	number	The type of centered symbol to be drawn before the label. This value must be in the range 1 to 15. Values of this parameter are associated with the following symbols: 1 Square 2 Circle 3 Triangle 4 Plus 5 Upper case X 6 Diamond 7 Up-arrow 8 Roofed upper case X 9 Upper case Z 10 Upper case Y 11 Curved square 12 Asterisk 13 Hourglass 14 Bar 15 Star If LABEL is specified, the symbol is placed to the left of the label with one character space between the symbol and the label text. If LABEL is not specified, the rectangle is centered at the point given by X and Y. Units: none Default: 1
C.SYMBOL	number	The color of the symbol (if any). Units: none Default: COLOR
RECTANGL	logical	Specifies that a filled rectangle be plotted with the label. If LABEL is specified, the rectangle is placed to the left of the label with one character space between the rectangle and the label text. If LABEL is not specified, the rectangle is centered at the point given by X and Y. Default: false
C.RECTAN	number	The color of the filled rectangle. Units: none Default: COLOR
W.RECTAN	number	The width of the filled rectangle. Units: cm Default: SIZE
H.RECTAN	number	The height of the filled rectangle. Units: cm Default: SIZE

Description

The **LABEL** statement is used to add text, symbols, and/or filled rectangles to a plot. This statement is meaningless unless a **PLOT . 1D**, **PLOT . 2D**, or **PLOT . 3D** statement has been previously specified.

Label Placement

The rules for placing these annotations are as follows:

1. Labels are always placed at the location specified by **X** and **Y**. The label is left justified, centered, or right justified at this location, depending on whether **LEFT**, **CENTER**, or **RIGHT** is specified.
2. The placement of line segments depends on whether a **LABEL** is specified:
 - a. If a **LABEL** is specified, the line segment is placed one character width to the left of the label.
 - b. If no **LABEL** is specified, the line segment is centered at the location specified by **X** and **Y**.
3. The placement of symbols and filled rectangles depends on whether a line segment or label is specified:
 - a. If a line segment is specified, the symbol or filled rectangle is centered on the line segment.
 - b. If no line segment is specified but a **LABEL** is specified, the symbol or filled rectangle is placed one character width to the left of the label.
 - c. If neither a line segment nor a **LABEL** is specified, the symbol or filled rectangle is centered at the location specified by **X** and **Y**.
4. The coordinates **X** and **Y** should be in the units of the plot axes, e.g., microns or $1/\text{cm}^3$, unless **CM** is specified.



Note:

*Some graphics devices have a cursor whose position can be read by the program. On such devices, a **LABEL** statement without **X** and **Y** coordinates attempts to read the cursor position and plot the label at that point. On terminals from which the cursor position cannot be read, a **LABEL** statement without **X** and **Y** coordinates may produce unpredictable results.*

Line, Symbol, and Rectangle

If **LINE . TYP**, **C . LINE**, or **LENGTH** is specified, a line segment is drawn. **LINE . TYP** specifies the dashed line type of the line segment. Type 1 produces a solid line, while types 2 through 10 produce various styles of dashed lines. **C . LINE** specifies the color of the line and **LENGTH** gives the length. If either

SYMBOL or **C . SYMBOL** is specified, a symbol is drawn. If **RECTANGL**, **C . RECTAN**, **W . RECTAN**, or **H . RECTAN** is specified, a filled rectangle is drawn.

The **SIZE** parameter specifies the character size to be used for the label and the default width and height for filled rectangles.

Color

The **COLOR** parameter specifies the color to be used for the label and the default color for any line segment, symbol, or filled rectangle. Color 1 contrasts with the background (e.g., black on white or white on black). On most color devices, colors 2 through 7 produce red, green, blue, cyan (light blue), magenta (light purple), and yellow, while colors 8 and above give a repeating sequence of 12 colors in rainbow order (red through violet). The **COLOR** parameter has no effect on monochrome devices.

Examples

1. The following statements put two labels on the plot starting at $x=3$ microns and $y=1.4$ and 1.6 microns, with a short line of the specified type before each one:

```
LABEL X=3.0 Y=1.4 LABEL="Arsenic" LINE=3
LABEL X=3.0 Y=1.6 LABEL="Phosphorus" LINE=4
```

2. The following statement plots a label preceded by a filled rectangle:

```
LABEL RIGHT X=12.5 Y=9.0 CM LABEL="Oxide" C.RECT=2
```

The label ends at a point 12.5 cm from the x axis and 9.0 cm from the y axis. It is preceded by a rectangle filled with color 2.

3. The following statement stores the coordinate of the position at which a mouse is clicked.

```
LABEL LABEL=x X.CLICK=px Y.CLICK=py
```

The variables, px , py store the coordinate of the position at which a mouse is clicked.



Note:

*The unit of the stored value in **X . CLICK** is the same as the x -coordinate unit. However, in the case of **Y . CLICK**, the unit is cm for the distance. In **PLOT . 2D** graph, for example, the variable of **Y . CLICK** stores the y -coordinate value in cm unit, while the variable of **X . CLICK** value stores the x -coordinate value in μm unit.*

AMBIENT

The **AMBIENT** statement is used to specify oxidation coefficients. **OXIDE** is a valid synonym for the **AMBIENT** statement.

AMBIENT

```
[ { DRY02 | WET02 | STEAM | INERT | AMB.1 | AMB.2 | AMB.3 | AMB.4
  | AMB.5}
  [F.O2=<n>] [F.H2O=<n>] [F.H2=<n>] [F.N2=<n>] [F.HCL=<n>]
  [PRESSURE=<n>] [HCL=<n>]
]
[ {02 | H2O}
  [ {<111> | <110> | <100> | ORIENTAT=<n> | POLYSILI}
    [THINOX.0=<n>] [THINOX.E=<n>] [THINOX.L=<n>]
    [L.LIN.0=<n>] [L.LIN.E=<n>] [H.LIN.0=<n>] [H.LIN.E=<n>]
  ]
  [L.PAR.0=<n>] [L.PAR.E=<n>] [H.PAR.0=<n>] [H.PAR.E=<n>]
  [LIN.BREA=<n>] [PAR.BREA=<n>] [LIN.PDEP=<n>] [PAR.PDEP=<n>]
  [GAMMA.0=<n>] [GAMMA.E=<n>]
  [ { LIN.PCT | PAR.PCT
    | ( {LIN.CLDE | PAR.CLDE} COLUMN=<n> )
  }
  TABLE=<c>
]
[ { MATERIAL=<c> | SILICON | OXIDE | OXYNITRI | NITRIDE | POLYSILI
  | AMBIENT}
  [D.0=<n>] [D.E=<n>] [VC=<c>]
  [HENRY.CO=<n>] [THETA=<n>]
  [ { /MATERIA=<c> | /SILICON | /OXIDE | /OXYNITR
    | /NITRIDE | /POLYSIL | /AMBIENT
  }
  [SEG.0=<n>] [SEG.E=<n>] [TRANS.0=<n>] [TRANS.E=<n>]
  [ALPHA=<n>]
]
]
]
[STRESS.D] [VR=<c>] [VT=<c>] [VD=<c>] [VDLIM=<n>]
[INITIAL=<n>] [SPREAD=<n>] [MASK.EDG=<n>]
[ERF.Q=<n>] [ERF.DELT=<n>] [ERF.LBB=<c>] [ERF.H=<c>]
[NIT.THIC=<n>]
[CLEAR]
[TEMPERAT=<c>]
[CM.SEC]
```

Parameter	Type	Definition
DRY02	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with the dry oxygen ambient. Default: false

Parameter	Type	Definition
WET02	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with the wet oxygen ambient. Default: false
STEAM	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with the steam ambient. Default: false
INERT	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with the inert ambient. Default: false Synonyms: NEUTRAL, NITROGEN
AMB . 1	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with ambient number one. Ambient number one is defined by the user. Default: false
AMB . 2	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with ambient number two. Ambient number two is defined by the user. Default: false
AMB . 3	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with ambient number three. Ambient number three is defined by the user. Default: false
AMB . 4	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with ambient number four. Ambient number four is defined by the user. Default: false
AMB . 5	logical	Specifies that the pressure, chlorine percentage, and flows of oxidizing and non-oxidizing species are associated with ambient number five. Ambient number five is defined by the user. Default: false
F . O2	number	The flow of O ₂ associated with the specified ambient. If H ₂ is also present, the O ₂ and H ₂ are assumed to react completely to form H ₂ O. The flows of O ₂ and H ₂ are reduced and the flow of H ₂ O is increased. Units: none Default: 0.0
F . H2O	number	The flow of H ₂ O associated with the specified ambient. If O ₂ and H ₂ are also present, the O ₂ and H ₂ are assumed to react completely to form H ₂ O. The flows of O ₂ and H ₂ are reduced and the flow of H ₂ O is increased. Units: none Default: 0.0
F . H2	number	The flow of H ₂ associated with the specified ambient. If O ₂ is also present, the O ₂ and H ₂ are assumed to react completely to form H ₂ O. The flows of O ₂ and H ₂ are reduced and the flow of H ₂ O is increased. Units: none Default: 0.0

Parameter	Type	Definition
F . N2	number	The flow of N2 (or other inert gasses) associated with the specified ambient. Units: none Default: 0.0
F . HCL	number	The flow of chlorine associated with the specified ambient. Units: none Default: 0.0
PRESSURE	number	The default value of total gas pressure for the specified ambient. Units: atmospheres Default: the current value for this ambient; initially 1.0
HCL	number	The default percentage of chlorine present for the specified ambient. Units: percent Default: calculated from F . HCL
O2	logical	Specifies that the oxidation coefficients are associated with the O ₂ oxidizing species. Default: false
H2O	logical	Specifies that the oxidation coefficients are associated with the H ₂ O oxidizing species. Default: false
<111>	logical	Specifies that linear and thin oxide growth rate coefficients apply to <111> orientation silicon. Default: false
<110>	logical	Specifies that linear and thin oxide growth rate coefficients apply to <110> orientation silicon. Default: false
<100>	logical	Specifies that linear and thin oxide growth rate coefficients apply to <100> orientation silicon. Default: false
ORIENTAT	number	Specifies that linear and thin oxide growth rate coefficients apply to silicon of the specified orientation. Allowed values are 111, 110, and 100. Units: none Default: 100
POLYSILI	logical	The specified coefficients apply to polysilicon, or the interface between polysilicon and some other material. Default: false
THINOX . 0	number	The pre-exponential constant in the expression for the thin oxide growth rate parameter. Units: microns/min or cm/sec Default: current value for this orientation and oxidant
THINOX . E	number	The activation energy in the expression for the thin oxide growth rate parameter. Units: electron volts Default: current value for this orientation and oxidant

Parameter	Type	Definition
THINOX.L	number	The characteristic length in the expression for the thin oxide growth rate parameter. Units: microns Default: current value for this orientation and oxidant
L.LIN.0	number	The pre-exponential constant in the expression for the linear oxidation rate for temperatures below the temperature breakpoint set by LIN.BREA . Units: microns/min or cm/sec Default: current value for this orientation and oxidant Synonyms: LIN.L.0
L.LIN.E	number	The activation energy in the expression for the linear oxidation rate for temperatures below the temperature breakpoint set by LIN.BREA . Units: electron volts Default: current value for this orientation and oxidant Synonyms: LIN.L.E
H.LIN.0	number	The pre-exponential constant in the expression for the linear oxidation rate for temperatures above the temperature breakpoint set by LIN.BREA . Units: microns/min or cm/sec Default: current value for this orientation and oxidant Synonyms: LIN.H.0
H.LIN.E	number	The activation energy in the expression for the linear oxidation rate for temperatures above the temperature breakpoint set by LIN.BREA . Units: electron volts Default: current value for this orientation and oxidant Synonyms: LIN.H.E
L.PAR.0	number	The pre-exponential constant in the expression for the parabolic oxidation rate for temperatures below the temperature breakpoint set by PAR.BREA . Units: microns ² /min or cm ² /sec Default: current value for this oxidant Synonyms: PAR.L.0
L.PAR.E	number	The activation energy in the expression for the parabolic oxidation rate for temperatures below the temperature breakpoint set by PAR.BREA . Units: electron volts Default: current value for this oxidant Synonyms: PAR.L.E
H.PAR.0	number	The pre-exponential constant in the expression for the parabolic oxidation rate for temperatures above the temperature breakpoint set by PAR.BREA . Units: microns ² /min or cm ² /sec Default: current value for this oxidant Synonyms: PAR.H.0
H.PAR.E	number	The activation energy in the expression for the parabolic oxidation rate for temperatures above the temperature breakpoint set by PAR.BREA . Units: electron volts Default: current value for this oxidant Synonyms: PAR.H.E

Parameter	Type	Definition
LIN . BREA	number	The temperature breakpoint at which the temperature dependence of the linear oxidation rate changes. Units: degrees Celsius Default: current value for this oxidant Synonyms: L . BREAK
PAR . BREA	number	The temperature breakpoint at which the temperature dependence of the parabolic oxidation rate changes. Units: degrees Celsius Default: current value for this oxidant Synonyms: P . BREAK
LIN . PDEP	number	The exponent of the pressure in the expression for the linear oxidation rate. Units: none Default: current value for this oxidant Synonyms: L . PDEP
PAR . PDEP	number	The exponent of the pressure in the expression for the parabolic oxidation rate. Units: none Default: current value for this oxidant Synonyms: P . PDEP
GAMMA . 0	number	The pre-exponential constant in the expression for the impurity concentration dependence of the linear oxidation rate. Units: none Default: current value for this oxidant
GAMMA . E	number	The activation energy in the expression for the impurity concentration dependence of the linear oxidation rate. Units: electron volts Default: current value for this oxidant
LIN . PCT	logical	Specifies that the TABLE parameter defines chlorine percentages associated with the rows in the table of coefficients modifying the linear oxidation rate in the presence of chlorine. Default: false
PAR . PCT	logical	Specifies that the TABLE parameter defines chlorine percentages associated with the rows in the table of coefficients modifying the parabolic oxidation rate in the presence of chlorine. Default: false
LIN . CLDE	logical	Specifies that the TABLE parameter defines entries in a column of the table of coefficients modifying the linear oxidation rate in the presence of chlorine. The column number is specified with the COLUMN parameter and is associated with the temperature specified by the TEMPERAT parameter. Default: false
PAR . CLDE	logical	Specifies that the TABLE parameter defines entries in a column of the table of coefficients modifying the parabolic oxidation rate in the presence of chlorine. The column number is specified with the COLUMN parameter and is associated with the temperature specified by the TEMPERAT parameter. Default: false

Parameter	Type	Definition
COLUMN	number	The column number in the tables of coefficients modifying the linear or parabolic oxidation rates. The coefficients defined by the TABLE parameter are stored in this column of a table. The column number is associated with the temperature specified by the TEMPERAT parameter. There can be at most 8 columns in a table and each column corresponds to one temperature. Units: none Default: none
TABLE	character	This parameter is interpreted as a series of numeric values, separated by spaces or commas. If the LIN.PCT or PAR.PCT parameter is specified, the TABLE parameter defines the chlorine percentages associated with the rows in the table of coefficients modifying the linear or parabolic oxidation rates, respectively. If the LIN.CLDE or PAR.CLDE parameter is specified, the TABLE parameter defines the entries in a column of the table of coefficients modifying the linear or parabolic oxidation rates, respectively. There can be at most eight rows in a table and each row corresponds to one chlorine percentage. At most eight values can be defined with this parameter. Units: percent or none Default: none
MATERIAL	character	The specified coefficients apply to the named material or to the interface between the named material and some other material. Default: none
SILICON	logical	The specified coefficients apply to silicon, or the interface between silicon and some other material. Default: false
OXIDE	logical	The specified coefficients apply to oxide, or the interface between oxide and some other material. Default: true if no other first material is specified
OXYNITRI	logical	The specified coefficients apply to oxynitride, or the interface between oxynitride and some other material. Default: false
NITRIDE	logical	The specified coefficients apply to nitride, or the interface between nitride and some other material. Default: false
POLYSILI	logical	The specified coefficients apply to polysilicon, or the interface between polysilicon and some other material. Default: false
AMBIENT	logical	The specified coefficients apply to gas, or the interface between gas and some other material. Default: false Synonyms: GAS
D.0	number	The pre-exponential constant in the expression for the diffusivity of oxidant in the specified material. Units: microns²/min or cm²/sec Default: current value for this oxidant and material Synonyms: DIFF.0

Parameter	Type	Definition
D . E	number	The activation energy in the expression for the diffusion of oxidant in the specified material. Units: electron volts Default: current value for this oxidant and material Synonyms: DIFF . E
VC	character	A table of activation volumes as a function of temperature for the dependence of material viscosity on shear stress for the specified material and oxidizing species (O2 or H2O). Entries in the table correspond to temperatures given by the TEMPERAT parameter (see text). Units: Å ³ Default: the current value; initially 300
HENRY . CO	number	The solubility of oxidant in the specified material at one atmosphere. Units: atoms/cm ³ /atm Default: current value for this oxidant and material
THETA	number	The number of oxide molecules per cubic centimeter of oxide. Units: atoms/cm ³ Default: current value
/MATERIA	character	The specified coefficients apply to the interface between the other specified material and this named material. Default: none
/SILICON	logical	The specified coefficients apply to the interface between the specified material and silicon. Default: True if no other second material is specified.
/OXIDE	logical	The specified coefficients apply to the interface between the specified material and oxide. Default: false
/OXYNITR	logical	The specified coefficients apply to the interface between the specified material and oxynitride. Default: false
/NITRIDE	logical	The specified coefficients apply to the interface between the specified material and nitride. Default: false
/POLYSIL	logical	The specified coefficients apply to the interface between the specified material and polysilicon. Default: false
/AMBIENT	logical	The specified coefficients apply to the interface between the specified material and gas. Default: false Synonyms: /GAS
SEG . 0	number	The pre-exponential constant in the expression for segregation of oxidant between the two specified materials. Units: none Default: current value for this oxidant and these materials

Parameter	Type	Definition
SEG . E	number	The activation energy in the expression for segregation of oxidant between the two specified materials. Units: electron volts Default: current value for this oxidant and these materials
TRANS . 0	number	The pre-exponential constant in the expression for transport of oxidant between the two specified materials. Units: microns/min or cm/sec Default: the current value for this oxidant and these materials Synonyms: TRN . 0
TRANS . E	number	The activation energy in the expression for transport of oxidant between the two specified materials. Units: electron volts Default: the current value for this oxidant and these materials Synonyms: TRN . E
ALPHA	number	The volume expansion ratio between the two specified materials. The defaults are 0.44 for silicon/oxide and polysilicon/oxide, and 1.0 for all other combinations. Units: none Default: the current value for these materials
STRESS . D	logical	Specifies that the stress-dependent models for oxide viscosity, oxidant diffusivity, and surface reaction rate are to be used. Default: the current value
VR	character	A table of activation volumes as a function of temperature for the dependence of oxidation rate at the Si/SiO ₂ interface on normal stress for the specified oxidizing species (02 or H2O). Entries in the table correspond to temperatures given by the TEMPERAT parameter (see text). Units: Å ³ Default: the current value; initially 15
VT	character	A table of activation volumes as a function of temperature for the dependence of oxidation rate at the Si/SiO ₂ interface on tangential stress for the specified oxidizing species (02 or H2O). Entries in the table correspond to temperatures given by the TEMPERAT parameter (see text). Units: Å ³ Default: the current value; initially 0.0.
VD	character	A table of activation volumes as a function of temperature for the dependence of oxidant diffusivity in oxide on pressure for the specified oxidizing species (02 or H2O). Entries in the table correspond to temperatures given by the TEMPERAT parameter (see text). Units: Å ³ Default: the current value; initially 75.
VDLIM	number	The maximum increase in oxidant diffusivity produced by the VD parameter. Units: none Default: the current value; initially 1.2.

Parameter	Type	Definition
INITIAL	number	The thickness of the existing oxide at the start of oxidation. Exposed silicon surfaces are covered with this thickness of native oxide before oxidation begins. Units: microns Default: the current value; initially 0.002
SPREAD	number	The ratio of width to height for the bird's beak, used in the ERFC model of local oxide shape. Units: none Default: the current value; initially 1.0
MASK . EDG	number	The assumed position of the mask, used by the analytical models for local oxidation. Oxide grows to the right of the mask edge. Units: microns Default: the current value; initially -200
ERF . Q	number	The q parameter for the ERFG (Guillemot) model. Units: microns Default: the current value; initially 0.05.
ERF . DELT	number	The δ parameter for the ERFG (Guillemot) model. Units: microns Default: the current value; initially 0.04.
ERF . LBB	character	The length of the bird's beak for the ERFG (Guillemot) model. This is an arithmetic expression involving the variables Fox (the field oxide thickness, in microns), eo (the pad oxide thickness, in microns), Tox (the oxidation temperature, in degrees Kelvin), and en (the nitride thickness, in microns). Units: microns Default: the current value; initially $(8.25e-3*(1580.3-Tox)*(Fox^{0.67})*(eo^{0.3})*exp(-((en-0.08)^2)/0.06))$.
ERF . H	character	The ratio of the nitride lifting to the field oxide thickness for the ERFG (Guillemot) model. This is an arithmetic expression involving the variables Fox (the field oxide thickness, in microns), eo (the pad oxide thickness, in microns), Tox (the oxidation temperature, in degrees Kelvin), and en (the nitride thickness, in microns). Units: none Default: the current value; initially $(402*(0.445-1.75*en)*exp(-Tox/200))$
NIT . THIC	number	The nitride thickness, en used in the equations for ERF . LBB and ERF . H . Units: microns Default: none
TEMPERAT	character	The temperature associated with the column in the chlorine tables given by the COLUMN parameter, or a list of temperatures corresponding to the values of the VC , VD , VR , and/or VT parameters. Units: degrees Celsius Default: none
CLEAR	logical	Clear table(s) specified by the VC , VD , VR , and/or VT parameters before adding new values (see text). Default: none

Parameter	Type	Definition
CM . SEC	logical	If true, parameters involving time are specified in centimeters and seconds; if false, parameters involving time are in microns and minutes. Default: false

Description

All parameters relating to oxidation are specified on this statement. The necessary parameters are set by **AMBIENT** statements in the *s4init* file, but can be changed by the user.

Oxidation Models

The following models are available:

1. An error-function fit to bird's beak shapes (the **ERFC** model)
2. A parameterized error-function model from the literature (the Guillemot or **ERFG** model)
3. A model in which oxidant diffuses and the oxide grows vertically at a rate determined by the local oxidant concentration (the **VERTICAL** model)
4. A compressible viscous flow model (the **COMPRESS** model)
5. A viscoelastic flow model (the **VISCOELA** model)
6. An incompressible viscous flow model (the **VISCOUS** model)

A summary of the features and characteristics of these models follows; full descriptions are given in [Chapter 2, "Oxidation" on page 2-44](#).



Note:

*Oxidation of polycrystalline silicon is modeled by the **COMPRESS**, **VISCOELA**, and **VISCOUS** models only.*

ERFC Model

The **ERFC** model is the fastest of the oxidation models. It can be used for uniform oxidation of bare silicon, provided that modeling of the concentration dependence of the oxidation rate is not needed. It can be used for nonuniform oxidation of planar surfaces provided that fitting data for the lateral spread of the bird's beak is available.

The **ERFC** model is controlled by the **SPREAD**, **MASK . EDG**, and **INITIAL** parameters. The growth rate vs. time is computed assuming an initial oxide thickness **INITIAL** at the start of each diffusion step. This model should not be used with a structure having an unmasked initial oxide thickness other than **INITIAL**.

- ERFG Model** The **ERFG** model is by Guillemot, et al., *IEEE Transactions on Electron Devices*, ED-34, May 1987. The bird's beak shape and nitride lifting are functions of process conditions. The **ERFG** model is controlled by the **ERF . Q**, **ERF . DELT**, **ERF . LBB**, **ERF . H**, **NIT . THIC**, and **INITIAL** parameters. The above comments regarding **INITIAL** apply the **ERFG** model as well. The **ERF1** and **ERF2** models use the two shapes derived by Guillemot, et al; the **ERFG** model chooses between them based on process conditions.
- VERTICAL Model** The **VERTICAL** model has no fitting parameters, but is only accurate when the growth is approximately vertical (within about 30° of vertical). The **VERTICAL** model does not simulate oxidation of polysilicon. The **VERTICAL** model can be used for oxidation of uniform substrates with arbitrary initial oxide thicknesses, and for approximating nonrecessed LOCOS processes. Concentration dependence of the oxidation rate is included in the **VERTICAL** model.
- COMPRESS Model** The **COMPRESS** model simulates the viscous flow of the oxide in two dimensions. It uses simple (three nodes per triangle) elements for speed, but must allow some compressibility as a consequence. It is more accurate than the **VERTICAL** model, but requires more computer time. It uses Young's modulus (**YOUNG . M**) and Poisson's ratio (**POISS . R**), specified for each material with the **MATERIAL** statement. The **COMPRESS** model is recommended for general use on arbitrary structures. It includes the concentration dependence of oxidation rate and models the oxidation of polysilicon.
- VISCOELA Model** The **VISCOELA** model simulates viscoelastic flow in two dimensions. It uses simple (three nodes per triangle) elements for speed, but simulates elastic deformation as well as viscous flow. When used with stress dependent parameters (i.e., **STRESS . D** true), it can produce very accurate results with reasonable simulation times. It is slower than the **COMPRESS** model, but 10-100 times faster than the **VISCOUS** model with stress dependence. It uses the **YOUNG . M**, **POISS . R**, **VISC . 0**, **VISC . E**, and **VISC . X** parameters for mechanical properties of materials plus the **VC**, **VR**, **VD**, and **VDLIM** parameters for describing stress dependence.
- VISCOUS Model** The **VISCOUS** model simulates incompressible viscous flow of the oxide using more complicated (seven nodes per triangle) elements. It calculates stresses and is the only model that models reflow. The **VISCOUS** model is slower than the **COMPRESS**, and **VISCOELA** models and may require large amounts of memory; it may be impossible to simulate large structures with this model on some computers, due to memory limitations. It uses the viscosity parameters (**VISC . 0**, **VISC . E**, and **VISC . X**) specified for each material with the **MATERIAL** statement.
- The **VISCOUS** model is needed only when stress calculations are required, when the stress-dependent oxidation parameters are used, or when **SKIP . SIL** must be set false in order to simulate structures with floating silicon mesas.

Stress Dependence

The parameter **STRESS.D** determines whether the stress dependence of oxidant diffusivity, surface reaction rate, and oxide viscosity are included when oxidizing with the **VISCOELA** or **VISCOUS** models. When **STRESS.D** is true, these stress dependencies are included; when **STRESS.D** is false, they are not.

The magnitude of the various stress effects are specified by the **VC**, **VR**, **VT**, **VD**, and **VDLIM** parameters.

- **VC** is the activation volume for the dependence of oxide viscosity on shear stress. **VC** can be specified for arbitrary materials using the **MATERIAL** statement.
- **VR** and **VT** are the activation volumes for the dependence of the surface reaction rate on normal and tangential stresses, respectively.
- **VD** is the activation volume for the dependence on pressure of the diffusivity of the oxidizing species in the oxide.
- **VDLIM** is the maximum increase in oxidant diffusivity produced by **VD**.

The parameters **VC**, **VD**, **VR**, **VT**, and **TEMPERAT** are used to specify the activation volumes as functions of temperature. A separate table is maintained for each oxidizing species, and for each material in the case of **VC**. Table entries are added or changed by specifying lists of values (with **VC**, **VD**, **VR**, or **VT**) and temperatures (with **TEMPERAT**). The portion of the table spanned by the specified temperatures is replaced by the specified values; the number of values must be the same as the number of temperatures, and the temperatures must be given in order, lowest to highest. The **CLEAR** parameter is used to clear a table before setting any values.

For example, the statement

```
AMBIENT O2 CLEAR VD="40 50 60" TEMP="800 900 1050"
```

removes any old values from the table of **VD** vs. temperature for O₂ and adds three new values. The statement

```
AMBIENT O2 VD="55 75" TEMP="900 1100"
```

would then replace the values at 900° C and 1050° C with new values at 900° C and 1100° C.

If no oxidizing species is specified, the values apply to ambients containing either O₂ or H₂O. The material should be specified when setting **VC**; if no material is specified, **OXIDE** is assumed. If **V.COMPAT** (on the **OPTION** statement) is less than 6.6, the specified values of the activation volumes apply to oxide in all ambients, including inert ambients.

An Arrhenius interpolation is used between values in the table. For temperatures outside the range of the table the nearest value is used.

Coefficients

The diffusion and segregation coefficients can be used to model oxidant diffusion in arbitrary layers, but the diffusion coefficient in oxide is derived from the parabolic rate constant. The transport coefficient between the ambient and oxide is interpreted as the gas-phase mass-transport coefficient for the specified oxidizing species.

Chlorine

The effects of chlorine in the ambient gas on the oxidation rate of silicon are specified by tables of coefficients that modify the linear and parabolic oxidation rates. There are two tables for each oxidizing species, one each for the linear and parabolic oxidation rates. The tables are two-dimensional with at most 8 rows corresponding to chlorine percentages and at most 8 columns corresponding to ambient temperatures. Linear interpolation is used to obtain values for temperatures or percentages between the values in the table. For temperatures or percentages outside of the range of values present in the table, the values in the first or last rows or columns, as appropriate, are used.

Examples

For example, consider the following table of chlorine coefficients with six rows of chlorine percentages and five columns of temperatures:

		1	2	3	4	5	column
row	%	800	900	1000	1100	1200	temperature
---	-	---	---	----	----	----	
1	0	1.0	1.0	1.0	1.0	1.0	
2	1	1.1	1.2	1.3	1.4	1.5	
3	3	1.6	1.7	1.8	1.9	2.0	
4	5	2.1	2.2	2.3	2.4	2.5	
5	7	2.6	2.7	2.8	2.9	3.0	
6	10	3.1	3.2	3.3	3.4	3.5	

If this table represented the modification coefficients for the linear oxidation rates for the O₂ oxidizing species, it could have been defined with the following series of input statements:

```

AMBIENT 02 LIN.PCT TABLE="0, 1, 3, 5, 7, 10"
AMBIENT 02 LIN.CLDE COLUMN=1 TEMPERAT=800 +
TABLE="1.0, 1.1, 1.6, 2.1, 2.6, 3.1"
AMBIENT 02 LIN.CLDE COLUMN=2 TEMPERAT=900
TABLE="1.0, 1.2, 1.7, 2.2, 2.7, 3.2"
AMBIENT 02 LIN.CLDE COLUMN=3 TEMPERAT=1000 +
TABLE="1.0, 1.3, 1.8, 2.3, 2.8, 3.3"
AMBIENT 02 LIN.CLDE COLUMN=4 TEMPERAT=1100 +
TABLE="1.0, 1.4, 1.9, 2.4, 2.9, 3.4"
AMBIENT 02 LIN.CLDE COLUMN=5 TEMPERAT=1200 +
TABLE="1.0, 1.5, 2.0, 2.5, 3.0, 3.5"

```

The following values are obtained from this table for the indicated percentages and temperatures:

percent	temperature	table value	row	column
1.0	1000	1.3	2	3
1.0	1050	1.35	2	3, 4
2.0	1000	1.55	2, 3	3
12.0	1000	3.3	6	3
1.0	700	1.1	2	1
1.0	1250	1.5	2	5
2.0	1250	1.75	2, 3	5

Parameter Dependencies

Parameters which have special dependencies are listed below. If insufficient information is given with a parameter (e.g., **L.LIN.0** without an orientation and an oxidant), the parameter is ignored (without warning).

Orientation

The following parameters are dependent on the specified orientation: **L.LIN.0**, **L.LIN.E**, **H.LIN.0**, **H.LIN.E**, **THINOX.0**, **THINOX.E**, and **THINOX.L**. Note that **POLYSILI** can be used in place of the orientation to specify coefficients for oxidation of polysilicon.

Oxidizing Species

The following parameters are dependent on the oxidizing species (O_2 or H_2O): **L.LIN.0**, **L.LIN.E**, **H.LIN.0**, **H.LIN.E**, **LIN.BREA**, **LIN.PDEP**, **L.PAR.0**, **L.PAR.E**, **H.PAR.0**, **H.PAR.E**, **PAR.BREA**, **PAR.PDEP**, **GAMMA.0**, **GAMMA.E**, **LIN.PCT**, **PAR.PCT**, **LIN.CLDE**, **PAR.CLDE**, **COLUMN**, **TEMPERAT**, **TABLE**, **THINOX.0**, **THINOX.E**, **THINOX.L**, **D.0**, **D.E**, **VC**, **HENRY.CO**, **SEG.0**, **SEG.E**, **TRANS.0**, and **TRANS.E**.

VD, **VR**, and **VT** also depend on the oxidizing species but apply to both O_2 and H_2O if neither is specified.

Specified Material

The following parameters are dependent only on the first material specified: **D.0**, **D.E**, **VC**, **HENRY.CO**, and **THETA**.

The following parameters are dependent on both materials specified: **SEG.0**, **SEG.E**, **TRANS.0**, **TRANS.E**, and **ALPHA**.

Specified Units

Parameters whose units include time are specified in units of microns and minutes, unless **CM.SEC** is true, in which case units of centimeters and seconds are assumed.

Examples

1. The statement

```
AMBIENT AMB.1 F.O2=0.90 F.N2=0.08 F.HCL=0.02 +  
PRESSURE=2.0
```

defines ambient **AMB.1** to consist of 90% oxygen and 2% chlorine at a pressure of two atmospheres.

2. The statement

```
AMBIENT H2O MAT=NITRIDE +  
VC="130 170" TEMP="900 1000"
```

replaces any values for temperatures between 900°C and 1000°C in the table for **VC** of nitride in ambients containing H₂O.

3. The initialization file *s4init* contains the definitive set of examples of use of the **AMBIENT** statement.

Additional AMBIENT Notes

1. Oxidant in materials other than oxide is allowed to diffuse and segregate, but its concentration is then ignored (no oxynitridation, for instance). The diffusion coefficients in oxide and transport coefficients between oxide and silicon are derived from the Deal-Grove coefficients, so these parameters are ignored if read from input statements.
2. The analytic models use the thickness of the oxide to compute the growth rate, and the **ERFG** model also uses the nitride thickness. These values are *not* inferred from the structure. Instead, the value of **NIT.THIC** is used for the nitride thickness, and the oxide thickness is calculated by adding the oxide grown in a given high-temperature step to the specified **INITIAL** oxide thickness. Thus if the structure has other than **INITIAL** microns of oxide on it at the start of a diffusion step, the thickness must be specified with the **INITIAL** parameter. (If there is no oxide on an exposed silicon surface, a layer of oxide of thickness **INITIAL** is deposited.) If the **INITIAL** parameter doesn't correspond to the actual oxide thickness, the growth rate is incorrect. The **INITIAL** parameter need not be set when an oxidation is continued with the **CONTINUE** parameter on the **DIFFUSION** statement.
3. The analytic models do not recognize masking layers in the structure. The location of the presumed mask edge must be specified by the **MASK.EDG** parameter.
4. The material viscosities have been calibrated for the **VISCOELA** model with stress dependence enabled. For use without stress dependence (with either the **VISCOELA** or **VISCOUS** model), it may be necessary to modify the viscosity values.