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# SUPREM-III User's Manual

Version 8628

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## 2. Introduction

SUPREM-III is a computer program that allows the user to simulate the various processing steps used in the manufacture of silicon integrated circuits or discrete devices. The types of processing steps simulated by the current version of the program are: inert ambient drive-in; oxidation of silicon and silicon-nitride; ion implantation, epitaxial growth of silicon; and low temperature deposition or etching of various materials. SUPREM-III simulates in one dimension the changes in a semiconductor structure as a result of the various processing steps used in its manufacture. The primary results of interest are the thicknesses of the various layers of materials that make up the structure and the distribution of impurities within those layers. The program will also determine certain material properties such as polysilicon grain size and the sheet resistivity of diffused regions in silicon layers.

## 3. The Simulation Structure

In SUPREM-III, a structure whose processing is being simulated is made up of from one to ten layers, each of which is composed of one of ten possible materials. The same material may appear in more than one layer. The default materials defined in SUPREM-III are single crystal silicon, poly-crystalline silicon, silicon dioxide, silicon nitride, and aluminum. The layers in a structure are numbered sequentially, the bottommost layer being layer one. Diffused regions within a layer are also numbered sequentially with the bottommost region in each layer being region one of that layer. A SUPREM-III structure may be doped with up to four impurities, with the default impurities being boron, phosphorus, arsenic, and antimony.

## 4. Using SUPREM-III

To begin a SUPREM-III simulation, all of the coefficients and parameters for the materials and impurities must be input and the initial structure defined. Both of these functions are accomplished by the INITIALIZE statement. In its simplest form the initial structure is a single layer of substrate material, though a more complicated multi-layer structure generated by a previous simulation may be specified. The coefficients are normally read from the default coefficient file and the structure may either be read from a previously saved structure file or defined through the parameters of the INITIALIZE statement. In the data file containing the input statements that control the SUPREM-III simulation, the INITIALIZE statement must precede all other statements except TITLE, COMMENT, or STOP statements.

Once the coefficients and the initial structure have been defined, process simulation can begin. If the user wishes to change any of the material or impurity coefficients, new values may be input by using the model parameter statements. The coefficients defining the impurities are accessed through the impurity statements, BORON, PHOSPHORUS, ARSENIC, ANTIMONY, and IMPURITY. The material coefficients are accessed through the SILICON, POLYSILICON, OXIDE, NITRIDE, ALUMINUM, and MATERIAL statements. Other coefficients that apply to the interaction of materials and impurities may be controlled through the SEGREGATION, VOL.RATIO, and MOBILITY statements. Oxidation rates are controlled by the parameters of the DRYO2, WETO2, and NITROGEN statements. If a user alters any of the coefficients, by using the SAVEFILE statement he may save the modified set of coefficients either into the default coefficient file, S3cof0, creating a new set of defaults, or into an alternate coefficient file that can be read in with either the INITIALIZE or the LOADFILE statements.

## 5. The SUPREM-III Grid Structure

In SUPREM-III, the structure is made up of a series of cells. These cells are laid out on a one-dimensional grid of points called nodes. Within each layer, each cell is centered about a single node point. The cells at either end of a layer are half-cells, with one cell boundary at the endpoint node and the other halfway to the adjacent node within the layer. Within each cell, the physical coefficients and any impurity concentrations are treated as constant. In the current version of the program there may be a maximum of 500 node points or 499 cells or spaces. If an attempt is made to use more than the maximum number of node points during a simulation, the program will terminate with an error.

The distance between adjacent node points within each layer can be controlled by the user, either when a layer is first defined in an INITIALIZE or DEPOSITION statement or at any time in the simulation through the GRID statement. The grid placement is controlled by five parameters; the layer thickness (THICKNESS), the nominal grid spacing (DX), the location of the nominal grid spacing relative to the top surface of the layer (XDX), the number of spaces in the layer (SPACES), and the minimum allowed grid spacing (DX.MIN). The way these parameters are used to control the grid spacing is described below. For the purposes of example, assume that a layer is being deposited on the structure.

In the simplest case the user need only specify the layer's thickness. In this case the program will assume that XDX is zero, placing the nominal grid spacing, DX, at the surface of the layer and will use the default DX for the deposited material. The deposited material, specified by name, has its characteristics, including its default DX, defined by the appropriate material statement. The program will use the number of spaces necessary to achieve a uniform grid spacing throughout the layer.

If the default DX is not adequate, then the user may specify both the thickness and the DX, and the program will work as above except that the specified DX will be used instead of the default value.

In many cases, both to save execution time and to have the structure fit within the limit of 499 grid spaces, a fewer number of spaces may be specified than the program would allocate for uniform grid spacing within the layer. In this case a non-uniform grid spacing will be set up within the affected layer. If the number of spaces specified is less than the number needed for a uniform grid spacing, the program will place a grid spacing of DX at the location specified by XDX, and cause the grid spacings to increase parabolically to either side (figure 1). If the number of spaces specified is greater than the number needed for uniform grid spacings, then the grid spacings will decrease from the DX value on either side of XDX (figure 2).

```
    |                |       |                |
    |               *| dX2  dX |      *          |
dX1 |*             *   |       |   *     *      |
    |   *     *     |    dX1 |*            *   |
dX  |      *         |       |               *| dX2
    |_______________________|      |_______________________|
    0      XdX      thickness    0      XdX       thickness
```

figure 1 figure 2

When a non-uniform grid is set up, the program first determines what the maximum grid spacing would be at either end of the layer assuming a linear variation in grid spacing from XDX, given DX, XDX, the layer thickness and the number of spaces to use. Then with the nominal DX and the two endpoint grid spacings, the grid is made to vary parabolically from DX to the endpoints in such a way that the resulting grid gives a layer of the specified thickness. With this algorithm the user can minimize the number of grid spacings used in the solution and yet place a fine mesh where it is needed to accurately represent a rapidly varying impurity distribution.

## 6. SUPREM-III Output

The results of a SUPREM-III simulation are available in both printed and graphic forms. Printed output can consist of the following: all material and impurity coefficients as might have been specified by one or more of the MATERIAL, IMPURITY, SEGREGATION, or VOL.RATIO statements; information about the current structure such as the thicknesses and composition of the various layers, impurity junction depths, or resistivity of layers or diffused regions; and the impurity concentrations at each node point and the distance of that point from the structure surface. Plotted or graphic output consists of plots of the specified impurity concentrations versus distance.

## 7. SUPREM-III Input Statements

SUPREM-III normally takes its input from a user specified disk file. This file is made up of various statements identified by a statement name followed by a parameter list. The statement name is delimited from the parameter list by either a comma and/or one or more blanks. If a comma is present, it may be preceded or followed by any number of blanks. Parameters in a SUPREM-III parameter list are delimited from each other in the same way the statement name is delimited. If more than one line of input is required for a particular statement, it may be continued on subsequent lines by placing a plus sign as the first non-blank character on the continuation lines.

Parameters in a SUPREM-III parameter list may be one of three types that correspond to the types of values that they may take on. These types are; logical, numerical, and character. Logical parameters take on a value of true if the parameter name appears by itself and a value of false if it is preceded by the NOT, (^), character. Numerical type parameters are assigned values in the parameter list by having the parameter name followed by an equal sign and the value. Blanks on either side of the equal sign are ignored. Character parameters may appear in one of two ways depending of the statement involved. In one case they have a formal parameter name and they are assigned a character string by use of an equal sign in the same way as a numerical parameter. In the other case the statement has the character parameter as the only valid parameter and the character string appears by itself following the statement name without an associated parameter name.

## 8. Manual Format

This manual presents each statement showing the statement name and the associated list of parameters. There are a number of special characters that are used to aid in the description of the parameter lists. These characters are <, >, [, ], (, ), and |.

The <> characters are used to indicate classes of things. For example a parameter description might appear as:

CONCENTRATION=<n>

which indicates that the parameter name is concentration and it is assigned a numerical value. The <n> defines a class of things represented by n, where n represents the set of numerical values. Valid numerical values are of the form:

9 1.2 -.345 6.7E8 -9.01E-2

The only other class defined in this manual is that of character strings represented by <c>.

The [] characters enclose sets of optional items, usually parameters. For example:

STMT1 [ PARM1 ] [ PARM2 PARM3 ] [ PARM4 [ PARM5 ] ]

indicates that on the STMT1 statement, the PARM1 parameter is optional. PARM2 and PARM3 are optional but if one is specified, both must be specified. PARM4 and PARM5 are optional but PARM5 may be specified only if PARM4 is specified.

When one or more of a list of items are to be chosen from, they are separated by a | character and enclosed in parenthesis. For example:

STMT2 (PARM1 | PARM2 | (PARM3 PARM4))

This indicates that statement STMT2 requires that either PARM1, PARM2, or both PARM3 and PARM4 be specified.

In none of the above examples are the special characters actually typed by the user when inputting a SUPREM-III input sequence.

## 9. Aluminum Statement

The ALUMINUM statement is used to input or modify the characteristics of aluminum as a layer material.

```
ALUMINUM

  [ NAME=<c> ] [ DX.DEFAU=<n> ]
  [ CONDUCTO ]
  [ SPECIES=<n> ] [ DENSITY=<n> ]
  [ AT.WT.1=<n> ] [ AT.NUM.1=<n> ] [ ABUND.1=<n> ]
  [ WORK.FUN=<n> ] [ EPSILONF=<n> ]
```

| Name | Type | Description |
|---|---|---|
| ABUND.1 | Num | The relative abundance of element one in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.1 | Num | The atomic number of element one in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.1 | Num | The atomic weight of element one in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| CONDUCTO | Log | Specifies that the material is a conductor.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| DENSITY | Num | The density of the material.<br>(unit: grams/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| DX.DEFAU | Num | The default nominal grid spacing for any layer containing this material.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| EPSILONF | Num | The dielectric constant of the material relative the dielectric constant of air.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| NAME | Char | The name of the material.<br>(unit: )<br>(default: the current name of the material.)<br>(synonym: ) |
| SPECIES | Num | The number of different elements in this material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| WORK.FUN | Num | The work function of the material.<br>(unit: volts)<br>(default: the current value.)<br>(synonym: ) |

The ALUMINUM statement is an alias for the MATERIAL statement with an index of five and is used to define or modify the parameters and coefficients associated with the material aluminum. Not all of the parameters of the MATERIAL statement apply to aluminum and so are not listed here.

## 10. Aluminum Statement

The ALUMINUM statement is used to input or modify the characteristics of aluminum as a layer material.

```
ALUMINUM

  [ NAME=<c> ] [ DX.DEFAU=<n> ]
  [ CONDUCTO ]
  [ SPECIES=<n> ] [ DENSITY=<n> ]
  [ AT.WT.1=<n> ] [ AT.NUM.1=<n> ] [ ABUND.1=<n> ]
  [ WORK.FUN=<n> ] [ EPSILONF=<n> ]
```

| Name | Type | Description |
|---|---|---|
| ABUND.1 | Num | The relative abundance of element one in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.1 | Num | The atomic number of element one in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.1 | Num | The atomic weight of element one in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| CONDUCTO | Log | Specifies that the material is a conductor.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| DENSITY | Num | The density of the material.<br>(unit: grams/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| DX.DEFAU | Num | The default nominal grid spacing for any layer containing this material.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| EPSILONF | Num | The dielectric constant of the material relative the dielectric constant of air.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| NAME | Char | The name of the material.<br>(unit: )<br>(default: the current name of the material.)<br>(synonym: ) |
| SPECIES | Num | The number of different elements in this material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| WORK.FUN | Num | The work function of the material.<br>(unit: volts)<br>(default: the current value.)<br>(synonym: ) |

The ALUMINUM statement is an alias for the MATERIAL statement with an index of five and is used to define or modify the parameters and coefficients associated with the material aluminum. Not all of the parameters of the MATERIAL statement apply to aluminum and so are not listed here.

11. Antimony Statement
------------------------------

The ANTIMONY statement is used to input or modify the physical or model coefficients associated with antimony as a dopant impurity.

```
ANTIMONY

  [ NAME=<c> ] [ DONOR ]
  [ AT.WT=<n> ] [ AT.NUMB=<n> ]
  [ IONFILE1=<c> ] [ IONFILE2=<c> ]
  [ (  ( SILICON
                [ FII.0=<n> ] [ FII.E=<n> ]
                [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
     )
    | ( POLYSILI
                [ FII.0=<n> ] [ FII.E=<n> ]
      [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
     )
    | ( OXIDE | NITRIDE | ALUMINUM )
   [ ELECT.ST=<n> ]
   [ DIX.0=<n> ] [ DIX.E=<n> ]
   [ DIM.0=<n> ] [ DIM.E=<n> ]
   [ DIMM.0=<n> ] [ DIMM.E=<n> ]
  ]
```

| Name | Type | Description |
|---|---|---|
| ALUMINUM | Log | Specifies that the material dependent parameters apply to antimony in aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| AT.NUMB | Num | The atomic number of the impurity.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT | Num | The atomic weight of the impurity.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| DIM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DIMM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIMM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DONOR | Log | Specifies that the impurity is a donor.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| ELECT.ST | Num | The electric stopping power of the impurity in the specified material.<br>(unit: KeV/micron.)<br>(default: the current value.)<br>(synonym: ) |
| ENTROPY | Num | The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| FII.0 | Num | The pre-exponential constant of the fractional partial-interstitialcy contribution.<br>(unit: (microns/minute)^(-1/2))<br>(default: the current value.)<br>(synonym: ) |
| FII.E | Num | The activation energy of the fractional partial-interstitialcy contribution.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| HEAT.SEG | Num | The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| IONFILE1 | Char | Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting atomic antimony.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |
| IONFILE2 | Char | Specifies the secondary ion implant range data file for implants using the analytic distrbutions. This file will be searched for the range statistics when implanting the compound ions containing antimony.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |
| K.A | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.<br>(unit: centimeters)<br>(default: the current value.)<br>(synonym: ) |
| K.MF | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controlling the rate-limiting step of the dopant incorporation process.<br>(unit: centimetersˆ(-2) minutesˆ(-1) atmospheresˆ(-1))<br>(default: the current value.)<br>(synonym: ) |
| K.P | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.<br>(unit: centimetersˆ(-3) atmospheresˆ(-1))<br>(default: the current value.)<br>(synonym: ) |
| NAME | Char | The name of the impurity.<br>(unit: )<br>(default: the last name specified.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material dependent parameters apply to antimony in silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material dependent parameters apply to antimony in silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material dependent parameters apply to antimony in polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| Q.SITES | Num | Effective density of segregation sites at a grain boundary.<br>(unit: sites/cm^2.)<br>(default: the current value.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material dependent parameters apply to antimony in silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The ANTIMONY statement is an alias for the IMPURITY statement with an index of four and is used to define or modify the parameters and coefficients associated with antimony as an impurity. Not all of the parameters of the IMPURITY statement apply to antimony and so are not listed here.

## 12. Arsenic Statement

The ARSENIC statement is used to input or modify the physical or model coefficients associated with arsenic as a dopant impurity.

```
ARSENIC

  [ NAME=<c> ] [ DONOR ]
  [ AT.WT=<n> ] [ AT.NUMB=<n> ]
  [ IONFILE1=<c> ] [ IONFILE2=<c> ]
  [ (  ( SILICON
       [ FII.0=<n> ] [ FII.E=<n> ]
                   [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
       [ ( IMPLANT | CHEMICAL )
         [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
       ]
      )
     | ( POLYSILI
       [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
       [ FII.0=<n> ] [ FII.E=<n> ]
       [ ( IMPLANT | CHEMICAL )
          [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
       ]
      )
     | ( OXIDE | NITRIDE | ALUMINUM )
    [ ELECT.ST=<n> ]
    [ DIX.0=<n> ] [ DIX.E=<n> ]
    [ DIM.0=<n> ] [ DIM.E=<n> ]
    [ DIMM.0=<n> ] [ DIMM.E=<n> ]
  ]
```

| Name | Type | Description |
| --- | --- | --- |
| ALUMINUM | Log | Specifies that the material dependent parameters apply to arsenic in aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| AT.NUMB | Num | The atomic number of the impurity.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT | Num | The atomic weight of the impurity.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| CHEMICAL | Log | Specifies that the clustering coefficients apply to the impurity from a chemical source.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| CTN.0 | Num | The pre-exponential constant used in calculating the impurity clustering coefficient.<br>(unit: atoms/cmˆ3.)<br>(default: the current value.)<br>(synonym: ) |
| CTN.E | Num | The activation energy used in calculating the impurity clustering coefficient.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| CTN.F | Num | The power dependence of the concentration used in calculating the impurity clustering coefficient.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| DIM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIMM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIMM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DONOR | Log | Specifies that the impurity is a donor in silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| ELECT.ST | Num | The electric stopping power of the impurity in the specified material.<br>(unit: KeV/micron.)<br>(default: the current value.)<br>(synonym: ) |
| ENTROPY | Num | The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| FII.0 | Num | The pre-exponential constant of the fractional partial-interstitialcy contribution.<br>(unit: (microns/minute)^(-1/2))<br>(default: the current value.)<br>(synonym: ) |
| FII.E | Num | The activation energy of the fractional partial-interstitialcy contribution.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| HEAT.SEG | Num | The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| IMPLANT | Log | Specifies that the impurity clustering coefficients apply to the impurity from an implanted source.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| IONFILE1 | Char | Specifies the primary ion implant range data file for implants using the analytic distrbutions. This file will be searched for the range statistics when implanting atomic arsenic.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |
| IONFILE2 | Char | Specifies the secondary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting the compound ions containing arsenic.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |
| K.A | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.<br>(unit: centimeters)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| K.MF | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controlling the rate-limiting step of the dopant incorporation process.<br>(unit: centimetersˆ(-2) minutesˆ(-1) atmospheresˆ(-1))<br>(default: the current value.)<br>(synonym: ) |
| K.P | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.<br>(unit: centimetersˆ(-3) atmospheresˆ(-1))<br>(default: the current value.)<br>(synonym: ) |
| NAME | Char | The name of the impurity.<br>(unit: )<br>(default: the last name specified.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material dependent parameters apply to arsenic in silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material dependent parameters apply to arsenic in silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material dependent parameters apply to arsenic in polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| Q.SITES | Num | Effective density of segregation sites at a grain boundary.<br>(unit: sites/cmˆ2.)<br>(default: the current value.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material dependent parameters apply to silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The ARSENIC statement is an alias for the IMPURITY statement with an index of three and is used to define or modify the parameters and coefficients associated with arsenic as an impurity. Not all of the parameters of the IMPURITY statement apply to arsenic and so are not listed here.

## 13. Bias Statement

The BIAS statement is used to specify the bias of conductor and semiconductor layers during a Poisson solution initiated by the ELECTRICAL statement.

```
BIAS

   LAYER=<n>
     ( [ V.ELECTR=<n> ] [ DV.ELECTR=<n> ] )
   | (  ( [ DIFFUSIO=<n> ]
          [ V.MAJORI=<n> ] [ DV.MAJOR=<n> ]
          [ V.MINORI=<n> ] [ DV.MINOR=<n> ]
        )
       | [ FLOAT ]
     )
```

| Name | Type | Description |
|---|---|---|
| DIFFUSIO | Num | The index of the diffused region for which the quasi-Fermi potentials are specified. The parameter is valid only for a semiconductor layer.<br>(unit: )<br>(default: All diffused regions in the layer.)<br>(synonym: ) |
| LAYER | Num | The index of the conductor or semiconductor layer for which a bias is being specified.<br>(unit: )<br>(default: )<br>(synonym: ) |
| DV.ELECT | Num | The increment for the bias applied to a conductor layer. This parameter is valid only for a conductor layer.<br>(unit: volts.)<br>(default: 0.0)<br>(synonym: ) |
| DV.MAJOR | Num | The increment for the quasi-Fermi potential of majority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer.<br>(unit: volts.)<br>(default: 0.0)<br>(synonym: ) |
| DV.MINOR | Num | The increment for the quasi-Fermi potential of minority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer.<br>(unit: volts.)<br>(default: 0.0)<br>(synonym: ) |
| FLOAT | Log | Specifies that a polysilicon layer is to be treated as a neutral dielectric. This parameter is valid only for a polysilicon layer.<br>(unit: )<br>(default: false.) |

| | | |
|---|---|---|
| | | (synonym: ) |
| V.ELECTR | Num | The initial value for the bias applied to a conductor layer. This parameter is valid only for a conductor layer.<br>(unit: volts.)<br>(default: 0.0)<br>(synonym: ) |
| V.MAJORI | Num | The initial value for the quasi-Fermi potential of majority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer.<br>(unit: volts.)<br>(default: 0.0)<br>(synonym: ) |
| V.MINORI | Num | The initial value for the quasi-Fermi potential of minority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer.<br>(unit: volts.)<br>(default: 0.0)<br>(synonym: ) |

The BIAS statement specifies the bias of a material layer. One BIAS statement may appear for each conductor layer and for each diffused region of a semiconductor layer. Diffused regions are bounded by material interfaces and metallurgical junctions.

For a semiconductor layer, elimination of the DIFFUSIO parameter applies the specified biases to all diffused regions in the layer. Additional BIAS statements may be included to override these values, which are used as the default values in regions for which specific BIAS statements do not appear.

The increment parameters on the BIAS statement are used to advance the bias values for each Poisson solution, where the number of solutions is controlled by the STEPS parameter on the ELECTRICAL statement.

## 14. Boron Statement

The BORON statement is used to input or modify the physical or model coefficients associated with boron as a dopant impurity.

```
BORON

   [ NAME=<c> ] [ ACCEPTOR ]
   [ AT.WT=<n> ] [ AT.NUMB=<n> ]
   [ IONFILE1=<c> ] [ IONFILE2=<c> ]
   [ (  ( SILICON
         [ FII.0=<n> ] [ FII.E=<n> ]
                    [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
        )
      | ( POLYSILI
         [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
         [ FII.0=<n> ] [ FII.E=<n> ]
        )
      | ( OXIDE | NITRIDE | ALUMINUM )
    [ ELECT.ST=<n> ]
    [ DIX.0=<n> ] [ DIX.E=<n> ]
    [ DIP.0=<n> ] [ DIP.E=<n> ]
   ]
```

| Name | Type | Description |
| --- | --- | --- |
| ACCEPTOR | Log | Specifies that the impurity is an acceptor in silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ALUMINUM | Log | Specifies that the material dependent parameters apply to boron in aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| AT.NUMB | Num | The atomic number of the impurity.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT | Num | The atomic weight of the impurity.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| DIP.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with positive vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DIP.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with positive vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| ELECT.ST | Num | The electric stopping power of the impurity in the specified material.<br>(unit: KeV/micron.)<br>(default: the current value.)<br>(synonym: ) |
| ENTROPY | Num | The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| FII.0 | Num | The pre-exponential constant of the fractional partial-interstitialcy contribution.<br>(unit: (microns/minute)^(-1/2))<br>(default: the current value.)<br>(synonym: ) |
| FII.E | Num | The activation energy of the fractional partial-interstitialcy contribution.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| HEAT.SEG | Num | The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| IONFILE1 | Char | Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting atomic boron.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |
| IONFILE2 | Char | Specifies the secondary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting BF2 ions.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |

| | | |
|---|---|---|
| K.A | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.<br>(unit: centimeters)<br>(default: the current value.)<br>(synonym: ) |
| K.MF | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controling the rate-limiting step of the dopant incorporation process.<br>(unit: centimeters^(-2) minutes^(-1) atmospheres^(-1))<br>(default: the current value.)<br>(synonym: ) |
| K.P | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.<br>(unit: centimeters^(-3) atmospheres^(-1))<br>(default: the current value.)<br>(synonym: ) |
| NAME | Char | The name of the impurity.<br>(unit: )<br>(default: the last name specified.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material dependent parameters apply to boron in silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material dependent parameters apply to boron in silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material dependent parameters apply to boron in polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| Q.SITES | Num | Effective density of segregation sites at a grain boundary.<br>(unit: sites/cm^2.)<br>(default: the current value.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material dependent parameters apply to boron in silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The BORON statement is an alias for the IMPURITY statement with an index of one and is used to define or modify the parameters and coefficients associated with boron as an impurity. Not all of the parameters of the

IMPURITY statement apply to boron and so are not listed here.

## 15. Comment Statement

The COMMENT statement is used to input a character string to label the following input sequence.

```
  COMMENT  [<c>]
or
  $        [<c>]
```

The character string associated with the COMMENT statement is output to the standard output device. If the previous statement was neither another COMMENT statement nor a TITLE statement, then a line feed is issued before the character string is output.

## 16. Deposition Statement

The DEPOSITION statement is used to deposit a specified material on top of the current structure. The material may be doped or undoped.

```
DEPOSITION

  THICKNES=<n>
  (  SILICON ( <111> | <110> | <100> )
   | POLYSILI
      TEMPERAT=<n> [ PRESSURE=<n> | GRAINSIZ=<n> ]
   | OXIDE
   | NITRIDE
   | ALUMINUM
  )
  [ DX=<n> ] [ XDX=<n> ] [ SPACES=<n> ] [ MIN.DX=<n> ]
                [ CONCENTRATION=<n>
    (ANTIMONY | ARSENIC | BORON | PHOSPHOR)
  ]
```

| Name | Type | Description |
|---|---|---|
| ALUMINUM | Log | Specifies that the material to be deposited is aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the deposited material is to be uniformly doped with antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the deposited material is to be uniformly doped with arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | Log | Specifies that the deposited material is to be uniformly doped with boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| CONCENTR | Num | The concentration at which the deposited material is to be uniformly doped.<br>(unit: atoms/cmˆ3.)<br>(default: 0.0)<br>(synonym: ) |
| DX | Num | The nominal grid spacing to be used in the deposited layer at the location associated with the XDX parameter.<br>(unit: microns.)<br>(default: the nominal dx of the top layer if its material is the same as is |

| | | |
|---|---|---|
| | | being deposited, otherwise, the default dx of the deposited material.)<br>(synonym: ) |
| GRAINSIZ | Num | The as-deposited grain size of the deposited polysilicon layer.<br>(unit: microns.)<br>(default: calculated from the deposition temperature and pressure.)<br>(synonym: ) |
| MIN.DX | Num | The minimum grid spacing that can be used in the layer on which the layer is to be deposited.<br>(unit: microns.)<br>(default: the last value specified.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material to be deposited is silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material to be deposited is silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the deposited material is to be uniformly doped with phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material to be deposited is poly-crystalline silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PRESSURE | Num | The pressure during the deposition of a polysilicon layer.<br>(unit: atmospheres.)<br>(default: 1.0)<br>(synonym: ) |
| SILICON | Log | Specifies that the material to be deposited is single crystal silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SPACES | Num | The number of spaces to be used in the deposited layer.<br>(unit: )<br>(default: thickness/dx.)<br>(synonym: ) |
| TEMPERAT | Num | The temperature during deposition of a polysilicon layer.<br>(unit: )<br>(default: degrees Centigrade.)<br>(synonym: ) |
| THICKNES | Num | The thickness of the deposited layer.<br>(unit: microns.)<br>(default: )<br>(synonym: ) |

| | | |
|---|---|---|
| XDX | Num | The distance from the surface of the layer at which the nominal grid spacing, DX, applies.<br>(unit: microns.)<br>(default: 0.)<br>(synonym: ) |
| <100> | Log | Specifies that the crystalline orientation of the deposited silicon is <100>.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <110> | Log | Specifies that the crystalline orientation of the deposited silicon is <110>.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <111> | Log | Specifies that the crystalline orientation of the deposited silicon is <111>.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The DEPOSITION statement is used to deposit a given thickness of the specified material on top of the existing structure. The material deposited may be either undoped or doped uniformly with one of the available impurity types. If the material to be deposited is of the same type as is already present in the top layer of the structure, then the material is added to the existing top layer. If the top layer material is of a different type than that being deposited, then a new layer is created for the deposited material.

If single crystal silicon is being deposited, then the crystalline orientation must also be specified. If polysilicon is being deposited, then the deposition temperature must also be specified. The resulting polysilicon grain size will be calculated from the deposition temperature and pressure unless overridden by the user via the GRAINSIZE parameters.

## 17. Diffusion Statement

The DIFFUSION statement is used to model high temperature diffusion in both oxidizing and non-oxidizing ambients.

```
DIFFUSION

  TIME=<n> TEMPERAT=<n> [ T.RATE=<n> ]
  [ ( GAS.CONC=<n> | SOLIDSOL )
    ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  ]
  [ ( DRYO2 | WETO2 | NITROGEN )
    [ PRESSURE=<n> ] [ P.RATE=<n> ] [ HCL%=<n> ]
  ]
  [ DTMIN=<n> ] [ DTMAX=<n> ]
  [ ABS.ERR=<n> ] [ REL.ERR=<n> ]
```

| Name | Type | Description |
| --- | --- | --- |
| ABS.ERR | Num | Specifies the maximum desired absolute truncation error. Used to control the time step as described below.<br>(unit: centimeters^(-3))<br>(default: 1.0E14)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the impurity in the ambient gas is antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the impurity in the ambient gas is arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | Log | Specifies that the impurity in the ambient gas is boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| DTMAX | Num | The largest time increment to be used during the solution.<br>(unit: minutes.)<br>(default: 5.0)<br>(synonym: ) |
| DTMIN | Num | The smallest time increment to be used during the solution.<br>(unit: minutes.)<br>(default: 0.005)<br>(synonym: ) |
| DRYO2 | Log | Specifies that the ambient gas consists of dry oxygen.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| GAS.CONC | Num | The concentration of the specified impurity in the ambient gas at the surface of the structure.<br>(unit: atoms/cmˆ3.)<br>(default: 0.0)<br>(synonym: CONCENTRATION) |
| HCL% | Num | The percentage of chlorine present in the ambient gas.<br>(unit: percent)<br>(default: percentage specified in corresponding ambient statement (DryO2, WetO2, Nitrogen))<br>(synonym: ) |
| NITROGEN | Log | Specifies that the ambient consists of nitrogen (non-oxidizing ambient).<br>(unit: )<br>(default: true.)<br>(synonym: ) |
| P.RATE | Num | The rate of change in the ambient gas pressure.<br>(unit: atmospheres/minute.)<br>(default: 0.0)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the impurity in the ambient gas is phosphorus.<br>(unit: false.)<br>(default: )<br>(synonym: ) |
| PRESSURE | Num | The pressure of the ambient gas. (See note below.)<br>(unit: atmospheres.)<br>(default: pressure specified in corresponding ambient statement (DryO2, WetO2, Nitrogen))<br>(synonym: ) |
| REL.ERR | Num | Specifies the maximum desired relative truncation error. Used to control the time step as described below.<br>(unit: )<br>(default: 0.5)<br>(synonym: ) |
| SOLIDSOL | Log | Sets the concentration of the specified impurity in the ambient gas at the surface of the structure to the solid solubility of the impurity in silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| TIME | Num | The total elapsed time of the diffusion step being simulated.<br>(unit: minutes.)<br>(default: )<br>(synonym: ) |
| TEMPERAT | Num | The temperature of the ambient at the beginning of the step.<br>(unit: degrees Centigrade.)<br>(default: )<br>(synonym: ) |
| T.RATE | Num | The rate of change of the ambient temperature.<br>(unit: degrees Centigrade/minute.)<br>(default: 0.0)<br>(synonym: ) |

| | | |
|---|---|---|
| WETO2 | Log | Specifies that the ambient gas consists of wet oxygen or pyrogenic steam.<br>(See note below.)<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The DIFFUSION statement simulates impurity diffusion in the structure under a variety of oxidizing and non-oxidizing conditions. At a minimum, only the time and temperature of a step needs to be specified. In this case a non-oxidizing drive-in is assumed. For oxidizing ambients or gaseous predepositions additional parameters need to be specified. The default pressures and chlorine percentages are set previously by the oxidation ambient model cards (e.g. DRYO2, WETO2, NITROGEN), while the defaults of the other optional parameters are set in the GENII key file S3FKY0.

The numerical solution of the diffusion equations requires that the total step time be divided into a number of smaller time increments, dt's, in order to insure sufficient accuracy. There are two mechanisms that control the choice of dt's, one is due to a restriction on interface movement such that no interface moves more than one cell spacing during a dt. The other time step control algorithm has been chosen to give the desired accuracy without using excessive amounts of computation time. Unless the interface control chooses a smaller dt, it will attempt to use a dt equal to that specified by the DTMIN parameter. Subsequent dt's are chosen in the following manner.

1. At each point in the current structure a projected concentration is calculated from the previous two solutions.

   Cp = C' + (C' - C'')*dt/dt'

   Where C' is the previous concentration, C'' is the concentration before that, and dt' is the previous dt.

2. From the current solution value, C, and the absolute and relative truncation error parameters, an 'error' term at each point is then calculated.

   Cerr = abs(C - Cp) / (ABS.ERR + abs(C)*REL.ERR)

3. The next dt is then calculated from the following expression.

   dtnext = dt * sqrt( (1. + dt/dt')/Cerrmax )

   Where Cerrmax is the maximum value of Cerr calculated at each point in the structure.

4. A value of dtnext is calculated for each impurity present with the smallest value being the one that is ultimately used.

NOTE: The effective oxidant partial pressure for pyrogenic steam reactors has been found to vary significantly from facility to facility. It is recommended that the user set the default pressure for WetO2 to a value that gives the best agreement with measured oxide thicknesses from his facility.

## 18. DryO2 Statement

The DRYO2 statement allows the user to modify the coefficients used to model the oxidation of the various materials under dry ambient oxidation conditions.

```
DRYO2

  [ ( <111> | <110> | <100> )
    [ LIN.L.0=<n> ] [ LIN.L.E=<n> ]
    [ LIN.H.0=<n> ] [ LIN.H.E=<n> ]
    [ THINOX.0=<n> ] [ THINOX.E=<n> ] [ THINOX.L=<n> ]
  ]
  [ PAR.L.0=<n> ] [ PAR.L.E=<n> ]
  [ PAR.H.0=<n> ] [ PAR.H.E=<n> ]
  [ LIN.BREA=<n> ] [ PAR.BREA=<n> ]
  [ LIN.PDEP=<n> ] [ PAR.PDEP=<n> ]
  [ PRESSURE=<n> ] [ HCL%=<n> ]
  [ GAMMA.0=<n> ] [ GAMMA.E=<n> ]
  [ DELTA.0=<n> ] [ DELTA.E=<n> ]
  [ EXP.0=<n> ] [ EXP.E=<n> ]
  [ NIOX.0=<n> ] [ NIOX.E=<n> ] [ NIOX.F=<n> ]
  [ CL.ROW=<n> [ CL.PCT=<n> ]
    CL.COLUM=<n> [ CL.TEMPE=<n> ]
    [ CL.DEP.L=<n> ] [ CL.DEP.P=<n> ]
  ]
```

| Name | Type | Description |
| --- | --- | --- |
| CL.COLUM | Num | The column number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.DEP.L | Num | The coefficient modifying the linear oxidation rate in the presence of chlorine at the specified row and column.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.DEP.P | Num | The coefficient modifying the parabolic oxidation rate in the presence of chlorine at the specified row and column.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.PCT | Num | The percentage of chlorine for which the coefficients in the specified row are valid.<br>(unit: percent.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| CL.ROW | Num | The row number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.TEMPE | Num | The temperature for which the coefficients in the specified column are valid.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |
| DELTA.0 | Num | The pre-exponential factor of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: cm^3/atom.)<br>(default: the current value.)<br>(synonym: ) |
| DELTA.E | Num | The activation energy of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| EXP.0 | Num | The pre-exponential factor of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| EXP.E | Num | The activation energy of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| GAMMA.0 | Num | The pre-exponential factor of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GAMMA.E | Num | The activation energy of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| HCL% | Num | The default percentage of chlorine present in the ambient.<br>(unit: percent.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.BREA | Num | The temperature at which the temperature dependence of the linear oxidation rate changes.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| LIN.H.0 | Num | The pre-exponential constant of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.H.E | Num | The activation energy of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.L.0 | Num | The pre-exponential constant of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.L.E | Num | The activation energy of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.PDEP | Num | The pressure dependence factor for the linear oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| NIOX.0 | Num | The pre-exponential constant used to determine the oxidation rate of silicon nitride.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| NIOX.E | Num | The activation energy used to determine the oxidation rate of silicon nitride.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| NIOX.F | Num | The exponent factor used to determine the oxidation rate of silicon nitride.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| PAR.BREA | Num | The temperature at which the temperature dependence of the parabolic oxidation rate changes.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.H.0 | Num | The pre-exponential constant of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| PAR.H.E | Num | The activation energy of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.L.0 | Num | The pre-exponential constant of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.L.E | Num | The activation energy of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.PDEP | Num | The pressure dependence factor for the parabolic oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| PRESSURE | Num | The default ambient pressure.<br>(unit: atmospheres.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.0 | Num | The pre-exponential constant of the thin oxide growth rate parameter.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.E | Num | The activation energy of the thin oxide growth rate parameter.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.L | Num | The characteristic length of the thin oxide growth rate parameter.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| <100> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <100> orientation silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <110> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <110> orientation silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <111> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <111> orientation silicon.<br>(unit: )<br>(default: false.) |

(synonym: )

The three oxidation model statements, DRYO2, WETO2, and NITROGEN, use identical parameters, differing only in the values assigned. The parameters NIOX.C, NIOX.E, and NIOX.F are used in modeling the oxidation of silicon nitride while the others deal with the oxidation of single and polycrystalline silicon.

The effects of chlorine in the ambient gas on the oxidation rate of silicon are currently modeled by an empirical expression whose only variable is defined by the L.CLDEP and P.CLDEP for the linear and parabolic rates respectively. To date no convenient function is available to calculate the chlorine dependence as a function of temperature and amount of chlorine present, therefor a table of values defines the chlorine dependence factors at those temperatures and percentages for which reliable data is available. For those temperatures and chlorine percentages between the values in the table, linear interpolation is employed to calculate the value used. For temperatures or percentages outside the range of values present in the table, the values whose conditions most nearly match the current conditions are used. For example, if the current conditions are a temperature of 1175 degrees with three percent chlorine, but the highest temperature entry in the table is 1150 degrees and the nearest chlorine percentages are for two and four percent, then a value halfway between the values at 1150 degrees and two and four percent chlorine will be used.

## 19. Electrical Statement

The ELECTRICAL statement begins a series of numerical solutions of Poisson's equation for the current structure.

```
ELECTRICAL

  [ STEPS=<n> ] [ EXTENT=<n> ] [ TEMPERAT=<n> ]
  [ ERROR=<n> ] [ MAX.ITER=<n> ] [ FILE.OUT=<c> ]
```

| Name | Type | Description |
|---|---|---|
| ERROR | Num | The allowed relative error between successive approximations during the iterative solution of Poisson's equation.<br>(unit: )<br>(default: 1 x 10ˆ-4.)<br>(synonym: ) |
| EXTENT | Num | The distance by which the bottom layer of the structure is extended for the numerical solution of Poisson's equation. This extension is necessary to allow for the proper treatment of depletion regions which extend beyond the bottom of the simulated structure.<br>(unit: microns.)<br>(default: 0.0)<br>(synonym: ) |
| FILE.OUT | char | The name of the file to which the results of the electrical calculations are to be output. The total hole and electron concentrations and their respective conductivities and resistivities are normally written to the standard output, but if a file is specified, they are also written to that file. The potential, net active impurity concentration and the distance from the surface at each node are also written to the file.<br>(unit: )<br>(default: )<br>(synonym: ) |
| MAX.ITER | Num | The maximum number of iterations allowed for each solution of Poisson's equation.<br>(unit: )<br>(default: 50)<br>(synonym: ) |
| STEPS | Num | The number of bias steps for which Poisson's equation is solved.<br>(unit: )<br>(default: 1)<br>(synonym: ) |
| TEMPERAT | Num | The device temperature used during the solutions of Poisson's equation.<br>(unit: degrees Centigrade.)<br>(default: 26.84)<br>(synonym: ) |

The ELECTRICAL statement performs the number of solutions of Poisson's equation specified by the STEPS parameter for the current physical structure. The solution region can be extended below the structure used for process simulation by using the EXTEND parameter. For a structure having an insulator layer at the top or bottom, reflection symmetry is used as the boundary condition at the associated external boundary.

Insulator layers in the structure are treated as charge-neutral dielectrics. Conductor layers are treated as regions having constant specified bias. Semiconductor layers have constant specified quasi-Fermi potentials for electrons and holes within each diffused region. Polysilicon layers can also be treated as charge-neutral dielectric layers. The above bias information is specified through a series of BIAS statements which follow the ELECTRICAL statement and are terminated by an END.ELECTRICAL statement.

For each Poisson solution, the total electron and hole concentrations, conductivities, and sheet resistances are calculated and printed for all diffused regions in the semiconductor layers.

## 20. End.Electrical Statement

The END.ELEC statement terminates a sequence of BIAS statements associated with the ELECTRIC statement.

```
END.ELEC  [ <c> ]
```

## 21. Epitaxy Statement

The EPITAXY statement simulates the epitaxial growth of silicon layers.

```
EPITAXY

  TEMPERAT=<n>  TIME=<n> [ DX=<n> ]
  ( GROWTH.R=<n> | PP.SILAN=<n> )
  [ ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
    ( CONCENTR=<n> | PP.DOPAN=<n> )
  [ DTMIN=<n> ] [ DTMAX=<n> ]
  [ ABS.ERR=<n> ] [ REL.ERR=<n> ]
```

| Name | Type | Description |
|---|---|---|
| ABS.ERR | Num | Specifies the maximum desired absolute truncation error. Used to control the time step as described below.<br>(unit: centimeters^(-3))<br>(default: 1.0E14)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the impurity in the ambient gas is antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the impurity in the ambient gas is arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | Log | Specifies that the impurity in the ambient gas is boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| CONCENTR | Num | The concentration of the specified impurity in the ambient gas at the surface of the structure.<br>(unit: atoms/cm^3.)<br>(default: 0.0)<br>(synonym: GAS.CONC) |
| DX | Num | Specifies a width of the grid spaces used in the epi-layer grown.<br>(unit: microns)<br>(default: the current nominal dx for this layer)<br>(synonym: ) |
| DTMAX | Num | The largest time increment to be used during the solution.<br>(unit: minutes.)<br>(default: 5.0)<br>(synonym: ) |

| | | |
|---|---|---|
| DTMIN | Num | The smallest time increment to be used during the solution.<br>(unit: minutes.)<br>(default: 0.005)<br>(synonym: ) |
| GROWTH.R | Num | The growth rate of the epitaxial layer.<br>(unit: microns/minute.)<br>(default: )<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the impurity in the ambient gas is phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PP.DOPAN | Num | Specifies the input dopant partial pressure. This is approximately equal to the dopant input flow rate divided by the hydrogen carrier input flow rate. See the R. Reif reference below.<br>(unit: atmospheres)<br>(default: 0.0)<br>(synonym: ) |
| PP.SILAN | Num | Specifies the input silane partial pressure. This is approximately equal to the silane input flow rate divided by the hydrogen carrier input flow rate. See the R. Reif reference below.<br>(unit: atmospheres)<br>(default: 0.0)<br>(synonym: ) |
| REL.ERR | Num | Specifies the maximum desired relative truncation error. Used to control the time step as described below.<br>(unit: )<br>(default: 0.5)<br>(synonym: ) |
| TEMPERAT | Num | The temperature at the beginning of the step.<br>(unit: degrees Centigrade.)<br>(default: )<br>(synonym: ) |
| TIME | Num | The total elapsed time of the epitaxy step being simulated.<br>(unit: minutes.)<br>(default: )<br>(synonym: ) |

The EPITAXY statement is used to grow a layer of single crystal silicon on top of the current structure. The epitaxial layer may be either doped or undoped. To grow an epitaxial layer, the top layer must be single crystal silicon.

The growth rate used in the simulation may be specified in one of two ways. The first is to explicitly specify it with the GROWTH.R parameter. The second is to specify the input partial pressure of silane with the PP.SILAN parameter causing the rate to be determined from the product of the partial pressure and the mass transport coefficient of silane in hydrogen as specified by the SILICON statement. (Reference, ‘Computer Simulation in Silicon Epitaxy’, by R. Reif and R. W. Dutton, J. Electrochem. Soc., Vol. 128, No. 4, April 1981, pp 909-918.)

Analogous to the growth rate, the impurity concentration in doped epi-layers may be specified in one of two ways. The first is to explicitly specify the surface concentration with the CONCENTR parameter. The second is to specify the input partial pressure of the dopant with the PP.DOPAN parameter. The surface concentration is then calculated as a function of the partial pressure, time increment, growth rate, and the mass transport and kinetic coefficients, K.a, K.p, and K.mf as specified by the SILICON statement. (See the previous reference.)

The numerical solution of the diffusion equations requires that the total step time be divided into a number of smaller time increments, dt's, in order to insure sufficient accuracy. There are two mechanisms that control the choice of dt's, one is due to a restriction on interface movement such that no interface moves more than one cell spacing during a dt. The other time step control algorithm has been chosen to give the desired accuracy without using excessive amounts of computation time. Unless the interface control chooses a smaller dt, it will attempt to use a dt equal to that specified by the DTMIN parameter. Subsequent dt's are chosen in the following manner.

1. At each point in the current structure a projected concentration is calculated from the previous two solutions.

   Cp = C' + (C' - C'')*dt/dt'

   Where C' is the previous concentration, C'' is the concentration before that, and dt' is the previous dt.

2. From the current solution value, C, and the absolute and relative truncation error parameters, an 'error' term at each point is then calculated.

   Cerr = abs(C - Cp) / (ABS.ERR + abs(C)*REL.ERR)

3. The next dt is then calculated from the following expression.

   dtnext = dt * sqrt( (1. + dt/dt')/Cerrmax )

   Where Cerrmax is the maximum value of Cerr calculated at each point in the structure.

4. A value of dtnext is calculated for each impurity present with the smallest value being the one that is ultimately used.

## 22. Etch Statement

The ETCH statement is used to etch a specified material from the top of the current structure.

```
ETCH

  ( SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM )
  [ ( THICKNES=<n> | ALL ) ]
```

| Name | Type | Description |
|---|---|---|
| ALL | Log | Specifies that all of the specified material is to be etched.<br>(unit: )<br>(default: true.)<br>(synonym: ) |
| ALUMINUM | Log | Specifies that the material to be etched is aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material to be etched is silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material to be etched is silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material to be etched is poly-crystalline silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material to be etched is single crystal silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| THICKNESS | Num | The amount of the material to be etched.<br>(unit: microns.)<br>(default: the surface layer thickness.)<br>(synonym: AMOUNT) |

The ETCH statement is used to etch a specified amount of the specified material from the top of the existing structure. If the material at the top of the structure is not the material specified then no etching takes place. If the amount to be etched is not specified then the entire layer is removed.

## 23. Grid Statement

The GRID statement specifies the grid spacing parameters for one or more of the layers in a structure. For the first layer, the thickness may also be extended.

```
GRID

   LAYER.<n> [ THICKNES=<n> ] [ DX=<n> ] [ MIN.DX=<n> ]
   [ XDX=<n> ] [ SPACES=<n> ]
```

| Name | Type | Description |
|---|---|---|
| DX | Num | The nominal grid spacing in to be used in the specified layer(s) at the location associated with the XDX parameter.<br>(unit: microns.)<br>(default: The current nominal grid spacing.)<br>(synonym: ) |
| LAYER.<n> | Log | Specifies that the grid parameters are to apply to the n'th layer of the structure.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| MIN.DX | Num | The minimum grid spacing that can be used in the specified layer(s).<br>(unit: microns.)<br>(default: The current minimum grid spacing.)<br>(synonym: ) |
| SPACES | Num | The number of spaces to be used in the specified layer(s).<br>(unit: )<br>(default: The current number of spaces in the layer.)<br>(synonym: ) |
| THICKNESS | Num | The thickness of the first layer. If the specified thickness is greater than the current layer thickness, then additional material is added to the bottom of the layer. The value specified must be greater than or equal to the current thickness.<br>(unit: microns.)<br>(default: The current layer thickness.)<br>(synonym: ) |
| XDX | Num | The distance from the surface of the layer at which the nominal grid spacing, DX, applies.<br>(unit: microns.)<br>(default: The last value specified.)<br>(synonym: ) |

The GRID statement is used primarily to change the grid spacing of one or more layers of the current structure. In the case of the first, or bottom layer, the GRID statement may be used to extend the depth of the layer by adding additional material to the bottom of the structure. In this case, the impurity concentration at the bottommost cell in the structure is used uniformly in the added region.

## 24. Implant Statement

The IMPLANT statement is used to simulate the ion-implantation of impurities into the structure. Four types of implantation models are available, a numerical method based on the Boltzman transport equation, and three analytical methods based on simple Gaussian, two sided Gaussian, or Pearson type-IV distributions.

```
IMPLANT

  DOSE=<n> ENERGY=<n>
  ( ANTIMONY | ARSENIC | BF2 | BORON | PHOSPHOR )
  (  GAUSSIAN
   | 2-GAUSSI
   | PEARSON
   | ( BOLTZMAN [ MINSTEPS=<n> ] [ AT.WT=<n> ] [ AT.NUMB=<n> ] )
  )
```

| Name | Type | Description |
|---|---|---|
| ANTIMONY | Log | Specifies that the ion to be implanted is antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the ion to be implanted is arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| AT.NUMB | Num | The atomic number of the ion to be implanted.<br>(unit: )<br>(default: The last value specified in the corresponding impurity coefficient statement)<br>(synonym: ) |
| AT.WT | Num | The atomic weight of the ion to be implanted.<br>(unit: amu)<br>(default: The last value specified in the corresponding impurity coefficient statement)<br>(synonym: AT.MASS) |
| BF2 | Log | Specifies that the ion to be implanted is boron-difluoride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| BOLTZMAN | Log | Specifies that the Boltzman transport model is to be used in simulating the implantation.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| BORON | Log | Specifies that the ion to be implanted is atomic boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| DOSE | Num | The implanted dose.<br>(unit: atoms/cmˆ2.)<br>(default: )<br>(synonym: ) |
| ENERGY | Num | The energy of the implant beam.<br>(unit: thousand electron volts.)<br>(default: )<br>(synonym: ) |
| GAUSSIAN | Log | Specifies that a simple Gaussian distribution is to be used to model the implanted profile.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| MINSTEPS | Num | The minimum number of steps between each grid point used in calculating the energy distribution during the solution of the Boltzman transport equation.<br>(unit: )<br>(default: 5.0)<br>(synonym: ) |
| PEARSON | Log | Specifies that a Pearson type-IV distribution is to be used to model the implanted profile.<br>(unit: )<br>(default: true, if no other model is specified.)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the ion to be implanted is phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| 2-GAUSSI | Log | Specifies that a two sided Gaussian distribution is to be used to model the implanted profile.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The IMPLANT statement is used to simulate ion-implantation of impurities into the structure. Four different ion-implantation models are available.

When the BOLTZMANN option is selected, the implanted ion distribution is calculated by a numerical solution of the Boltzmann transport equation [1]. In this method, the momentum distribution of the implanted ion is determined at each depth in the target. Then distribution in energy and angle is represented numerically by a two-dimensional array (default size 15 x 8).

The calculation proceeds starting from the surface, where the momentum distribution is known to be a delta function (mono-energetic beam moving normal to the target surface). A knowledge of the scattering cross section for both two-body atomic and electronic interactions, together with the transport equations, is then sufficient to determine how the momentum distribution evolves with depth. Material discontinuities are simple to handle, since only the cross sections change as the ions cross any interface. When any ion scatters to an energy less than about 5% of the initial energy, or when an ion is scattered back toward the target surface, that ion is considered stopped at that depth and becomes part of the range distribution. The calculation proceeds until the concentration of the implanted profile drops to 10ˆ-5 of its peak value.

The other three models are based on fitting the as-implanted distribution to an analytical function. The three functions available are a simple Gaussian, a two sided Gaussian, or a Pearson type-IV distribution. The necessary moments, or range statistics, are read from the implant moment data file specified via the appropriate impuritys statement.

## 25. Impurity Statement

The IMPURITY statement is used to input or modify the physical or model coefficients associated with a dopant impurity.

```
IMPURITY

  INDEX=<n>
  [ NAME=<c> ] [ (DONOR | ACCEPTOR) ]
  [ AT.WT=<n> ] [ AT.NUMB=<n> ]
  [ IONFILE1=<c> ] [ IONFILE2=<c> ]
  [ (  ( SILICON
        [ FII.0=<n> ] [ FII.E=<n> ]
                    [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
        [ MISFITST=<n> ] [ CD=<n> ]
        [ MSF111FA=<n> ] [ MSF110FA=<n> ] [ MSF100FA=<n> ]
        [ DAMAGEST=<n> ]
        [ NE.0=<n> ] [ NE.E=<n> ]
        [ ( IMPLANT | CHEMICAL )
          [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
        ]
      )
     | ( POLYSILI
        [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
        [ FII.0=<n> ] [ FII.E=<n> ]
        [ ( IMPLANT | CHEMICAL )
           [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
        ]
      )
     | ( OXIDE | NITRIDE | ALUMINUM )
    [ ELECT.ST=<n> ]
    [ DIX.0=<n> ] [ DIX.E=<n> ]
    [ DIM.0=<n> ] [ DIM.E=<n> ]
    [ DIMM.0=<n> ] [ DIMM.E=<n> ]
    [ DIP.0=<n> ] [ DIP.E=<n> ]
  ]
```

| Name | Type | Description |
|---|---|---|
| ACCEPTOR | Log | Specifies that the impurity is an acceptor in silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ALUMINUM | Log | Specifies that the material dependent parameters apply to the impurity in aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| AT.NUMB | Num | The atomic number of the impurity.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| AT.WT | Num | The atomic weight of the impurity.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| CD | Num | This parameter is used to calculate the temperature dependent part of the expression for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.<br>(unit: (atoms/cmˆ3)(degrees Centigradeˆ2).)<br>(default: the current value.)<br>(synonym: ) |
| CHEMICAL | Log | Specifies that the clustering coefficients apply to the impurity from a chemical source.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| CTN.0 | Num | The pre-exponential constant used in calculating the impurity clustering coefficient.<br>(unit: atoms/cmˆ3.)<br>(default: the current value.)<br>(synonym: ) |
| CTN.E | Num | The activation energy used in calculating the impurity clustering coefficient.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| CTN.F | Num | The power dependence of the concentration used in calculating the impurity clustering coefficient.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| DAMAGEST | Num | The factor in the implant dose dependent expression for calculating the bandgap narrowing due to the residual damage of phosphorus implants.<br>(unit: electron volts-cmˆ(1/2).)<br>(default: the current value.)<br>(synonym: ) |
| DIM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIMM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DIMM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIP.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with positive vacancies.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIP.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with positive vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DONOR | Log | Specifies that the impurity is a donor in silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| ELECT.ST | Num | The electric stopping power of the impurity in the specified material.<br>(unit: KeV/micron.)<br>(default: the current value.)<br>(synonym: ) |
| ENTROPY | Num | The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| FII.0 | Num | The pre-exponential constant of the fractional partial-interstitialcy contribution.<br>(unit: (microns/minute)ˆ(-1/2))<br>(default: the current value.)<br>(synonym: ) |
| FII.E | Num | The activation energy of the fractional partial-interstitialcy contribution.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| HEAT.SEG | Num | The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| IMPLANT | Log | Specifies that the impurity clustering coefficients apply to the impurity from an implanted source.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| IONFILE1 | Char | Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting the atomic ion of this impurity.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |
| IONFILE2 | Char | Specifies the secondary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting the compound ions containing this impurity.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |
| K.A | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.<br>(unit: centimeters)<br>(default: the current value.)<br>(synonym: ) |
| K.MF | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controling the rate-limiting step of the dopant incorporation process.<br>(unit: centimetersˆ(-2) minutesˆ(-1) atmospheresˆ(-1))<br>(default: the current value.)<br>(synonym: ) |
| K.P | Num | Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.<br>(unit: centimetersˆ(-3) atmospheresˆ(-1))<br>(default: the current value.)<br>(synonym: ) |
| MISFITST | Num | The prefactor in the high concentration dependent expression for calculating the bandgap narrowing due to the lattice misfit strain from high concentrations of phosphorus.<br>(unit: electron volts-cmˆ3.)<br>(default: the current value.)<br>(synonym: ) |
| MSF100FA | Num | The orientation factor in <100> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| MSF110FA | Num | The orientation factor in <110> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| MSF111FA | Num | The orientation factor in <111> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| NAME | Char | The name of the impurity.<br>(unit: )<br>(default: the last name specified.)<br>(synonym: ) |
| NE.0 | Num | The pre-exponential constant for Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of phosphorus at high concentrations.<br>(unit: atoms/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| NE.E | Num | The activation energy for calculating Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of phosphorus at high concentrations.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material dependent parameters apply to the impurity in silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material dependent parameters apply to the impurity in silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material dependent parameters apply to the impurity in polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| Q.SITES | Num | Effective density of segregation sites at a grain boundary.<br>(unit: sites/cm^2.)<br>(default: the current value.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material dependent parameters apply to the impurity in single crystal silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The IMPURITY statement is used to input or modify the coefficients and parameters that define a given impurity. Four impurities are defined, boron, phosphorus, arsenic, and antimony. These impurities each have their own impurity coefficient statements which are aliases of the general IMPURITY statement.

## 26. Initialize Statement

The INITIALIZE statement, as it's name implies, is used to set up the initial coefficients and structure to be used in the processing steps that follow.

```
INITIALIZE

  [ ( COEFFICI=<c> | FIRSTIME ) ]
  [ STRUCTUR=<c> ] [ MIN.DX=<n> ] [ SAVESTEP ]
  [ THICKNES=<n> ] [ DX=<n> ] [ XDX=<n> ] [ SPACES=<n> ]
  [ (  SILICON  ( <111> | <110> | <100> )
     | POLYSILI
        ( GRAINSIZ=<n> | ( TEMPERAT=<n> [ PRESSURE=<n> ] ) )
     | OXIDE
     | NITRIDE
     | ALUMINUM
    )
    [ CONCENTR=<n>
      ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
    ]
  ]
```

| Name | Type | Description |
| --- | --- | --- |
| ALUMINUM | Log | Specifies that aluminum is the material in the first layer.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | Log | Specified that the initial structure is to be doped uniformly with antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the initial structure is to be doped uniformly with arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | Log | Specifies that the initial structure is to be doped uniformly with boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| COEFFICI | Char | The name of the file containing the physical coefficients to be used by the program.<br>(unit: )<br>(default: S3cof0.)<br>(synonym: ) |

| | | |
|---|---|---|
| CONCENTR | Num | The impurity concentration at which the structure is to be uniformly doped.<br>(unit: atoms/cmˆ3.)<br>(default: 0.0)<br>(synonym: ) |
| DX | Num | The nominal grid spacing to be used in the first layer of the structure at the location specified by XDX.<br>(unit: microns.)<br>(default: That of the first layer of the input structure file; otherwise, the default for the material in the first layer.)<br>(synonym: ) |
| FIRSTIME | Log | Indicates that no coefficient file exists. Used the first time the program is executed to create the default coefficient file.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| GRAINSIZ | Num | Specifies the polysilicon grain size.<br>(unit: microns.)<br>(default: )<br>(synonym: ) |
| MIN.DX | Num | The minimum grid spacing to be used in the first layer of the structure.<br>(unit: microns.)<br>(default: That of the first layer of the input structure file; otherwise, 0.001.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that silicon nitride is the material in the first layer.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that silicon dioxide is the material in the first layer.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the initial structure is to be doped uniformly with phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that polycrystalline silicon is the material in the first layer.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PRESSURE | Num | Specifies the polysilicon deposition pressure.<br>(unit: atmospheres.)<br>(default: 1.0)<br>(synonym: ) |

| | | |
|---|---|---|
| SAVESTEP | Log | Causes the structure to be saved in the file S3sav0 after each step in which the structure is modified.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SILICON | Log | Specifies that single crystal silicon is the material in the first layer.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SPACES | Num | The number of spaces to be used in the layer.<br>(unit: )<br>(default: thickness/dx if no structure is input; otherwise, the current number of spaces.)<br>(synonym: ) |
| STRUCTUR | Char | The name of the file containing the initial structure information.<br>(unit: )<br>(default: )<br>(synonym: ) |
| TEMPERAT | Num | Specifies the polysilicon deposition temperature.<br>(unit: degrees Centigrade.)<br>(default: )<br>(synonym: ) |
| THICKNES | Num | The thickness of the first layer of the initial structure.<br>(unit: microns.)<br>(default: That of the first layer of the input structure file; otherwise, none.)<br>(synonym: ) |
| XDX | Num | The distance from the top of the first layer at which the nominal grid spacing applies.<br>(unit: microns.)<br>(default: That of the first layer of the input structure file; otherwise, 0.0)<br>(synonym: ) |
| <100> | Log | Specifies that the crystalline orientation of the material in the first layer is <100>.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <110> | Log | Specifies that the crystalline orientation of the material in the first layer is <110>.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <111> | Log | Specifies that the crystalline orientation of the material in the first layer is <111>.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

An INITIALIZE statement is required in every SUPREM-III input sequence and it must preceed all other statements except for TITLE or COMMENT statements. At the start of execution the SUPREM-III program contains no information about any of the materials or impurities that may be used in the processing sequence. All of the physical and model coefficients and any initial structure information is contained in one or two files and must be read into the programs internal storage before processing can proceed. Normally, all of the coefficient information is contained in a default file, S3COF0. If this is the case, and if a coefficient file is not specified in the INITIALIZE statement, the data is read from the default coefficient file.

The same is true with the structure information, an initial structure of at least one layer of material must be present before execution can continue. A previously defined structure of arbitrary complexity can be input from a file specified by the STRUCTUR parameter. The other parameters of the INITIALIZE statement may be used to redefine the structure input from a file if the structure has only a single layer of material or, if no structure file is input, they may be used to set up the initial layer.

If no coefficient file is present, the FIRSTIME parameter must be specified and all of the needed coefficients explicitly specified by subsequent statements before processing statements can be executed. As it's name implies, the FIRSTIME parameter should only be needed the first time the program is brought up at a new installation.

## 27. Loadfile Statement

The LOADFILE statement is used to input either a new structure to be processed, the physical and model coefficients to be used by the program, or both.

```
LOADFILE

 FILENAME=<c> ( ALL | COEFFICI | STRUCTUR )
 [ FORMATTE ]
```

| Name | Type | Description |
|---|---|---|
| ALL | Log | Specifies that both the structure information and the model coefficients are to be input from the specified file.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| COEFFICI | Log | Specifies that the coefficient information is to be input from the specified file.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| FILENAME | Char | The name of the file from which the specified information is to be read.<br>(unit: )<br>(default: )<br>(synonym: NAME) |
| FORMATTE | Log | Specifies that the information in the file is formatted. If not specified then the information is assumed to be unformatted or binary.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| STRUCTUR | Log | Specifies that the information describing the structure is to be input from the specified file.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The LOADFILE statement inputs two classes of information about the process that is to be simulated. The first class is the physical structure and impurity distributions of the materials to be simulated. This file is used as the starting point for subsequent processing steps. The other class of information consists of all of the physical and model parameters or coefficients used by the program.

A LOADFILE statement may appear at any point in a processing sequence after the INITIALIZE statement and before the STOP statement. If both structure and coefficient information are to be input, it is recommended that an INITIALIZE statement be used instead of LOADFILE.

## 28. Lpplot Statement

The LPPLOT statement outputs a semi-logarithmic plot of the specified impurity concentrations versus depth into the structure to the output using the standard character set. This type of plotting is suitable for non-graphics terminals and line printers.

PLOT

[ ACTIVE ] [ CHEMICAL ] [ TOTAL ] [ NET ]
[ ANTIMONY ] [ ARSENIC ] [ BORON ] [ PHOSPHOR ]
[ XMIN=<n> ] [ XMAX=<n> ] [ CMIN=<n> ] [ CMAX=<n> ]
[ LINES/PA=<n> ] [ COLUMNS=<n> ]

| Name | Type | Description |
|---|---|---|
| ACTIVE | Log | Specifies that the electrically active concentrations of the specified impurities are to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the antimony concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the arsenic concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | Log | Specifies that the boron concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| CHEMICAL | Log | Specifies that the chemical concentration of the specified impurities are to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| COLUMNS | Num | The number of character columns of the output device.<br>(unit: columns)<br>(default: 80)<br>(synonym: ) |
| CMAX | Num | The maximum concentration value plotted.<br>(unit: atoms/cm^3.)<br>(default: 1x10^21)<br>(synonym: ) |

| | | |
|---|---|---|
| CMIN | Num | The minimum concentration value plotted.<br>(unit: atoms/cmˆ3.)<br>(default: 1x10ˆ14)<br>(synonym: ) |
| LINES/PA | Num | The number of line per page of the output device.<br>(unit: lines)<br>(default: 60)<br>(synonym: ) |
| NET | Log | Specifies that the difference of the sum of the n-type and the sum p-type active or chemical impurity concentrations present in the structure is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the phosphorus concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| TOTAL | Log | Specifies that the sum of the active or chemical impurity concentrations present in the structure is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| XMAX | Num | The distance from the top of the plotted layers to the point where the last concentration is to be plotted.<br>(unit: microns.)<br>(default: The current total width of the plotted layers.)<br>(synonym: ) |
| XMIN | Num | The distance from the top of the plotted layers to the point where the first concentration is to be plotted.<br>(unit: microns.)<br>(default: 0.0)<br>(synonym: ) |

The LPPLOT statement is used to output plots of the impurity distributions versus distance in the structure. The impurities present may be plotted either individually, added together, or as the difference between n- and p-type dopants. These plots may be of either the electrically active or total chemical concentrations.

If no range parameters (XMIN or XMAX) are specified, then the distributions are plotted over the entire structure. If no minimum or maximum plot concentrations (CMIN or CMAX) are specified, then the range between 1x10ˆ14 and 1x10ˆ21 is plotted.

## 29. Material Statement

The MATERIAL statement is used to input or modify the characteristics of a layer material. The program is presently configured to handle up to ten different material types. Materials with index numbers one through five are defaulted to silicon, silicon dioxide, polysilicon, silicon nitride, and aluminum, respectively. The parameter values for the defaulted materials may also be accessed via the SILICON, OXIDE, POLYSILI, NITRIDE, and ALUMINUM statements.

```
MATERIAL

  [ INDEX=<n> ]
  [ NAME=<c> ] [ DX.DEFAU=<n> ]
  [ ( SEMICOND | CONDUCTO | INSULATO ) ]
  [ SPECIES=<n> ] [ DENSITY=<n> ]
  [ AT.WT.1=<n> ] [ AT.WT.2=<n> ] [ AT.WT.3=<n> ]
  [ AT.NUM.1=<n> ] [ AT.NUM.2=<n> ] [ AT.NUM.3=<n> ]
  [ ABUND.1=<n> ] [ ABUND.2=<n> ] [ ABUND.3=<n> ]
  [ DIFX.0=<n> ] [ DIFX.E=<n> ]
  [ DIMX.0=<n> ] [ DIFM.E=<n> ]
  [ DIMMX.0=<n> ] [ DIFMM.E=<n> ]
  [ DIFP.0=<n> ] [ DIFP.E=<n> ]
  [ NI.0=<n> ] [ NI.E=<n> ] [ NI.F=<n> ] [ DEFECTLN=<n> ]
  [ OEDK.0=<n> ] [ OEDK.E=<n> ] [ OED.RATE=<n> ]
  [ 100.OEDF=<n> ] [ 110.OEDF=<n> ] [ 111.OEDF=<n> ]
  [ GSZ.H.0=<n> ] [ GSZ.H.E=<n> ]
  [ GSZ.L.0=<n> ] [ GSZ.L.E=<n> ]
  [ MIN.GRAI=<n> ] [ TEMP.BRE=<n> ]
  [ RATIO.0=<n> ] [ RATIO.E=<n> ]
  [ GEO.FACT=<n> ] [ GBE.0=<n> ] [ GBE.E=<n> ]
  [ TAU.0=<n> ] [ TAU.E=<n> ]
  [ AFFINITY=<n> ] [ WORK.FUN=<n> ] [ EPSILONF=<n> ]
  [ N.VALENC=<n> ] [ N.CONDUC=<n> ] [ BAND.GAP=<n> ]
  [ K.M=<n> ]
```

| Name | Type | Description |
|---|---|---|
| ABUND.1 | Num | The relative abundance of element one in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| ABUND.2 | Num | The relative abundance of element two in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| ABUND.3 | Num | The relative abundance of element three in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| AFFINITY | Num | The electron affinity of the material.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.1 | Num | The atomic number of element one in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.2 | Num | The atomic number of element two in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.3 | Num | The atomic number of element three in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.1 | Num | The atomic weight of element one in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.2 | Num | The atomic weight of element two in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.3 | Num | The atomic weight of element three in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| BAND.GAP | Num | The band gap of the material.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| CONDUCTO | Num | Specifies that the material is a conductor.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| DEFECTLN | Num | The decay length of point defects in the material.<br>(unit: microns)<br>(default: the current value.)<br>(synonym: ) |
| DENSITY | Num | The density of the material.<br>(unit: grams/cmˆ3.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DIFM.0 | Num | The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFM.E | Num | The activation energy used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIFMM.0 | Num | The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with doubly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFMM.E | Num | The activation energy used in the calculation the component of the self-diffusivity due to diffusion with doubly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIFP.0 | Num | The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFP.E | Num | The activation energy used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIFX.0 | Num | The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFX.E | Num | The activation energy used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DX.DEFAU | Num | The default nominal grid spacing for any layer containing this material.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| EPSILONF | Num | The dielectric constant of the material relative the dielectric constant of air.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| GBE.0 | Num | The pre-exponential constant used in calculating the grain-boundary energy<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GBE.E | Num | The activation energy used in calculating the grain-boundary energy.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| GEO.FACT | Num | A geometric factor used in calculating the grain growth driving force, F.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GSZ.H.0 | Num | The pre-exponential constant used in calculating the 'as deposited' polysilicon grain size for pressures near one atmosphere.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| GSZ.H.E | Num | The activation energy used in calculating the 'as deposited' polysilicon grain size for pressures near one atmosphere.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| GSZ.L.0 | Num | The pre-exponential constant used in calculating the 'as deposited' polysilicon grain size for low pressure CVD.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| GSZ.L.E | Num | The activation energy used in calculating the 'as deposited' polysilicon grain size for low pressure CVD.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| INDEX | Num | The material index of the material being modified. This number is used internally in the program to identify the material and point to its parameters.<br>(unit: )<br>(default: )<br>(synonym: ) |
| INSULATO | Log | Specifies that the material is an insulator.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| K.M | Num | Used in R. Reif's epitaxial growth model (see reference in EPITAXY statement). K.m is the mass transport coefficient for silane in hydrogen.<br>(unit: microns/minute/atmosphere)<br>(default: the current value)<br>(synonym: ) |

| | | |
|---|---|---|
| MIN.GRAI | Num | The minimum polysilicon grain size. Used for 'as deposited' LPCVD polysilicon when the temperature is below that specified by TEMP.BRE<br>(unit: microns)<br>(default: the current value.)<br>(synonym: ) |
| NAME | Char | The name of the material.<br>(unit: )<br>(default: the current name of the material.)<br>(synonym: ) |
| NI.0 | Num | The pre-factor used in the calculation of the intrinsic carrier concentration.<br>(unit: (carriers/cm^3)(degrees Kelvin)^(3/2).)<br>(default: the current value.)<br>(synonym: ) |
| NI.E | Num | The activation energy used in the calculation of the intrinsic carrier concentration.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| NI.F | Num | The exponent to the absolute temperature used in the calculation of the intrinsic carrier concentration.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| N.VALENC | Num | The carrier concentration in the valence band of the material.<br>(unit: carriers/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| N.CONDUC | Num | The carrier concentration in the conduction band of the material.<br>(unit: carriers/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| OEDK.0 | Num | The pre-exponential constant used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| OEDK.E | Num | The activation energy used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.<br>(unit: electron volts)<br>(default: the current value.)<br>(synonym: ) |
| OED.RATE | Num | The power dependence of oxidation enhanced diffusion on the oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| RATIO.0 | Num | The pre-exponential constant used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the ratio of the pre-exponential factors for the two self-diffusivities<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| RATIO.E | Num | The activation energy used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the difference between the activation energies of the two self-diffusivities<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| SEMICOND | Log | Specifies that the material is a semiconductor.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SPECIES | Num | The number of different elements in this material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| TAU.0 | Num | The pre-exponential constant used to calculate the time dependence of the grain interior concentration.<br>(unit: minutes.)<br>(default: the current value.)<br>(synonym: ) |
| TAU.E | Num | The activation energy used to calculate the time dependence of the grain interior concentration.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| TEMP.BRE | Num | For LPCVD the temperature below which the deposited polysilicon becomes amorphous.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |
| WORK.FUN | Num | The work function of the material.<br>(unit: volts)<br>(default: the current value.)<br>(synonym: ) |
| 100.OEDF | Num | The orientation dependent factor for the oxidation enhanced diffusion for <100> oriented silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| 110.OEDF | Num | The orientation dependent factor for the oxidation enhanced diffusion for <110> oriented silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| 111.OEDF | Num | The orientation dependent factor for the oxidation enhanced diffusion for <111> oriented silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

The MATERIAL statement is used to input or modify the coefficients and parameters that define a given material. Up to ten materials can be defined at one time. There are five default materials assigned the material indexes one through ten, these are single crystal silicon, silicon dioxide, polysilicon, silicon nitride, and aluminum. The first four of these should not be redefined as they are treated specially by several models in the program.

The current implementation of the program allows the definition of materials made up of at most three elements.

## 30. Nitride Statement

The NITRIDE statement is used to input or modify the characteristics of silicon nitride as a layer material.

```
NITRIDE

  [ NAME=<c> ] [ DX.DEFAU=<n> ]
  [ INSULATO ]
  [ SPECIES=<n> ] [ DENSITY=<n> ]
  [ AT.WT.1=<n> ] [ AT.WT.2=<n> ]
  [ AT.NUM.1=<n> ] [ AT.NUM.2=<n> ]
  [ ABUND.1=<n> ] [ ABUND.2=<n> ]
  [ EPSILONF=<n> ]
```

| Name | Type | Description |
|---|---|---|
| ABUND.1 | Num | The relative abundance of element one in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| ABUND.2 | Num | The relative abundance of element two in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.1 | Num | The atomic number of element one in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.2 | Num | The atomic number of element two in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.1 | Num | The atomic weight of element one in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.2 | Num | The atomic weight of element two in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| DENSITY | Num | The density of the material.<br>(unit: grams/cm^3.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DX.DEFAU | Num | The default nominal grid spacing for any layer containing this material.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| EPSILONF | Num | The dielectric constant of the material relative the dielectric constant of air.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| INSULATO | Log | Specifies that the material is an insulator.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| NAME | Char | The name of the material.<br>(unit: )<br>(default: the current name of the material.)<br>(synonym: ) |
| SPECIES | Num | The number of different elements in this material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

The NITRIDE statement is an alias for the MATERIAL statement with an index of four and is used to define or modify the parameters and coefficients associated with the material silicon nitride. Not all of the parameters of the MATERIAL statement apply to silicon nitride and so are not listed here.

## 31. Nitrogen Statement

The NITROGEN statement allows the user to modify the coefficients used to model the oxidation of the various materials under nitrogen ambient or non-oxidizing conditions.

```
NITROGEN

  [ ( <111> | <110> | <100> )
    [ LIN.L.0=<n> ] [ LIN.L.E=<n> ]
    [ LIN.H.0=<n> ] [ LIN.H.E=<n> ]
    [ THINOX.0=<n> ] [ THINOX.E=<n> ] [ THINOX.L=<n> ]
  ]
  [ PAR.L.0=<n> ] [ PAR.L.E=<n> ]
  [ PAR.H.0=<n> ] [ PAR.H.E=<n> ]
  [ LIN.BREA=<n> ] [ PAR.BREA=<n> ]
  [ LIN.PDEP=<n> ] [ PAR.PDEP=<n> ]
  [ PRESSURE=<n> ] [ HCL%=<n> ]
  [ GAMMA.0=<n> ] [ GAMMA.E=<n> ]
  [ DELTA.0=<n> ] [ DELTA.E=<n> ]
  [ EXP.0=<n> ] [ EXP.E=<n> ]
  [ NIOX.0=<n> ] [ NIOX.E=<n> ] [ NIOX.F=<n> ]
  [ CL.ROW=<n> [ CL.PCT=<n> ]
    CL.COLUM=<n> [ CL.TEMPE=<n> ]
    [ CL.DEP.L=<n> ] [ CL.DEP.P=<n> ]
  ]
```

| Name | Type | Description |
|---|---|---|
| CL.COLUM | Num | The column number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.DEP.L | Num | The coefficient modifying the linear oxidation rate in the presence of chlorine at the specified row and column.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.DEP.P | Num | The coefficient modifying the parabolic oxidation rate in the presence of chlorine at the specified row and column.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.PCT | Num | The percentage of chlorine for which the coefficients in the specified row are valid.<br>(unit: percent.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| CL.ROW | Num | The row number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.TEMPE | Num | The temperature for which the coefficients in the specified column are valid.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |
| DELTA.0 | Num | The pre-exponential factor of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: cmˆ3/atom.)<br>(default: the current value.)<br>(synonym: ) |
| DELTA.E | Num | The activation energy of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| EXP.0 | Num | The pre-exponential factor of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| EXP.E | Num | The activation energy of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| GAMMA.0 | Num | The pre-exponential factor of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GAMMA.E | Num | The activation energy of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| HCL% | Num | The default percentage of chlorine present in the ambient.<br>(unit: percent.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.BREA | Num | The temperature at which the temperature dependence of the linear oxidation rate changes.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| LIN.H.0 | Num | The pre-exponential constant of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.H.E | Num | The activation energy of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.L.0 | Num | The pre-exponential constant of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.L.E | Num | The activation energy of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.PDEP | Num | The pressure dependence factor for the linear oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| NIOX.0 | Num | The pre-exponential constant used to determine the oxidation rate of silicon nitride.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| NIOX.E | Num | The activation energy used to determine the oxidation rate of silicon nitride.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| NIOX.F | Num | The exponent factor used to determine the oxidation rate of silicon nitride.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| PAR.BREA | Num | The temperature at which the temperature dependence of the parabolic oxidation rate changes.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.H.0 | Num | The pre-exponential constant of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| PAR.H.E | Num | The activation energy of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.L.0 | Num | The pre-exponential constant of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.<br>(unit: micronsˆ2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.L.E | Num | The activation energy of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.PDEP | Num | The pressure dependence factor for the parabolic oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| PRESSURE | Num | The default ambient pressure.<br>(unit: atmospheres.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.0 | Num | The pre-exponential constant of the thin oxide growth rate parameter.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.E | Num | The activation energy of the thin oxide growth rate parameter.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.L | Num | The characteristic length of the thin oxide growth rate parameter.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| <100> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <100> orientation silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <110> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <110> orientation silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <111> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <111> orientation silicon.<br>(unit: )<br>(default: false.) |

(synonym: )

The three oxidation model statements, DRYO2, WETO2, and NITROGEN, use identical parameters, differing only in the values assigned. The parameters NIOX.C, NIOX.E, and NIOX.F are used in modeling the oxidation of silicon nitride while the others deal with the oxidation of single and polycrystalline silicon.

The effects of chlorine in the ambient gas on the oxidation rate of silicon are currently modeled by an empirical expression whose only variable is defined by the L.CLDEP and P.CLDEP for the linear and parabolic rates respectively. To date no convenient function is available to calculate the chlorine dependence as a function of temperature and amount of chlorine present, therefor a table of values defines the chlorine dependence factors at those temperatures and percentages for which reliable data is available. For those temperatures and chlorine percentages between the values in the table, linear interpolation is employed to calculate the value used. For temperatures or percentages outside the range of values present in the table, the values whose conditions most nearly match the current conditions are used. For example, if the current conditions are a temperature of 1175 degrees with three percent chlorine, but the highest temperature entry in the table is 1150 degrees and the nearest chlorine percentages are for two and four percent, then a value halfway between the values at 1150 degrees and two and four percent chlorine will be used.

## 32. Oxide Statement

The OXIDE statement is used to input or modify the characteristics of silicon dioxide as a layer material.

```
OXIDE

  [ NAME=<c> ] [ DX.DEFAU=<n> ]
  [ INSULATO ]
  [ SPECIES=<n> ] [ DENSITY=<n> ]
  [ AT.WT.1=<n> ] [ AT.WT.2=<n> ]
  [ AT.NUM.1=<n> ] [ AT.NUM.2=<n> ]
  [ ABUND.1=<n> ] [ ABUND.2=<n> ]
  [ EPSILONF=<n> ]
```

| Name | Type | Description |
| --- | --- | --- |
| ABUND.1 | Num | The relative abundance of element one in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| ABUND.2 | Num | The relative abundance of element two in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.1 | Num | The atomic number of element one in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.2 | Num | The atomic number of element two in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.1 | Num | The atomic weight of element one in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.2 | Num | The atomic weight of element two in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| DENSITY | Num | The density of the material.<br>(unit: grams/cm^3.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DX.DEFAU | Num | The default nominal grid spacing for any layer containing this material.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| EPSILONF | Num | The dielectric constant of the material relative the dielectric constant of air.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| INSULATO | Log | Specifies that the material is an insulator.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| NAME | Char | The name of the material.<br>(unit: )<br>(default: the current name of the material.)<br>(synonym: ) |
| SPECIES | Num | The number of different elements in this material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

The OXIDE statement is an alias for the MATERIAL statement with an index of two and is used to define or modify the parameters and coefficients associated with the material silicon dioxide. Not all of the parameters of the MATERIAL statement apply to silicon dioxide and so are not listed here.

## 33. Phosphorus Statement

--------------------------------

The PHOSPHOR statement is used to input or modify the physical or model coefficients associated with phosphorus as a dopant impurity.

```
PHOSPHOR

   [ NAME=<c> ] [ DONOR ]
   [ AT.WT=<n> ] [ AT.NUMB=<n> ]
   [ IONFILE1=<c> ] [ IONFILE2=<c> ]
   [ (  ( SILICON
         [ FII.0=<n> ] [ FII.E=<n> ]
                     [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
         [ MISFITST=<n> ] [ CD=<n> ]
         [ MSF111FA=<n> ] [ MSF110FA=<n> ] [ MSF100FA=<n> ]
         [ DAMAGEST=<n> ]
         [ NE.0=<n> ] [ NE.E=<n> ]
         [ ( IMPLANT | CHEMICAL )
           [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
         ]
       )
      | ( POLYSILI
         [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
         [ FII.0=<n> ] [ FII.E=<n> ]
         [ ( IMPLANT | CHEMICAL )
            [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
         ]
       )
      | ( OXIDE | NITRIDE | ALUMINUM )
     [ ELECT.ST=<n> ]
     [ DIX.0=<n> ] [ DIX.E=<n> ]
     [ DIM.0=<n> ] [ DIM.E=<n> ]
     [ DIMM.0=<n> ] [ DIMM.E=<n> ]
   ]
```

| Name | Type | Description |
|---|---|---|
| ALUMINUM | Log | Specifies that the material dependent parameters apply to phosphorus in aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| AT.NUMB | Num | The atomic number of the impurity.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT | Num | The atomic weight of the impurity.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| CD | Num | This parameter is used to calculate the temperature dependent part of the expression for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.<br>(unit: (atoms/cm^3)(degrees Centigrade^2).)<br>(default: the current value.)<br>(synonym: ) |
| CHEMICAL | Log | Specifies that the clustering coefficients apply to the impurity from a chemical source.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| CTN.0 | Num | The pre-exponential constant used in calculating the impurity clustering coefficient.<br>(unit: atoms/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| CTN.E | Num | The activation energy used in calculating the impurity clustering coefficient.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| CTN.F | Num | The power dependence of the concentration used in calculating the impurity clustering coefficient.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| DAMAGEST | Num | The factor in the implant dose dependent expression for calculating the bandgap narrowing due to the residual damage of phosphorus implants.<br>(unit: electron volts-cm^(1/2).)<br>(default: the current value.)<br>(synonym: ) |
| DIM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIMM.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIMM.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.) |

(synonym: )

| | | |
|---|---|---|
| DIX.0 | Num | The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIX.E | Num | The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DONOR | Log | Specifies that the impurity is a donor in silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| ELECT.ST | Num | The electric stopping power of the impurity in the specified material.<br>(unit: KeV/micron.)<br>(default: the current value.)<br>(synonym: ) |
| ENTROPY | Num | The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| FII.0 | Num | The pre-exponential constant of the fractional partial-interstitialcy contribution.<br>(unit: (microns/minute)^(-1/2))<br>(default: the current value.)<br>(synonym: ) |
| FII.E | Num | The activation energy of the fractional partial-interstitialcy contribution.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| HEAT.SEG | Num | The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| IMPLANT | Log | Specifies that the impurity clustering coefficients apply to the impurity from an implanted source.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| IONFILE1 | Char | Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting atomic phosphorus.<br>(unit: )<br>(default: the last file specified.)<br>(synonym: ) |

IONFILE2 Char
Specifies the secondary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting the compound ions containing phosphorus.
(unit: )
(default: the last file specified.)
(synonym: )

K.A Num
Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.
(unit: centimeters)
(default: the current value.)
(synonym: )

K.MF Num
Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controlling the rate-limiting step of the dopant incorporation process.
(unit: centimeters^(-2) minutes^(-1) atmospheres^(-1))
(default: the current value.)
(synonym: )

K.P Num
Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.
(unit: centimeters^(-3) atmospheres^(-1))
(default: the current value.)
(synonym: )

MISFITST Num
The prefactor in the high concentration dependent expression for calculating the bandgap narrowing due to the lattice misfit strain from high concentrations of phosphorus.
(unit: electron volts-cm^3.)
(default: the current value.)
(synonym: )

MSF100FA Num
The orientation factor in <100> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.
(unit: )
(default: the current value.)
(synonym: )

MSF110FA Num
The orientation factor in <110> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.
(unit: )
(default: the current value.)
(synonym: )

MSF111FA Num
The orientation factor in <111> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.
(unit: )
(default: the current value.)
(synonym: )

NAME Char
The name of the impurity.
(unit: )
(default: the last name specified.)
(synonym: )

| | | |
|---|---|---|
| NE.0 | Num | The pre-exponential constant for Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of phosphorus at high concentrations.<br>(unit: atoms/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| NE.E | Num | The activation energy for calculating Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of phosphorus at high concentrations.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material dependent parameters apply to phosphorus in silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material dependent parameters apply to phosphorus in silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material dependent parameters apply to phosphorus in polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| Q.SITES | Num | Effective density of segregation sites at a grain boundary.<br>(unit: sites/cm^2.)<br>(default: the current value.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material dependent parameters apply to phosphorus in silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The PHOSPHOR statement is an alias for the IMPURITY statement with an index of two and is used to define or modify the parameters and coefficients associated with phosphorus as an impurity. Not all of the parameters of the IMPURITY statement apply to phosphorus and so are not listed here.

## 34. Plot Statement

The PLOT statement outputs a semi-logarithmic plot of the specified impurity concentrations versus depth into the structure.

```
PLOT

  [ ACTIVE ] [ CHEMICAL ] [ TOTAL ] [ NET ]
  [ ANTIMONY ] [ ARSENIC ] [ BORON ] [ PHOSPHOR ]
  [ XMIN=<n> ] [ XMAX=<n> ] [ CMIN=<n> ] [ CMAX=<n> ]
  [ LAYER1 ] [ LAYER2 ] ... [ LAYER10 ]
  [ CLEAR ] [ AXIS ] [ LINETYPE=<n> ]
            [ TITLE=<c> ] [ LABEL=<c> ]
  [ XPWIDTH=<n> ] [ YPWIDTH=<n> ]
  [ XOFFSET=<n> ] [ YOFFSET=<n> ]
  [ DEVICE=<c> ] [ FILENAME=<c> ]
```

| Name | Type | Description |
|---|---|---|
| ACTIVE | Log | Specifies that the electrically active concentrations of the specified impurities are to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the antimony concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the arsenic concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| AXIS | Log | Specifies that the axis is to be plotted.<br>(unit: )<br>(default: true.)<br>(synonym: ) |
| BORON | Log | Specifies that the boron concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| CHEMICAL | Log | Specifies that the chemical concentration of the specified impurities are to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| CLEAR | Log | Causes the plot area to be cleared.<br>(unit: )<br>(default: true.)<br>(synonym: ) |
| CMAX | Num | The maximum concentration value plotted.<br>(unit: atoms/cmˆ3.)<br>(default: 1x10ˆ21)<br>(synonym: ) |
| CMIN | Num | The minimum concentration value plotted.<br>(unit: atoms/cmˆ3.)<br>(default: 1x10ˆ14)<br>(synonym: ) |
| DEVICE | Char | Specifies the type of plot device used. If this is not specified, on a system with full gplot support the user's terminal will be used if it has graphics capabilities or the default graphics device if it does not. On a system without full gplot support the device types are limited to those distributed with the code or added by the person providing local Suprem-III support. This person should be contacted for a list of the devices available.<br>(unit: )<br>(default: See above.)<br>(synonym: PLOTDEV) |
| FILENAME | Char | Specifies that the plot output is to be re-routed to the named file.<br>(unit: )<br>(default: )<br>(synonym: ) |
| LABEL | Char | Specifies the string to be plotted to the right of the plotted structure along with a short segment of the current linetype. If not specified then the type of data plotted is used.<br>(unit: )<br>(default: The type of data plotted.)<br>(synonym: ) |
| LAYERn | Log | If not negated, specifies that the indicated layer is to be plotted. If negated, specifies that the layer is not to be included in the plot. If no layers are specified then all layers present in the current structure are plotted. If any layer is negated then all layers not explicitly negated are plotted, if any layer is specified and not negated then only those layers so specified are plotted.<br>(unit: )<br>(default: true.)<br>(synonym: ) |
| LINETYPE | Num | Sets the line type used when plotting the impurity distribution. A solid line and various dotted and dashed line types are available.<br>(unit: )<br>(default: 1 i.e. solid line.)<br>(synonym: ) |
| NET | Log | Specifies that the difference of the sum of the n-type and the sum p-type active or chemical impurity concentrations present in the structure is to be plotted.<br>(unit: )<br>(default: false.) |

| | | |
|---|---|---|
| | | (synonym: ) |
| PHOSPHOR | Log | Specifies that the phosphorus concentration, either active and/or chemical, is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| TITLE | Log | Specifies the title string to be plotted at the top of the the plotted structure.<br>(unit: )<br>(default: Suprem-III-8628)<br>(synonym: ) |
| TOTAL | Log | Specifies that the sum of the active or chemical impurity concentrations present in the structure is to be plotted.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| XMAX | Num | The distance from the top of the plotted layers to the point where the last concentration is to be plotted.<br>(unit: microns.)<br>(default: The current total width of the plotted layers.)<br>(synonym: ) |
| XMIN | Num | The distance from the top of the plotted layers to the point where the first concentration is to be plotted.<br>(unit: microns.)<br>(default: 0.0)<br>(synonym: ) |
| XOFFSET | Num | The distance that the plot is to be offset from the origin of the plot device in the horizontal direction. The value should be normalized to the horizontal width of the plot field with a value between 0 and 1.<br>(unit: )<br>(default: 0.0)<br>(synonym: ) |
| XPWIDTH | Num | The plot width (horizontal direction). This is normalized to the total width of the plot device and should therefore have a value between 0 and 1.<br>(unit: )<br>(default: 1.0)<br>(synonym: ) |
| YOFSET | Num | The distance that the plot is to be offset from the origin of the plot device in the vertical direction. The value should be normalized to the vertical height of the plot field with a value between 0 and 1.<br>(unit: )<br>(default: 1.0)<br>(synonym: ) |
| YPWIDTH | Num | The plot height (vertical direction). This is normalized to the total height of the plot device and should therefore have a value between 0 and 1.<br>(unit: )<br>(default: 1.0.)<br>(synonym: ) |

The PLOT statement is used to output plots of the impurity distributions versus distance in the structure. On a system with full gplot support the user's terminal will be used as the plot device if it has graphics capabilities or the default graphics device will be used if it does not. On a system without full gplot support the device types are limited to those distributed with the code or added by the person providing local Suprem-III support. This person should be contacted for a list of the devices available.

The impurities present may be plotted either individually, added together, or as the difference between n- and p-type dopants. These plots may be of either the electrically active or total chemical concentrations.

By default the entire structure is plotted, however the user may specify those layers that are to be plotted and those layers which are not to be plotted via the various LAYERn parameters (where n is 1 to the maximum number of layers). If it is not negated, the layer parameter specifies that that layer is to be plotted. If it is negated, the layer parameter specifies that the layer is not to be included in the plot. If any layer is negated then all layers not explicitly negated are plotted. If any layer is specified and not negated then only those layers so specified are plotted. If no range parameters (XMIN or XMAX) are specified, then the distributions are plotted over the entire structure. If no minimum or maximum plot concentrations (CMIN or CMAX) are specified, then the range between 1x10ˆ14 and 1x10ˆ21 is plotted.

## 35. Polysilicon Statement

The POLYSILI statement is used to input or modify the characteristics of polycrystalline silicon as a layer material.

```
POLYSILI

  [ NAME=<c> ] [ DX.DEFAU=<n> ]
  [ SEMICOND ]
  [ SPECIES=<n> ] [ DENSITY=<n> ]
  [ AT.WT.1=<n> ] [ AT.NUM.1=<n> ] [ ABUND.1=<n> ]
  [ DIFX.0=<n> ] [ DIFX.E=<n> ]
  [ DIMX.0=<n> ] [ DIFM.E=<n> ]
  [ DIMMX.0=<n> ] [ DIFMM.E=<n> ]
  [ DIFP.0=<n> ] [ DIFP.E=<n> ]
  [ NI.0=<n> ] [ NI.E=<n> ] [ NI.F=<n> ] [ DEFECTLN=<n> ]
  [ OEDK.0=<n> ] [ OEDK.E=<n> ] [ OED.RATE=<n> ]
  [ GSZ.H.0=<n> ] [ GSZ.H.E=<n> ]
  [ GSZ.L.0=<n> ] [ GSZ.L.E=<n> ]
  [ MIN.GRAI=<n> ] [ TEMP.BRE=<n> ]
  [ RATIO.0=<n> ] [ RATIO.E=<n> ]
  [ GEO.FACT=<n> ] [ GBE.0=<n> ] [ GBE.E=<n> ]
  [ TAU.0=<n> ] [ TAU.E=<n> ]
  [ AFFINITY=<n> ] [ EPSILONF=<n> ]
  [ N.VALENC=<n> ] [ N.CONDUC=<n> ] [ BAND.GAP=<n> ]
```

| Name | Type | Description |
|---|---|---|
| ABUND.1 | Num | The relative abundance of element one in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AFFINITY | Num | The electron affinity of the material.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.1 | Num | The atomic number of element one in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.1 | Num | The atomic weight of element one in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| BAND.GAP | Num | The band gap of the material.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DEFECTLN | Num | The decay length of point defects in the material.<br>(unit: microns)<br>(default: the current value.)<br>(synonym: ) |
| DENSITY | Num | The density of the material.<br>(unit: grams/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| DIFM.0 | Num | The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFM.E | Num | The activation energy used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIFMM.0 | Num | The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with doubly negative vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFMM.0 | Num | The activation energy used in the calculation the component of the self-diffusivity due to diffusion with doubly negative vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIFP.0 | Num | The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFP.E | Num | The activation energy used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DIFX.0 | Num | The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| DIFX.E | Num | The activation energy used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DX.DEFAU | Num | The default nominal grid spacing for any layer containing this material.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| EPSILONF | Num | The dielectric constant of the material relative the dielectric constant of air.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GBE.0 | Num | The pre-exponential constant used in calculating the grain-boundary energy<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GBE.E | Num | The activation energy used in calculating the grain-boundary energy.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| GEO.FACT | Num | A geometric factor used in calculating the grain growth driving force, F.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GSZ.H.0 | Num | The pre-exponential constant used in calculating the ‘as deposited’ polysilicon grain size for pressures near one atmosphere.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| GSZ.H.E | Num | The activation energy used in calculating the ‘as deposited’ polysilicon grain size for pressures near one atmosphere.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| GSZ.L.0 | Num | The pre-exponential constant used in calculating the ‘as deposited’ polysilicon grain size for low pressure CVD.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| GSZ.L.E | Num | The activation energy used in calculating the ‘as deposited’ polysilicon grain size for low pressure CVD.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| MIN.GRAI | Num | The minimum polysilicon grain size. Used for ‘as deposited’ LPCVD polysilicon when the temperature is below that specified by TEMP.BRE<br>(unit: microns)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| NAME | Char | The name of the material.<br>(unit: )<br>(default: the current name of the material.)<br>(synonym: ) |
| NI.0 | Num | The pre-factor used in the calculation of the intrinsic carrier concentration.<br>(unit: (carriers/cm^3)(degrees Kelvin)^(3/2).)<br>(default: the current value.)<br>(synonym: ) |
| NI.E | Num | The activation energy used in the calculation of the intrinsic carrier concentration.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| NI.F | Num | The exponent to the absolute temperature used in the calculation of the intrinsic carrier concentration.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| N.CONDUC | Num | The carrier concentration in the conduction band of the material.<br>(unit: carriers/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| N.VALENC | Num | The carrier concentration in the valence band of the material.<br>(unit: carriers/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| OEDK.0 | Num | The pre-exponential constant used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| OEDK.E | Num | The activation energy used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.<br>(unit: electron volts)<br>(default: the current value.)<br>(synonym: ) |
| OED.RATE | Num | The power dependence of oxidation enhanced diffusion on the oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| RATIO.0 | Num | The pre-exponential constant used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the ratio of the pre-exponential factors for the two self-diffusivities<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| RATIO.E | Num | The activation energy used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the difference between the activation energies of the two self-diffusivities<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| SEMICOND | Log | Specifies that the material is a semiconductor.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SPECIES | Num | The number of different elements in this material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| TAU.0 | Num | The pre-exponential constant used to calculate the time dependence of the grain interior concentration.<br>(unit: minutes.)<br>(default: the current value.)<br>(synonym: ) |
| TAU.E | Num | The activation energy used to calculate the time dependence of the grain interior concentration.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| TEMP.BRE | Num | For LPCVD the temperature below which the deposited polysilicon becomes amorphous.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |

The POLYSILI statement is an alias for the MATERIAL statement with an index of three and is used to define or modify the parameters and coefficients associated with the material polysilicon. Not all of the parameters of the MATERIAL statement apply to polysilicon and so are not listed here.

## 36. Print Statement

The PRINT statement outputs information about the structure being simulated and the coefficients used in the simulation. The printed output may consist of the impurity concentrations versus depth into the structure, junction depths, sheet resistivities, layer thicknesses, diffusion or oxidation rates, etc.

```
PRINT

  [ CONCENTR
    [ ACTIVE ] [ CHEMICAL ] [ ALL ] [ TOTAL ] [ NET ]
    [ ANTIMONY ] [ ARSENIC ] [ BORON ] [ PHOSPHOR ]
    [ XMIN=<n> ] [ XMAX=<n> ]
  ]
  [ IMPURITY
     [  ALL
      | ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
     ]
  ]
  [ MATERIAL
     [  ALL
      | ( SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM )
     ]
  ]
  [ LAYERS ] [ SEGREGAT ] [ OXIDATIO ]
  [ LINES/PA=<n> ] [ COLUMNS=<n> ]
  [ LU=<n> | FILENAME=<c> ]
```

| Name | Type | Description |
|---|---|---|
| ACTIVE | Log | Specifies that the electrically active concentration of the specified impurities are to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ALL | Log | Specifies that the impurity coefficient information for all impurities is to be printed, or that the impurity distributions of all impurities present in the structure are to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ALUMINUM | Log | Specifies that the material coefficient information for aluminum is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the antimony concentration, either active or chemical, is to be printed, or that the antimony coefficient information is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |

| | | |
|---|---|---|
| ARSENIC | Log | Specifies that the arsenic concentration, either active or chemical, is to be printed, or that the arsenic coefficient information is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | Log | Specifies that the boron concentration, either active or chemical, is to be printed, or that the boron coefficient information is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| CHEMICAL | Log | Specifies that the chemical concentration of the specified impurities are to be printed.<br>(unit: false.)<br>(default: )<br>(synonym: ) |
| COLUMNS | Num | The number of columns to be used in the printed output.<br>(unit: columns.)<br>(default: 80)<br>(synonym: ) |
| CONCENTR | Log | Causes the specified impurity concentrations versus depth to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| FILENAME | Char | The name of a file to which the information is to be output.<br>(unit: )<br>(default: )<br>(synonym: ) |
| IMPURITY | Log | Specifies that the coefficient information concerning the specified impurities is to be printed (e.g. diffusion coefficients, atomic number and mass, etc.)<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| LAYERS | Log | Specifies that information concerning the layers of the current structure is to be printed (e.g. layer thickness, junction depths, integrated dopant concentrations, etc.)<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| LINES/PA | Num | The number of lines per page in the printed output.<br>(unit: lines/page.)<br>(default: 60)<br>(synonym: ) |
| LU | Num | The logical unit number to which the information is to be output.<br>(unit: )<br>(default: the standard output lu.)<br>(synonym: ) |

| | | |
|---|---|---|
| MATERIAL | Log | Specifies that the coefficient information concerning the specified materials is to be printed (e.g. band gap, intrinsic carrier concentration coefficients, electric stopping powers, etc.)<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| NET | Log | Specifies that the sum of the n-type minus the sum of the p-type active or chemical impurity concentrations are to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material coefficient information for silicon nitride is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDATIO | Log | Specifies that the coefficients that determine the oxidation of silicon, polysilicon and silicon nitride are to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material coefficient information for silicon dioxide is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the phosphorus concentration, either active or chemical, is to be printed, or that the phosphorus coefficient information is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material coefficient information for polysilicon is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SEGREGAT | Log | Specifies that the coefficients that determine the segregation of impurities across material interfaces are to be printed. The mass transport coefficients and the volume ratios are also printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material coefficient information for single crystal silicon is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| TOTAL | Log | Specifies that the sum of all of the active or chemical impurity concentrations present in the structure is to be printed.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| XMAX | Num | The distance from the top of the structure to the point where the last concentration is to be printed.<br>(unit: microns.)<br>(default: The current depth of the structure.)<br>(synonym: ) |
| XMIN | Num | The distance from the top of the structure to the point where the first concentration is to be printed.<br>(unit: microns.)<br>(default: 0.0)<br>(synonym: ) |

The PRINT statement is used to output printed information. This information may consist of structural information such as junction depths, layer thicknesses or various impurity distributions versus distance in the structure, or coefficient information such as the coefficients for impurity diffusion or segregation, the oxidation of silicon, or the atomic number and mass of impurities or materials.

The impurities present may be printed either individually, added together, or as the difference between n- and p-type dopants. These prints may be of either electrically or total chemical concentrations. If no range is specified, then the distributions are printed over the entire structure.

Normally the output of the print statement goes to the standard output device (usually the line printer), but the user may override the output logical unit number by specifying the output lu, or he may direct it into a specified file.

## 37. Profile Statement

The PROFILE statement is used to input an arbitrary impurity profile from a data file. The data must be stored as two columns, one being the distance from the origin and the other being the concentration at that point.

```
PROFILE

  FILE=<c>  CONC.COL=<n>  X.COL=<n>  [ LAYER=<n> ]
            [ SKIP=<n> ]  [ COUNT=<n> ]  [ COM.CHAR=<c> ]
  ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
```

| Name | Type | Description |
|---|---|---|
| ANTIMONY | log | Specifies that the profile data is for the dopant antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | log | Specifies that the profile data is for the dopant arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | log | Specifies that the profile data is for the dopant boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| COM.CHAR | Char | Specifies the comment character for the lines in the file. Any line with this character in column one is ignored.<br>(unit: )<br>(default: *)<br>(synonym: ) |
| CONC.COL | Num | Specifies the column in the file containing the concentration data.<br>(unit: )<br>(default: )<br>(synonym: ) |
| COUNT | Num | Specifies the number of data points to be input.<br>(unit: )<br>(default: Input all data points.)<br>(synonym: ) |
| LAYER | Num | Specifies the layer at which the first data point is to be placed.<br>(unit: )<br>(default: Topmost layer.)<br>(synonym: ) |
| PHOSPHOR | log | Specifies that the profile data is for the dopant phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| SKIP | Num | Specifies the number of data points to be skipped on input.<br>(unit: )<br>(default: 0)<br>(synonym: ) |
| X.COL | Num | Specifies the column in the file containing the distance of each data point from the origin.<br>(unit: )<br>(default: )<br>(synonym: ) |

The PROFILE statement inputs an arbitrary impurity distribution of the specified dopant from a data file. The data files must be organized in columns, with one column containing the concentration data and another containing the distance from the origin at which the corresponding concentration applies. The data in the columns must be organized such that the locations are in increasing order. Comment lines may appear at any point as long as they are preceded the comment character in column one.

## 38. Resistivity Statement

The RESISTIVITY statement is used to input a table of ordered resistivity/concentration pairs. This data is used by the program to calculate the resistivity of diffused layers in the current structure.

```
RESISTIVITY

  FILE=<c>  CONC.COL=<n>  RES.COL=<n>
                 [ SKIP=<n> ]  [ COUNT=<n> ]  [ COM.CHAR=<c> ]
  ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  ( ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON )
```

| Name | Type | Description |
|---|---|---|
| ALUMINUM | Log | Specifies that the resistivity data applies to the impurity in the material aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the resistivity data applies to the dopant antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | Log | Specifies that the resistivity data applies to the dopant arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | Log | Specifies that the resistivity data applies to the dopant boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| COM.CHAR | Char | Specifies the comment character for the lines in the file. Any line with this character in column one is ignored.<br>(unit: )<br>(default: *)<br>(synonym: ) |
| CONC.COL | Num | Specifies the column in the data file containing the concentrations at which the resistivity data applies.<br>(unit: )<br>(default: )<br>(synonym: CON.COL) |
| COUNT | Num | Specifies the number of data points to be input.<br>(unit: )<br>(default: Input all every data point.)<br>(synonym: ) |

| | | |
|---|---|---|
| NITRIDE | Log | Specifies that the resistivity data applies to the impurity in the material nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the resistivity data applies to the impurity in the material oxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the resistivity data applies to the dopant phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the resistivity data applies to the impurity in the material polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| RES.COL | Num | Specifies the column in the data file containing the resistivities associated with the corresponding concentration values.<br>(unit: )<br>(default: )<br>(synonym: ) |
| SKIP | Num | Specifies the number of data points to be skipped on input.<br>(unit: )<br>(default: 0)<br>(synonym: ) |
| SILICON | Log | Specifies that the resistivity data applies to the impurity in the material silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The RESISTIVITY statement inputs the resistivity vs. concentration data from the specified file and associates it with one or more impurities in one or more materials. The data files must be organized in columns, with one column containing the resistivity values and another containing corresponding impurity concentrations. The data in the columns must be organized such that the concentration values are in increasing order. Comment lines may appear at any point as long as they are preceded with the comment character in column one.

## 39. Savefile Statement

The SAVEFILE statement is used to save either the current structure being processed, the physical and model coefficients being used, or both.

```
SAVEFILE

 FILENAME=<c> ( ALL | COEFFICI | STRUCTUR | EXPORT )
 [ FORMATTE ]
```

| Name | Type | Description |
|---|---|---|
| ALL | Log | Specifies that both the structure information and the model coefficients are to be written to the specified file.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| COEFFICI | Log | Specifies that the coefficient information is to be written to the specified file.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| EXPORT | Log | Specifies that the structure information be written in export format for use by a post-processor or device simulation program such as SEDAN-II or PISCES-II<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| FILENAME | Char | The name of the file to which the specified information is to be written.<br>(unit: )<br>(default: )<br>(synonym: NAME) |
| FORMATTE | Log | Specifies that the information is to be formatted on output, if not specified then the information will be output will be unformatted or binary.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| STRUCTUR | Log | Specifies that the information describing the current structure is to be written to the specified file.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

The SAVEFILE statement saves two classes of information. One is class contains all of the physical and model parameters or coefficients used by the program. A file containing this information is used by the INITIALIZATION statement at the beginning of each processing sequence to initialize the program. The other class of information contains the physical structure and impurity distributions of the materials being simulated. There are two types of files that can be written containing this class of information. One, the structure file, may be used as the starting point for subsequent processing simulations in order to model process run splits or examine process sensitivity. The other is the export file which stores the current structure information in a format that is designed to be read by either post-processors or device simulation programs such as SEDAN-II or PISCES-II.

The information stored by the SAVEFILE statement, except for export files, can be read into the program either by the INITIALIZE statement at the start of a process, or at any time by a LOADFILE statement.

## 40. Segregation Statement

The SEGREGAT statement is used to define or modify the impurity segregation coefficient and the impurity transport coefficient across the interface between two material layers.

```
SEGREGAT

  (  ( SILICON
       [ 100.FACT=<n> ] [ 110.FACT=<n> ] [ 111.FACT=<n> ]
     )
   |  OXIDE | POLYSILI | NITRIDE | ALUMINUM | AIR
  )
  (  ( /SILICON
       [ 100.FACT=<n> ] [ 110.FACT=<n> ] [ 111.FACT=<n> ]
     )
   |  /OXIDE | /POLYSIL | /NITRIDE | /ALUMINU | /AIR
  )
  ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  [ SEG.0=<n> ] [ SEG.E=<n> ]
  [ TRANS.0=<n> ] [ TRANS.E=<n> ]
              [ MAX.0=<n> ] [ MAX.E=<n> ]
              [ ( MODEL.1 | MODEL.2 ) ]
  [ MUI.0=<n> ] [ MUI.E=<n> ]
              [ GRATE.0=<n> ] [ GRATE.E=<n> ]
              [ C.INIT=<n> ] [ C.THRESH=<n> ] [ L.THICK=<n> ]
```

| Name | Type | Description |
|---|---|---|
| AIR | Log | Specifies that the material above the interface is the ambient gas.<br>(unit: )<br>(default: false.)<br>(synonym: AMBIENT) |
| ALUMINUM | Log | Specifies that the material above the interface is aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | Log | Specifies that the coefficients apply to the dopant antimony.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ARSENIC | Log | Specifies that the coefficients apply to the dopant arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| BORON | Log | Specifies that the coefficients apply to the dopant boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| C.INIT | Num | Specifies the initial interface concentration level to be used in calculating model 2 segregation effects.<br>(unit: atoms/cc)<br>(default: the current value.)<br>(synonym: ) |
| C.THRESH | Num | Specifies the bulk concentration minimum threshold for model 2.<br>(unit: atoms/cc)<br>(default: the current value.)<br>(synonym: ) |
| GRATE.0 | Num | Specifies the pre-exponential constant of the rate of the interface pile up for model 2.<br>(unit: atoms/cc/minute)<br>(default: the current value.)<br>(synonym: ) |
| GRATE.E | Num | Specifies the activation energy of the rate of the interface pile up for model 2.<br>(unit: electron volts)<br>(default: the current value.)<br>(synonym: ) |
| L.THICK | Num | The effective thickness of the pile up region at the interface for model 2.<br>(unit: microns)<br>(default: the current value.)<br>(synonym: ) |
| MAX.0 | Num | The pre-exponential factor for the maximum concentration level at the interface.<br>(unit: atoms/cc)<br>(default: the current value.)<br>(synonym: ) |
| MAX.E | Num | The activation energy for the maximum concentration level at the interface.<br>(unit: electron volts)<br>(default: the current value.)<br>(synonym: ) |
| MODEL.1 | Log | Specifies that model 1, (Barton's model), is to be used for this impurity/material combination.<br>(unit: )<br>(default: false)<br>(synonym: ) |
| MODEL.2 | Log | Specifies that model 2, (Shone's model), is to be used for this impurity/material combination.<br>(unit: )<br>(default: false)<br>(synonym: ) |
| MUI.0 | Num | The pre-exponential factor for the chemical potential segregation term.<br>(unit: microns)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| MUI.E | Num | The activation energy for the chemical potential segregation term.<br>(unit: electron volts)<br>(default: the current value.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the material above the interface is silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the material above the interface is silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PHOSPHOR | Log | Specifies that the specified coefficients apply to the dopant phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the material above the interface is polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SEG.0 | Num | The pre-exponential factor of the segregation coefficient.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| SEG.E | Num | The activation energy of the segregation coefficient.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| SILICON | Log | Specifies that the material above the interface is single crystal silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| TRANS.0 | Num | The pre-exponential factor of the interface transport coefficient.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| TRANS.E | Num | The activation energy of the interface transport coefficient.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| /AIR | Log | Specifies that the material below the interface is air.<br>(unit: )<br>(default: false.)<br>(synonym: AMBIENT) |
| /ALUMINU | Log | Specifies that the material below the interface is aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| /NITRIDE | Log | Specifies that the material below the interface is silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| /OXIDE | Log | Specifies that the material below the interface is silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| /POLYSIL | Log | Specifies that the material below the interface is polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| /SILICON | Log | Specifies that the material below the interface is single crystal silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| 100.FACT | Num | The orientation factor of the impurity’s segregation coefficient for <100> orientation silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| 110.FACT | Num | The orientation factor of the impurity’s segregation coefficient for <110> orientation silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| 111.FACT | Num | The orientation factor of the impurity’s segregation coefficient for <111> orientation silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

The SEGREGAT statement defines those parameters that have to do with transport of impurities across material interfaces. The impurity type must be specified as well as the the material types on either side of the interface. The material above the interface is specified simply by name, while the material below the interface is specified by its name preceded by a slash ‘/’.

Where a parameter or quantity applies to only one side of a given interface, the parameter will apply to the side with the material that is not preceded by a slach ‘/’.

## 41. Silicon Statement

The SILICON statement is used to input or modify the characteristics of single crystal silicon as a layer material.

```
SILICON

   [ NAME=<c> ] [ DX.DEFAU=<n> ]
   [ SEMICOND ]
   [ SPECIES=<n> ] [ DENSITY=<n> ]
   [ AT.WT.1=<n> ] [ AT.NUM.1=<n> ] [ ABUND.1=<n> ]
   [ NI.0=<n> ] [ NI.E=<n> ] [ NI.F=<n> ] [ DEFECTLN=<n> ]
   [ OEDK.0=<n> ] [ OEDK.E=<n> ] [ OED.RATE=<n> ]
   [ 100.OEDF=<n> ] [ 110.OEDF=<n> ] [ 111.OEDF=<n> ]
   [ AFFINITY=<n> ] [ EPSILONF=<n> ]
   [ N.VALENC=<n> ] [ N.CONDUC=<n> ] [ BAND.GAP=<n> ]
   [ K.M=<n> ]
```

| Name | Type | Description |
|---|---|---|
| ABUND.1 | Num | The relative abundance of element one in the material. The sum of all abundances for a material must equal one.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AFFINITY | Num | The electron affinity of the material.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| AT.NUM.1 | Num | The atomic number of element one in the material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| AT.WT.1 | Num | The atomic weight of element one in the material.<br>(unit: amu)<br>(default: the current value.)<br>(synonym: ) |
| BAND.GAP | Num | The band gap of the material.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| DEFECTLN | Num | The decay length of point defects in the material.<br>(unit: microns)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| DENSITY | Num | The density of the material.<br>(unit: grams/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| DX.DEFAU | Num | The default nominal grid spacing for any layer containing this material.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| EPSILONF | Num | The dielectric constant of the material relative the dielectric constant of air.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| K.M | Num | Used in R. Reif's epitaxial growth model (see reference in EPITAXY statement). K.m is the mass transport coefficient for silane in hydrogen.<br>(unit: microns/minute/atmosphere)<br>(default: the current value)<br>(synonym: ) |
| NAME | Char | The name of the material.<br>(unit: )<br>(default: the current name of the material.)<br>(synonym: ) |
| NI.0 | Num | The pre-factor used in the calculation of the intrinsic carrier concentration.<br>(unit: (carriers/cm^3)(degrees Kelvin)^(3/2).)<br>(default: the current value.)<br>(synonym: ) |
| NI.E | Num | The activation energy used in the calculation of the intrinsic carrier concentration.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| NI.F | Num | The exponent to the absolute temperature used in the calculation of the intrinsic carrier concentration.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| N.CONDUC | Num | The carrier concentration in the conduction band of the material.<br>(unit: carriers/cm^3.)<br>(default: the current value.)<br>(synonym: ) |
| N.VALENC | Num | The carrier concentration in the valence band of the material.<br>(unit: carriers/cm^3.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| OEDK.0 | Num | The pre-exponential constant used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| OEDK.E | Num | The activation energy used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.<br>(unit: electron volts)<br>(default: the current value.)<br>(synonym: ) |
| OED.RATE | Num | The power dependence of oxidation enhanced diffusion on the oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| SEMICOND | Log | Specifies that the material is a semiconductor.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SPECIES | Num | The number of different elements in this material.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| 100.OEDF | Num | The orientation dependent factor for oxidation enhanced diffusion for <100> oriented silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| 110.OEDF | Num | The orientation dependent factor for oxidation enhanced diffusion for <110> oriented silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| 111.OEDF | Num | The orientation dependent factor for oxidation enhanced diffusion for <111> oriented silicon.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |

The SILICON statement is an alias for the MATERIAL statement with an index of one and is used to define or modify the parameters and coefficients associated with the material silicon. Not all of the parameters of the MATERIAL statement apply to silicon and so are not listed here.

## 42. Solubility Statement

The SOLUBILITY statement is used to input a table of ordered temperature/solubility pairs. This data is used by the program to calculate the solid solubility of the various impurities in the materials present in the structure.

SOLUBILITY

FILE=<c> CONC.COL=<n> TEMP.COL=<n>
[ SKIP=<n> ] [ COUNT=<n> ] [ COM.CHAR=<c> ]
( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
( ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON )

| Name | Type | Description |
|---|---|---|
| ALUMINUM | log | Specifies that the solubility data applies to the impurity in the material aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| ANTIMONY | log | Specifies that the solubility data applies to the dopant antimony.<br>(unit: )<br>(default: false.)<br>(synonym: SB) |
| ARSENIC | log | Specifies that the solubility data applies to the dopant arsenic.<br>(unit: )<br>(default: false.)<br>(synonym: AS) |
| BORON | log | Specifies that the solubility data applies to the dopant boron.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| COM.CHAR | Char | Specifies the comment character for the lines in the file. Any line with this character in column one is ignored.<br>(unit: )<br>(default: *)<br>(synonym: ) |
| CONC.COL | Num | Specifies the column in the data file containing the solubility associated with the corresponding temperature value.<br>(unit: )<br>(default: )<br>(synonym: ) |
| COUNT | Num | Specifies the number of data points to be input.<br>(unit: )<br>(default: Input all every data point.)<br>(synonym: ) |

| | | |
|---|---|---|
| NITRIDE | log | Specifies that the solubility data applies to the impurity in the material nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | log | Specifies that the solubility data applies to the impurity in the material oxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| PHOSPHOR | log | Specifies that the solubility data applies to the dopant phosphorus.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | log | Specifies that the solubility data applies to the impurity in the material polysilicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| SKIP | Num | Specifies the number of data points to be skipped on input.<br>(unit: )<br>(default: 0)<br>(synonym: ) |
| SILICON | log | Specifies that the solubility data applies to the impurity in the material silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| TEMP.COL | Num | Specifies the column in the data file containing the temperature associated with the corresponding solubility values.<br>(unit: )<br>(default: )<br>(synonym: ) |

The SOLUBILITY statement inputs the solubility vs. temperature data from the specified file and associates it with one or more impurities in one or more materials. The data files must be organized in columns, with one column containing the temperature values and another containing corresponding solubility concentrations. The data in the columns must be organized such that the temperature values are in increasing order. Comment lines may appear at any point as long as they are preceded the comment character in column one.

## 43. Stop Statement

The STOP statement terminates the SUPREM-III execution.

```
STOP  [ <c> ]
```

The STOP statement is usually the last statement in the input stream. Any statements following an STOP statement are ignored by the program. The optional character string on the STOP statement is ignored by the program and is used for input documentation purposes only.

## 44. Title Statement

The TITLE statement is used to input a character string to label the following input sequence.

TITLE [ <c> ]

The character string associated with the TITLE statement is output to the standard output device. If the previous statement was not either another TITLE statement nor a COMMENT statement, then a top-of-form is issued before the character string is output.

## 45. Vol.Ratio Statement

The VOL.RATIO statement is used to set the volume ratio between two materials, where one material might be converted into the material as in silicon to silicon dioxide.

```
VOL.RATIO

  ( SILICON | OXIDE | POLYSILI | NITRIDE | ALUMINUM )
  ( /SILICON | /OXIDE | /POLYSIL | /NITRIDE | /ALUMINUM )
  RATIO=<n>
```

| Name | Type | Description |
| --- | --- | --- |
| ALUMINUM | Num | Specifies that the constant is the volume ratio of aluminum to the other material specified.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| NITRIDE | Log | Specifies that the constant is the volume ratio of silicon nitride to the other material specified.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| OXIDE | Log | Specifies that the constant is the volume ratio of silicon dioxide to the other material specified.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| POLYSILI | Log | Specifies that the constant is the volume ratio of polycrystalline silicon to the other material specified.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| RATIO | Num | The volume ratio between the materials specified.<br>(unit: )<br>(default: the current value.)<br>(synonym: CONSTANT) |
| SILICON | Log | Specifies that the constant is the volume ratio of silicon to the other material specified.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| /ALUMINU | Log | Specifies that the constant is the volume ratio of the other material specified to aluminum.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

| | | |
|---|---|---|
| /NITRIDE | Log | Specifies that the constant is the volume ratio of the other material specified to silicon nitride.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| /OXIDE | Log | Specifies that the constant is the volume ratio of the other material specified to silicon dioxide.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| /POLYSIL | Log | Specifies that the constant is the volume ratio of the other material specified to polycrystalline silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| /SILICON | Log | Specifies that the constant is the volume ratio of the other material specified to silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |

When oxidizing silicon, whether single crystal, poly crystalline, or silicon nitride, the oxide formed may have a different volume from that of the original material. The ratio between the volume of the original material and the resulting oxide is needed for modeling the moving interface during oxidation.

The ratio between any of the materials defined in the program can be specified, but only those between the various silicon forms and silicon dioxide are used by the program.

## 46. V.Threshold Statement

The V.THRESHOLD statement is used to calculate and print out the threshold voltage as a function of substrate bias for the current structure.

```
V.THRESHOLD

  [ V.SUB1=<n> ] [ V.SUB2=<n> ] [ DV.SUB=<n> ]
  [ (SURFACE | BACKSIDE | (BULKCONC=<n> (PTYPE | NTYPE))) ]
  [ Q.F=<n> ] [ TEMPERAT=<n> ]
            [ FILENAME=<c> [ APPEND ] ]
```

| Name | Type | Description |
|---|---|---|
| APPEND | log | Specifies that the threshold voltage data is to be appended to the specified file. Otherwise the data will appear at the beginning of the file, deleting the previous contents of the file, if any.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| BACKSIDE | log | Specifies that the substrate bias contact is at the backside of the wafer. This causes the concentration at the last or bottommost point in the current structure to be used as the concentration at the point of contact.<br>(unit: )<br>(default: true)<br>(synonym: ) |
| BULKCONC | Num | Specifies the net active impurity concentration at the substrate bias contact.<br>(unit: atoms/centimeter^3)<br>(default: )<br>(synonym: ) |
| DV.SUB | Num | The incremental substrate bias voltage. The threshold and punchthrough calculations will be done at substrate bias voltages from V.SUB1 to V.SUB2 in DV.SUB steps. At most 20 steps will be attempted.<br>(unit: volts)<br>(default: 0.5)<br>(synonym: ) |
| FILENAME | Char | Specifies the name of a file in which the calculated threshold and punchthrough voltages as a function of substrate bias are to be output. If no file is specified the data is output to the standard output.<br>(unit: )<br>(default: )<br>(synonym: ) |
| NTYPE | log | Specifies that the majority impurity type at the bulk contact is n-type. Used only in conjunction with the BULKCONC parameter.<br>(unit: )<br>(default: false.)<br>(synonym: N-TYPE) |

| | | |
|---|---|---|
| PTYPE | log | Specifies that the majority impurity type at the bulk contact is p-type. Used only in conjunction with the BULKCONC parameter.<br>(unit: )<br>(default: false.)<br>(synonym: P-TYPE) |
| Q.F | Num | Specifies the fixed oxide charge density.<br>(unit: charges/unit area)<br>(default: 0.0)<br>(synonym: Q.SS) |
| SURFACE | log | Specifies that the substrate bias contact is at the top surface of the wafer. This causes the concentration at the first or topmost point in the current structure to be used as the concentration at the point of contact.<br>(unit: )<br>(default: true)<br>(synonym: ) |
| TEMPERAT | Num | The calculations are done assuming that the device is operating at the temperature specified.<br>(unit: degrees centigrade)<br>(default: 27.0)<br>(synonym: ) |
| V.SUB1 | Num | The initial substrate bias voltage used in calculating the threshold and punchthrough voltages. The threshold and punchthrough calculations will be done at substrate bias voltages from V.SUB1 to V.SUB2 in DV.SUB steps. At most 20 steps will be attempted.<br>(unit: volts)<br>(default: 0.0)<br>(synonym: ) |
| V.SUB2 | Num | The final substrate bias voltage used in calculating the threshold and punchthrough voltages. The threshold and punchthrough calculations will be done at substrate bias voltages from V.SUB1 to V.SUB2 in DV.SUB steps. At most 20 steps will be attempted.<br>(unit: volts)<br>(default: 5.0)<br>(synonym: ) |

The V.THRESHOLD statement calculates the threshold and punchthrough voltages for the current structure at one or more substrate biases. A MIS structure must exist for the calculations to be performed. If more than one substrate bias point is desired, then the first and last and optionally the increment bias voltages are specified. The oxide fixed charge density and the substrate bias contact point may also be specified.

Normally the results of the V.THRESHOLD calculations are output to the standard output, however if a file is specified, the results are instead sent to that file. The results of several V.THRESHOLD calculations may be sent to the same file if the APPEND parameter is used.

An explanation of the algorithm used by the V.THRESHOLD statement can be found in ‘Calculation of Threshold Voltage in Nonuniformly Doped MOSFETS’, by D. A. Antoniadis, IEEE Trans. E. D., Vol. ED-31, No. 3, March 1984, pp 303-307.

## 47. WetO2 Statement

The WETO2 statement allows the user to modify the coefficients used to model the oxidation of the various materials under wet ambient oxidation conditions.

```
WETO2

  [ ( <111> | <110> | <100> )
    [ LIN.L.0=<n> ] [ LIN.L.E=<n> ]
    [ LIN.H.0=<n> ] [ LIN.H.E=<n> ]
    [ THINOX.0=<n> ] [ THINOX.E=<n> ] [ THINOX.L=<n> ]
  ]
  [ PAR.L.0=<n> ] [ PAR.L.E=<n> ]
  [ PAR.H.0=<n> ] [ PAR.H.E=<n> ]
  [ LIN.BREA=<n> ] [ PAR.BREA=<n> ]
  [ LIN.PDEP=<n> ] [ PAR.PDEP=<n> ]
  [ PRESSURE=<n> ] [ HCL%=<n> ]
  [ GAMMA.0=<n> ] [ GAMMA.E=<n> ]
  [ DELTA.0=<n> ] [ DELTA.E=<n> ]
  [ EXP.0=<n> ] [ EXP.E=<n> ]
  [ NIOX.0=<n> ] [ NIOX.E=<n> ] [ NIOX.F=<n> ]
  [ CL.ROW=<n> [ CL.PCT=<n> ]
    CL.COLUM=<n> [ CL.TEMPE=<n> ]
    [ CL.DEP.L=<n> ] [ CL.DEP.P=<n> ]
  ]
```

| Name | Type | Description |
|---|---|---|
| CL.COLUM | Num | The column number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.DEP.L | Num | The coefficient modifying the linear oxidation rate in the presence of chlorine at the specified row and column.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.DEP.P | Num | The coefficient modifying the parabolic oxidation rate in the presence of chlorine at the specified row and column.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.PCT | Num | The percentage of chlorine for which the coefficients in the specified row are valid.<br>(unit: percent.)<br>(default: the current value.)<br>(synonym: ) |

| | | |
|---|---|---|
| CL.ROW | Num | The row number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| CL.TEMPE | Num | The temperature for which the coefficients in the specified column are valid.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |
| DELTA.0 | Num | The pre-exponential factor of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: cmˆ3/atom.)<br>(default: the current value.)<br>(synonym: ) |
| DELTA.E | Num | The activation energy of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| EXP.0 | Num | The pre-exponential factor of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| EXP.E | Num | The activation energy of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| GAMMA.0 | Num | The pre-exponential factor of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| GAMMA.E | Num | The activation energy of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| HCL% | Num | The default percentage of chlorine present in the ambient.<br>(unit: percent.)<br>(default: the current value.)<br>(synonym: ) |
| LIN.BREA | Num | The temperature at which the temperature dependence of the linear oxidation rate changes.<br>(unit: degrees Centigrade.)<br>(default: the current value.)<br>(synonym: ) |

LIN.H.0 Num The pre-exponential constant of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.
(unit: microns/minute.)
(default: the current value.)
(synonym: )

LIN.H.E Num The activation energy of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.
(unit: electron volts.)
(default: the current value.)
(synonym: )

LIN.L.0 Num The pre-exponential constant of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.
(unit: microns/minute.)
(default: the current value.)
(synonym: )

LIN.L.E Num The activation energy of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.
(unit: electron volts.)
(default: the current value.)
(synonym: )

LIN.PDEP Num The pressure dependence factor for the linear oxidation rate.
(unit: )
(default: the current value.)
(synonym: )

NIOX.0 Num The pre-exponential constant used to determine the oxidation rate of silicon nitride.
(unit: microns.)
(default: the current value.)
(synonym: )

NIOX.E Num The activation energy used to determine the oxidation rate of silicon nitride.
(unit: electron volts.)
(default: the current value.)
(synonym: )

NIOX.F Num The exponent factor used to determine the oxidation rate of silicon nitride.
(unit: )
(default: the current value.)
(synonym: )

PAR.BREA Num The temperature at which the temperature dependence of the parabolic oxidation rate changes.
(unit: degrees Centigrade.)
(default: the current value.)
(synonym: )

PAR.H.0 Num The pre-exponential constant of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.
(unit: microns^2/minute.)
(default: the current value.)
(synonym: )

| | | |
|---|---|---|
| PAR.H.E | Num | The activation energy of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.L.0 | Num | The pre-exponential constant of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.<br>(unit: microns^2/minute.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.L.E | Num | The activation energy of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| PAR.PDEP | Num | The pressure dependence factor for the parabolic oxidation rate.<br>(unit: )<br>(default: the current value.)<br>(synonym: ) |
| PRESSURE | Num | The default ambient pressure. (See note below.)<br>(unit: atmospheres.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.0 | Num | The pre-exponential constant of the thin oxide growth rate parameter.<br>(unit: microns/minute.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.E | Num | The activation energy of the thin oxide growth rate parameter.<br>(unit: electron volts.)<br>(default: the current value.)<br>(synonym: ) |
| THINOX.L | Num | The characteristic length of the thin oxide growth rate parameter.<br>(unit: microns.)<br>(default: the current value.)<br>(synonym: ) |
| <100> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <100> orientation silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <110> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <110> orientation silicon.<br>(unit: )<br>(default: false.)<br>(synonym: ) |
| <111> | Log | Specifies that the linear growth rate and thin oxide growth rate parameters apply to <111> orientation silicon.<br>(unit: )<br>(default: false.) |

(synonym: )

The three oxidation model statements, DRYO2, WETO2, and NITROGEN, use identical parameters, differing only in the values assigned. The parameters NIOX.C, NIOX.E, and NIOX.F are used in modeling the oxidation silicon nitride while the others deal with the oxidation of single and polycrystalline silicon.

The effects of chlorine in the ambient gas on the oxidation rate of silicon are currently modeled by an empirical expression whose only variable is defined by the L.CLDEP and P.CLDEP for the linear and parabolic rates respectively. To date no convenient function is available to calculate the chlorine dependence as a function of temperature and amount of chlorine present, therefor a table of values defines the chlorine dependence factors at those temperatures and percentages for which reliable data is available. For those temperatures and chlorine percentages between the values in the table, linear interpolation is employed to calculate the value used. For temperatures or percentages outside the range of values present in the table, the values whose conditions most nearly match the current conditions are used. For example, if the current conditions are a temperature of 1175 degrees with three percent chlorine, but the highest temperature entry in the table is 1150 degrees and the nearest chlorine percentages are for two and four percent, then a value halfway between the values at 1150 degrees and two and four percent chlorine will be used.

NOTE: The effective oxidant partial pressure for pyrogenic steam reactors has been found to vary significantly from facility to facility. It is recommended that the user set the default pressure for WetO2 to a value that gives the best agreement with measured oxide thicknesses from his facility.

## 48. Statement Summary

ALUMINUM

```
[ NAME=<c> ] [ DX.DEFAU=<n> ]
[ CONDUCTO ]
[ SPECIES=<n> ] [ DENSITY=<n> ]
[ AT.WT.1=<n> ] [ AT.NUM.1=<n> ] [ ABUND.1=<n> ]
[ WORK.FUN=<n> ] [ EPSILONF=<n> ]
```

ANTIMONY

```
[ NAME=<c> ] [ DONOR ]
[ AT.WT=<n> ] [ AT.NUMB=<n> ]
[ IONFILE1=<c> ] [ IONFILE2=<c> ]
[ (  ( SILICON
                [ FII.0=<n> ] [ FII.E=<n> ]
                [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
     )
   | ( POLYSILI
                [ FII.0=<n> ] [ FII.E=<n> ]
      [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
     )
   | ( OXIDE | NITRIDE | ALUMINUM )
  [ ELECT.ST=<n> ]
  [ DIX.0=<n> ] [ DIX.E=<n> ]
  [ DIM.0=<n> ] [ DIM.E=<n> ]
  [ DIMM.0=<n> ] [ DIMM.E=<n> ]
]
```

```
ARSENIC

  [ NAME=<c> ] [ DONOR ]
  [ AT.WT=<n> ] [ AT.NUMB=<n> ]
  [ IONFILE1=<c> ] [ IONFILE2=<c> ]
  [ (  ( SILICON
        [ FII.0=<n> ] [ FII.E=<n> ]
                          [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
        [ ( IMPLANT | CHEMICAL )
          [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
        ]
      )
    | ( POLYSILI
        [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
        [ FII.0=<n> ] [ FII.E=<n> ]
        [ ( IMPLANT | CHEMICAL )
            [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
        ]
      )
    | ( OXIDE | NITRIDE | ALUMINUM )
    [ ELECT.ST=<n> ]
    [ DIX.0=<n> ] [ DIX.E=<n> ]
    [ DIM.0=<n> ] [ DIM.E=<n> ]
    [ DIMM.0=<n> ] [ DIMM.E=<n> ]
  ]


BIAS

  LAYER=<n>
    ( [ V.ELECTR=<n> ] [ DV.ELECTR=<n> ] )
  | (  ( [ DIFFUSIO=<n> ]
        [ V.MAJORI=<n> ] [ DV.MAJOR=<n> ]
        [ V.MINORI=<n> ] [ DV.MINOR=<n> ]
      )
     |  [ FLOAT ]
    )
```

```
BORON

   [ NAME=<c> ] [ ACCEPTOR ]
   [ AT.WT=<n> ] [ AT.NUMB=<n> ]
   [ IONFILE1=<c> ] [ IONFILE2=<c> ]
   [ (  ( SILICON
          [ FII.0=<n> ] [ FII.E=<n> ]
                            [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
        )
      | ( POLYSILI
          [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
          [ FII.0=<n> ] [ FII.E=<n> ]
        )
      | ( OXIDE | NITRIDE | ALUMINUM )
     [ ELECT.ST=<n> ]
     [ DIX.0=<n> ] [ DIX.E=<n> ]
     [ DIP.0=<n> ] [ DIP.E=<n> ]
   ]


COMMENT  [<c>]
or
$       [<c>]


DEPOSITION

   THICKNES=<n>
   (  SILICON ( <111> | <110> | <100> )
    | POLYSILI
         TEMPERAT=<n> [ PRESSURE=<n> | GRAINSIZ=<n> ]
    | OXIDE
    | NITRIDE
    | ALUMINUM
   )
   [ DX=<n> ] [ XDX=<n> ] [ SPACES=<n> ] [ MIN.DX=<n> ]
                        [ CONCENTRATION=<n>
     (ANTIMONY | ARSENIC | BORON | PHOSPHOR)
   ]


DIFFUSION

   TIME=<n> TEMPERAT=<n> [ T.RATE=<n> ]
   [ ( GAS.CONC=<n> | SOLIDSOL )
     ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
   ]
   [ ( DRYO2 | WETO2 | NITROGEN )
     [ PRESSURE=<n> ] [ P.RATE=<n> ] [ HCL%=<n> ]
   ]
   [ DTMIN=<n> ] [ DTMAX=<n> ]
   [ ABS.ERR=<n> ] [ REL.ERR=<n> ]
```

DRYO2

```
[ ( <111> | <110> | <100> )
  [ LIN.L.0=<n> ] [ LIN.L.E=<n> ]
  [ LIN.H.0=<n> ] [ LIN.H.E=<n> ]
  [ THINOX.0=<n> ] [ THINOX.E=<n> ] [ THINOX.L=<n> ]
]
[ PAR.L.0=<n> ] [ PAR.L.E=<n> ]
[ PAR.H.0=<n> ] [ PAR.H.E=<n> ]
[ LIN.BREA=<n> ] [ PAR.BREA=<n> ]
[ LIN.PDEP=<n> ] [ PAR.PDEP=<n> ]
[ PRESSURE=<n> ] [ HCL%=<n> ]
[ GAMMA.0=<n> ] [ GAMMA.E=<n> ]
[ DELTA.0=<n> ] [ DELTA.E=<n> ]
[ EXP.0=<n> ] [ EXP.E=<n> ]
[ NIOX.0=<n> ] [ NIOX.E=<n> ] [ NIOX.F=<n> ]
[ CL.ROW=<n> [ CL.PCT=<n> ]
  CL.COLUM=<n> [ CL.TEMPE=<n> ]
  [ CL.DEP.L=<n> ] [ CL.DEP.P=<n> ]
]
```

ELECTRICAL

```
[ STEPS=<n> ] [ EXTENT=<n> ] [ TEMPERAT=<n> ]
[ ERROR=<n> ] [ MAX.ITER=<n> ] [ FILE.OUT=<c> ]
```

```
END.ELEC  [ <c> ]
```

EPITAXY

```
TEMPERAT=<n>  TIME=<n> [ DX=<n> ]
( GROWTH.R=<n> | PP.SILAN=<n> )
[ ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  ( CONCENTR=<n> | PP.DOPAN=<n> )
[ DTMIN=<n> ] [ DTMAX=<n> ]
[ ABS.ERR=<n> ] [ REL.ERR=<n> ]
```

ETCH

```
( SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM )
[ ( THICKNES=<n> | ALL ) ]
```

GRID

```
LAYER.<n> [ THICKNES=<n> ]  [ DX=<n> ]  [ MIN.DX=<n> ]
[ XDX=<n> ]  [ SPACES=<n> ]
```

IMPLANT

```
DOSE=<n> ENERGY=<n>
( ANTIMONY | ARSENIC | BF2 | BORON | PHOSPHOR )
(  GAUSSIAN
 | 2-GAUSSI
 | PEARSON
 | ( BOLTZMAN [ MINSTEPS=<n> ] [ AT.WT=<n> ] [ AT.NUMB=<n> ] )
)
```

IMPURITY

```
INDEX=<n>
[ NAME=<c> ] [ (DONOR | ACCEPTOR) ]
[ AT.WT=<n> ] [ AT.NUMB=<n> ]
[ IONFILE1=<c> ] [ IONFILE2=<c> ]
[ (  ( SILICON
       [ FII.0=<n> ] [ FII.E=<n> ]
                   [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
       [ MISFITST=<n> ] [ CD=<n> ]
       [ MSF111FA=<n> ] [ MSF110FA=<n> ] [ MSF100FA=<n> ]
       [ DAMAGEST=<n> ]
       [ NE.0=<n> ] [ NE.E=<n> ]
       [ ( IMPLANT | CHEMICAL )
         [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
       ]
     )
   | ( POLYSILI
       [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
       [ FII.0=<n> ] [ FII.E=<n> ]
       [ ( IMPLANT | CHEMICAL )
          [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
       ]
     )
   | ( OXIDE | NITRIDE | ALUMINUM )
  [ ELECT.ST=<n> ]
  [ DIX.0=<n> ] [ DIX.E=<n> ]
  [ DIM.0=<n> ] [ DIM.E=<n> ]
  [ DIMM.0=<n> ] [ DIMM.E=<n> ]
  [ DIP.0=<n> ] [ DIP.E=<n> ]
]
```

INITIALIZE

```
[ ( COEFFICI=<c> | FIRSTIME ) ]
[ STRUCTUR=<c> ] [ MIN.DX=<n> ] [ SAVESTEP ]
[ THICKNES=<n> ] [ DX=<n> ] [ XDX=<n> ] [ SPACES=<n> ]
[ (  SILICON  ( <111> | <110> | <100> )
   | POLYSILI
       ( GRAINSIZ=<n> | ( TEMPERAT=<n> [ PRESSURE=<n> ] ) )
   | OXIDE
   | NITRIDE
   | ALUMINUM
  )
  [ CONCENTR=<n>
    ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  ]
]
```

LOADFILE

```
FILENAME=<c> ( ALL | COEFFICI | STRUCTUR )
[ FORMATTE ]
```

PLOT

```
[ ACTIVE ] [ CHEMICAL ] [ TOTAL ] [ NET ]
[ ANTIMONY ] [ ARSENIC ] [ BORON ] [ PHOSPHOR ]
[ XMIN=<n> ] [ XMAX=<n> ] [ CMIN=<n> ] [ CMAX=<n> ]
[ LINES/PA=<n> ] [ COLUMNS=<n> ]
```

MATERIAL

[ INDEX=<n> ]
[ NAME=<c> ] [ DX.DEFAU=<n> ]
[ ( SEMICOND | CONDUCTO | INSULATO ) ]
[ SPECIES=<n> ] [ DENSITY=<n> ]
[ AT.WT.1=<n> ] [ AT.WT.2=<n> ] [ AT.WT.3=<n> ]
[ AT.NUM.1=<n> ] [ AT.NUM.2=<n> ] [ AT.NUM.3=<n> ]
[ ABUND.1=<n> ] [ ABUND.2=<n> ] [ ABUND.3=<n> ]
[ DIFX.0=<n> ] [ DIFX.E=<n> ]
[ DIMX.0=<n> ] [ DIFM.E=<n> ]
[ DIMMX.0=<n> ] [ DIFMM.E=<n> ]
[ DIFP.0=<n> ] [ DIFP.E=<n> ]
[ NI.0=<n> ] [ NI.E=<n> ] [ NI.F=<n> ] [ DEFECTLN=<n> ]
[ OEDK.0=<n> ] [ OEDK.E=<n> ] [ OED.RATE=<n> ]
[ 100.OEDF=<n> ] [ 110.OEDF=<n> ] [ 111.OEDF=<n> ]
[ GSZ.H.0=<n> ] [ GSZ.H.E=<n> ]
[ GSZ.L.0=<n> ] [ GSZ.L.E=<n> ]
[ MIN.GRAI=<n> ] [ TEMP.BRE=<n> ]
[ RATIO.0=<n> ] [ RATIO.E=<n> ]
[ GEO.FACT=<n> ] [ GBE.0=<n> ] [ GBE.E=<n> ]
[ TAU.0=<n> ] [ TAU.E=<n> ]
[ AFFINITY=<n> ] [ WORK.FUN=<n> ] [ EPSILONF=<n> ]
[ N.VALENC=<n> ] [ N.CONDUC=<n> ] [ BAND.GAP=<n> ]
[ K.M=<n> ]

NITRIDE

[ NAME=<c> ] [ DX.DEFAU=<n> ]
[ INSULATO ]
[ SPECIES=<n> ] [ DENSITY=<n> ]
[ AT.WT.1=<n> ] [ AT.WT.2=<n> ]
[ AT.NUM.1=<n> ] [ AT.NUM.2=<n> ]
[ ABUND.1=<n> ] [ ABUND.2=<n> ]
[ EPSILONF=<n> ]

NITROGEN

```
[ ( <111> | <110> | <100> )
  [ LIN.L.0=<n> ] [ LIN.L.E=<n> ]
  [ LIN.H.0=<n> ] [ LIN.H.E=<n> ]
  [ THINOX.0=<n> ] [ THINOX.E=<n> ] [ THINOX.L=<n> ]
]
[ PAR.L.0=<n> ] [ PAR.L.E=<n> ]
[ PAR.H.0=<n> ] [ PAR.H.E=<n> ]
[ LIN.BREA=<n> ] [ PAR.BREA=<n> ]
[ LIN.PDEP=<n> ] [ PAR.PDEP=<n> ]
[ PRESSURE=<n> ] [ HCL%=<n> ]
[ GAMMA.0=<n> ] [ GAMMA.E=<n> ]
[ DELTA.0=<n> ] [ DELTA.E=<n> ]
[ EXP.0=<n> ] [ EXP.E=<n> ]
[ NIOX.0=<n> ] [ NIOX.E=<n> ] [ NIOX.F=<n> ]
[ CL.ROW=<n> [ CL.PCT=<n> ]
  CL.COLUM=<n> [ CL.TEMPE=<n> ]
  [ CL.DEP.L=<n> ] [ CL.DEP.P=<n> ]
]
```

OXIDE

```
[ NAME=<c> ] [ DX.DEFAU=<n> ]
[ INSULATO ]
[ SPECIES=<n> ] [ DENSITY=<n> ]
[ AT.WT.1=<n> ] [ AT.WT.2=<n> ]
[ AT.NUM.1=<n> ] [ AT.NUM.2=<n> ]
[ ABUND.1=<n> ] [ ABUND.2=<n> ]
[ EPSILONF=<n> ]
```

```
PHOSPHOR

  [ NAME=<c> ] [ DONOR ]
  [ AT.WT=<n> ] [ AT.NUMB=<n> ]
  [ IONFILE1=<c> ] [ IONFILE2=<c> ]
  [ (  ( SILICON
       [ FII.0=<n> ] [ FII.E=<n> ]
                    [ K.MF=<n> ] [ K.A=<n> ] [ K.P=<n> ]
       [ MISFITST=<n> ] [ CD=<n> ]
       [ MSF111FA=<n> ] [ MSF110FA=<n> ] [ MSF100FA=<n> ]
       [ DAMAGEST=<n> ]
       [ NE.0=<n> ] [ NE.E=<n> ]
       [ ( IMPLANT | CHEMICAL )
         [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
       ]
      )
    | ( POLYSILI
       [ ENTROPY=<n> ] [ HEAT.SEG=<n> ] [ Q.SITES=<n> ]
       [ FII.0=<n> ] [ FII.E=<n> ]
       [ ( IMPLANT | CHEMICAL )
          [ CTN.0=<n> ] [ CTN.E=<n> ] [ CTN.F=<n> ]
       ]
      )
    | ( OXIDE | NITRIDE | ALUMINUM )
   [ ELECT.ST=<n> ]
   [ DIX.0=<n> ] [ DIX.E=<n> ]
   [ DIM.0=<n> ] [ DIM.E=<n> ]
   [ DIMM.0=<n> ] [ DIMM.E=<n> ]
  ]


PLOT

  [ ACTIVE ] [ CHEMICAL ] [ TOTAL ] [ NET ]
  [ ANTIMONY ] [ ARSENIC ] [ BORON ] [ PHOSPHOR ]
  [ XMIN=<n> ] [ XMAX=<n> ] [ CMIN=<n> ] [ CMAX=<n> ]
  [ LAYER1 ] [ LAYER2 ] ... [ LAYER10 ]
  [ CLEAR ] [ AXIS ] [ LINETYPE=<n> ]
                    [ TITLE=<c> ] [ LABEL=<c> ]
  [ XPWIDTH=<n> ] [ YPWIDTH=<n> ]
  [ XOFFSET=<n> ] [ YOFFSET=<n> ]
  [ DEVICE=<c> ] [ FILENAME=<c> ]
```

POLYSILI

```
[ NAME=<c> ] [ DX.DEFAU=<n> ]
[ SEMICOND ]
[ SPECIES=<n> ] [ DENSITY=<n> ]
[ AT.WT.1=<n> ] [ AT.NUM.1=<n> ] [ ABUND.1=<n> ]
[ DIFX.0=<n> ] [ DIFX.E=<n> ]
[ DIMX.0=<n> ] [ DIFM.E=<n> ]
[ DIMMX.0=<n> ] [ DIFMM.E=<n> ]
[ DIFP.0=<n> ] [ DIFP.E=<n> ]
[ NI.0=<n> ] [ NI.E=<n> ] [ NI.F=<n> ] [ DEFECTLN=<n> ]
[ OEDK.0=<n> ] [ OEDK.E=<n> ] [ OED.RATE=<n> ]
[ GSZ.H.0=<n> ] [ GSZ.H.E=<n> ]
[ GSZ.L.0=<n> ] [ GSZ.L.E=<n> ]
[ MIN.GRAI=<n> ] [ TEMP.BRE=<n> ]
[ RATIO.0=<n> ] [ RATIO.E=<n> ]
[ GEO.FACT=<n> ] [ GBE.0=<n> ] [ GBE.E=<n> ]
[ TAU.0=<n> ] [ TAU.E=<n> ]
[ AFFINITY=<n> ] [ EPSILONF=<n> ]
[ N.VALENC=<n> ] [ N.CONDUC=<n> ] [ BAND.GAP=<n> ]
```

PRINT

```
[ CONCENTR
   [ ACTIVE ] [ CHEMICAL ] [ ALL ] [ TOTAL ] [ NET ]
   [ ANTIMONY ] [ ARSENIC ] [ BORON ] [ PHOSPHOR ]
   [ XMIN=<n> ] [ XMAX=<n> ]
]
[ IMPURITY
     [  ALL
      | ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
     ]
]
[ MATERIAL
     [  ALL
      | ( SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM )
     ]
]
[ LAYERS ] [ SEGREGAT ] [ OXIDATIO ]
[ LINES/PA=<n> ] [ COLUMNS=<n> ]
[ LU=<n> | FILENAME=<c> ]
```

PROFILE

```
FILE=<c>  CONC.COL=<n>  X.COL=<n>  [ LAYER=<n> ]
                    [ SKIP=<n> ]  [ COUNT=<n> ]  [ COM.CHAR=<c> ]
( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
```

```
RESISTIVITY

  FILE=<c>  CONC.COL=<n>  RES.COL=<n>
                    [ SKIP=<n> ]  [ COUNT=<n> ]  [ COM.CHAR=<c> ]
  ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  ( ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON )


SAVEFILE

 FILENAME=<c> ( ALL | COEFFICI | STRUCTUR | EXPORT )
 [ FORMATTE ]


SEGREGAT

  (  ( SILICON
      [ 100.FACT=<n> ] [ 110.FACT=<n> ] [ 111.FACT=<n> ]
    )
   |   OXIDE | POLYSILI | NITRIDE | ALUMINUM | AIR
  )
  (  ( /SILICON
      [ 100.FACT=<n> ] [ 110.FACT=<n> ] [ 111.FACT=<n> ]
    )
   |   /OXIDE | /POLYSIL | /NITRIDE | /ALUMINU | /AIR
  )
  ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  [ SEG.0=<n> ] [ SEG.E=<n> ]
  [ TRANS.0=<n> ] [ TRANS.E=<n> ]
                    [ MAX.0=<n> ] [ MAX.E=<n> ]
                    [ ( MODEL.1 | MODEL.2 ) ]
  [ MUI.0=<n> ] [ MUI.E=<n> ]
                    [ GRATE.0=<n> ] [ GRATE.E=<n> ]
                    [ C.INIT=<n> ] [ C.THRESH=<n> ] [ L.THICK=<n> ]


SILICON

  [ NAME=<c> ] [ DX.DEFAU=<n> ]
  [ SEMICOND ]
  [ SPECIES=<n> ] [ DENSITY=<n> ]
  [ AT.WT.1=<n> ] [ AT.NUM.1=<n> ] [ ABUND.1=<n> ]
  [ NI.0=<n> ] [ NI.E=<n> ] [ NI.F=<n> ] [ DEFECTLN=<n> ]
  [ OEDK.0=<n> ] [ OEDK.E=<n> ] [ OED.RATE=<n> ]
  [ 100.OEDF=<n> ] [ 110.OEDF=<n> ] [ 111.OEDF=<n> ]
  [ AFFINITY=<n> ] [ EPSILONF=<n> ]
  [ N.VALENC=<n> ] [ N.CONDUC=<n> ] [ BAND.GAP=<n> ]
  [ K.M=<n> ]


SOLUBILITY

  FILE=<c>  CONC.COL=<n>  TEMP.COL=<n>
                    [ SKIP=<n> ]  [ COUNT=<n> ]  [ COM.CHAR=<c> ]
  ( ANTIMONY | ARSENIC | BORON | PHOSPHOR )
  ( ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON )
```

STOP [ <c> ]

TITLE [ <c> ]

VOL.RATIO

( SILICON | OXIDE | POLYSILI | NITRIDE | ALUMINUM )
( /SILICON | /OXIDE | /POLYSIL | /NITRIDE | /ALUMINUM )
RATIO=<n>

V.THRESHOLD

[ V.SUB1=<n> ] [ V.SUB2=<n> ] [ DV.SUB=<n> ]
[ (SURFACE | BACKSIDE | (BULKCONC=<n> (PTYPE | NTYPE))) ]
[ Q.F=<n> ] [ TEMPERAT=<n> ]
[ FILENAME=<c> [ APPEND ] ]

WETO2

[ ( <111> | <110> | <100> )
[ LIN.L.0=<n> ] [ LIN.L.E=<n> ]
[ LIN.H.0=<n> ] [ LIN.H.E=<n> ]
[ THINOX.0=<n> ] [ THINOX.E=<n> ] [ THINOX.L=<n> ]
]
[ PAR.L.0=<n> ] [ PAR.L.E=<n> ]
[ PAR.H.0=<n> ] [ PAR.H.E=<n> ]
[ LIN.BREA=<n> ] [ PAR.BREA=<n> ]
[ LIN.PDEP=<n> ] [ PAR.PDEP=<n> ]
[ PRESSURE=<n> ] [ HCL%=<n> ]
[ GAMMA.0=<n> ] [ GAMMA.E=<n> ]
[ DELTA.0=<n> ] [ DELTA.E=<n> ]
[ EXP.0=<n> ] [ EXP.E=<n> ]
[ NIOX.0=<n> ] [ NIOX.E=<n> ] [ NIOX.F=<n> ]
[ CL.ROW=<n> [ CL.PCT=<n> ]
CL.COLUM=<n> [ CL.TEMPE=<n> ]
[ CL.DEP.L=<n> ] [ CL.DEP.P=<n> ]
]

## 49. Example 1: NMOS Silicon Gate.

Presented here is an example of the simulation of a NMOS silicon gate process. Three vertical cross-sections are simulated, one through the center of the gate region, the second through the source or drain region, and the third through the isolation or field region.

The structure was simulated using six input files. The first file simulates the processing in the active region of the device, up to the point where the process diverges for the gate and the source/drain regions. The second and third files start with the result of this first file and complete the processing for the gate region and the source/drain region respectively. The fourth file performs an electrical parameter calculation on the resulting gate region. The fifth file is similar to the first one, except that the processing effecting the field region of the device is simulated. The sixth file completes the field region processing.

The processing sequence used is listed below.

1. The process begins with a high resistivity, <100>, p-type substrate.
2. A 400 Angstrom pad layer of silicon dioxide is grown.
3. An 800 Angstrom layer of silicon nitride is deposited on top of the silicon dioxide.
4. The nitride is stripped from the areas outside of the active regions.
5. Boron is ion-implanted to increase the p doping at the surface in the field regions.
6. The field regions are then oxidized for three hours at 1000 degrees centigrade in a wet oxygen ambient.
7. Etch to the silicon surface in the active regions.
8. Ion implant boron to set the threshold voltage of the device.
9. Grow the 400 Angstrom gate oxide.
10. Deposit a half micron layer of polysilicon.
11. Dope it with phosphorus using POCl3 in a predeposition furnace.
12. Etch the polysilicon from the areas outside of the gate regions.
13. Ion implant arsenic to form the source and gate regions.
14. Drive-in the source and drain diffusions for 30 minutes at 1000 degrees centigrade in a dry oxygen ambient.
15. Open the contact holes in the gate, source, and drain regions.
16. Use CVD to deposit phosphorus doped silicon dioxide over the wafer surface.
17. Reflow the glass at 1000 degrees for 30 minutes.
18. Reopen the contact holes and deposit aluminum.

Cross-section of locally oxidized NMOS device simulated in this example. Simulations through both the active (channel) region and through the field oxide region are shown. In addition, a Poisson solution through the channel region is used to extract threshold voltage.

```
*********************************
***        Suprem-III        ***
***   version 1B  rev. 8628   ***
*********************************

   Tue Oct 27 15:50:45 1987



  Commands input from file: s3ex1a.in

 1... Title          SUPREM-III Example 1.  NMOS Silicon Gate
 2... Comment        Active device region initial processing.
 3... $              File S3EX1A

 4... Comment        Initialize silicon substrate.
 5... Initialize     <100> Silicon, Boron Concentration=1e15
  ...  +             Thickness=1.5 dX=.005 XdX=.02  Spaces=150

 6... Comment        Grow pad oxide, 400A.
 7... Diffusion      Temperature=1000  Time=40  DryO2

 8... Comment        Deposit 800A of CVD Nitride.
 9... Deposit        Nitride  Thickness=.0800  Spaces=15

10... Comment        Grow field oxide.
11... Diffusion      Temperature=1000  Time=180  WetO2
12... Print          Layer

13... Comment        Etch to silicon surface.
14... Etch           Oxide all
15... Etch           Nitride all
16... Etch           Oxide all

17... Comment        Implant boron to shift the threshold voltage.
18... Implant        Boron  Dose=4e11  Energy=50

19... Comment        Grow gate oxide
20... Diffusion      Temperature=1050  Time=30  DryO2  HCL%=3

21... Comment        Deposit polysilicon
22... Deposit        Polysilicon  Thickness=0.5  Temperature=600

23... Comment        Heavily dope the polysilicon using POCl3
24... Diffusion      Temperature=1000  Time=25  dTmin=.3
  ...  +             Phosphorus  Solidsolubility

25... Print          Layer
26... Plot           Chemical Boron      Xmax=1.5   Clear ^Axis Linetype=2
27... Plot           Chemical Phosphorus  Xmax=1.5  ^Clear ^Axis Linetype=3
28... Plot           Chemical Net        Xmax=1.5  ^Clear  Axis

29... Comment        Save the structure at this point.  The simulation runs
30... $              are split for the gate and source/drain regions.
31... Save           Structure  File=s3e1as

32... Stop           End of SUPREM-III Example 1.
```

SUPREM-III Example 1. NMOS Silicon Gate
Active device region initial processing.
File S3EX1A
Initialize silicon substrate.

Grow pad oxide, 400A.

Deposit 800A of CVD Nitride.

Grow field oxide.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 4 | OXIDE | 0.0176 | 0.0100 | 0.0010 | 330 | 332 | |
| 3 | NITRIDE | 0.0694 | 0.0100 | 0.0010 | 333 | 347 | |
| 2 | OXIDE | 0.0376 | 0.0100 | 0.0010 | 348 | 352 | |
| 1 | SILICON | 1.4835 | 0.0050 | 0.0010 | 353 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 3 | 0.0000e+00 | -1.2524e+07 | 0.0000e+00 | 1.2524e+07 |
| 2 | 0.0000e+00 | -6.8527e+09 | 0.0000e+00 | 6.8527e+09 |
| 1 | -1.4225e+11 | -1.4225e+11 | 1.4225e+11 | 1.4225e+11 |
| sum | -1.4225e+11 | -1.4912e+11 | 1.4225e+11 | 1.4912e+11 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 |
| 3 | 0.0000e+00 | 1.2524e+07 |
| 2 | 0.0000e+00 | 6.8527e+09 |
| 1 | 1.4225e+11 | 1.4225e+11 |
| sum | 1.4225e+11 | 1.4912e+11 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 4 | 1 | n | 0.0000 | 0.0000e+00 | 0.0000e+00 |
| 3 | 2 | n | 0.0000 | 0.0000e+00 | 0.0000e+00 |
| 3 | 1 | p | 0.0694 | 0.0000e+00 | 0.0000e+00 |
| 2 | 1 | p | 0.0000 | 0.0000e+00 | 6.8527e+09 |
| 1 | 1 | p | 0.0000 | 1.4225e+11 | 1.4225e+11 |

Etch to silicon surface.

Implant boron to shift the threshold voltage.

Grow gate oxide

Deposit polysilicon

Heavily dope the polysilicon using POCl3

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 3 | POLYSILICON | 0.5000 | 0.0100 | 0.0010 | 300 | 350 | 0.6105 |
| 2 | OXIDE | 0.0672 | 0.0100 | 0.0010 | 351 | 358 | |
| 1 | SILICON | 1.4539 | 0.0050 | 0.0010 | 359 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 9.6442e+15 | 1.6986e+16 | 9.6442e+15 | 1.6986e+16 |
| 2 | 0.0000e+00 | 5.3176e+12 | 0.0000e+00 | 5.5242e+12 |
| 1 | -4.3757e+11 | -4.3757e+11 | 4.3757e+11 | 4.3757e+11 |
| sum | 9.6437e+15 | 1.6991e+16 | 9.6446e+15 | 1.6992e+16 |

Integrated Dopant

| layer | BORON | | PHOSPHORUS | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 1.0440e+08 | 1.0440e+08 | 9.6442e+15 | 1.6986e+16 |
| 2 | 0.0000e+00 | 1.0328e+11 | 0.0000e+00 | 5.4209e+12 |
| 1 | 4.3757e+11 | 4.3757e+11 | 5.9474e+03 | 5.9474e+03 |
| sum | 4.3767e+11 | 5.4096e+11 | 9.6442e+15 | 1.6991e+16 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 3 | 1 | n | 0.0000 | 9.6442e+15 | 1.6986e+16 |
| 2 | 2 | n | 0.0000 | 0.0000e+00 | 5.2968e+12 |
| 2 | 1 | p | 0.0242 | 0.0000e+00 | 8.0323e+10 |
| 1 | 1 | p | 0.0000 | 4.3757e+11 | 4.3757e+11 |

Save the structure at this point. The simulation runs are split for the gate and source/drain regions.

End Suprem-III

Suprem-III simulation after the channel implant, gate oxide growth, poly deposition and doping. Phosphorus diffusion from the poly gate into the gate oxide is evident.

```
*********************************
***       Suprem-III        ***
***   version 1B  rev. 8628   ***
*********************************

    Tue Oct 27 15:51:52 1987



  Commands input from file: s3ex1b.in

 1... Title          SUPREM-III Example 1.  NMOS Silicon Gate
 2... Comment        Gate region.
 3... $              File s3ex1b

 4... Comment        Initialize silicon substrate.
 5... Initialize     Structure=s3e1as

 6... Comment        Implant Arsenic for source/drain regions.
 7... Implant        Arsenic  Dose=5E15  Energy=150

 8... Comment        Drive-in Arsenic and re-oxidize source/drain regions.
 9... Diffusion      Temperature=1000  Time=30  DryO2

10... Comment        Etch contact holes to gate, source, and drain regions.
11... Etch           Oxide

12... Comment        Deposit Phosphorus doped SiO2 using CVD.
13... Deposit        Oxide  Thickness=.7500  Phosphorus Concentration=1.E21

14... Comment        Increase the diffusivity of phosphorus in oxide by
15... $              two orders of magnitude.
16... Phosphorus     Oxide  Dix.0=4.56E7

17... Comment        Reflow glass to smooth surface and dope contact holes.
18... Diffusion      Temperature=1000  Time=30

19... Comment        Reopen contact holes.
20... Etch           Oxide

21... Comment        Deposit Aluminum.
22... Deposit        Aluminum  Thickness=1.2  Spaces=10

23... Comment        Plot the chemical impurity distributions at this point.
24... Print          Layer
25... Plot           Chemical Boron       Xmax=2.5   Clear ^Axis Linetype=2
26... Plot           Chemical Arsenic     Xmax=2.5  ^Clear ^Axis Linetype=3
27... Plot           Chemical Phosphorus  Xmax=2.5  ^Clear ^Axis Linetype=6
28... Plot           Chemical Net         Xmax=2.5  ^Clear  Axis

29... Comment        Save the structure.
30... Save           Structure  File=s3e1bs

31... Stop           End of SUPREM-III Example 1.
```

SUPREM-III Example 1. NMOS Silicon Gate
Gate region.
File s3ex1b
Initialize silicon substrate.

Implant Arsenic for source/drain regions.

Drive-in Arsenic and re-oxidize source/drain regions.

Etch contact holes to gate, source, and drain regions.

Deposit Phosphorus doped SiO2 using CVD.

Increase the diffusivity of phosphorus in oxide by
two orders of magnitude.

Reflow glass to smooth surface and dope contact holes.

Reopen contact holes.

Deposit Aluminum.

Plot the chemical impurity distributions at this point.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 4 | ALUMINUM | 1.2000 | 0.0100 | 0.0010 | 292 | 302 | |
| 3 | POLYSILICON | 0.4646 | 0.0100 | 0.0010 | 303 | 350 | 0.9035 |
| 2 | OXIDE | 0.0672 | 0.0100 | 0.0010 | 351 | 358 | |
| 1 | SILICON | 1.4539 | 0.0050 | 0.0010 | 359 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 3 | 1.3770e+16 | 2.2278e+16 | 1.3770e+16 | 2.2278e+16 |
| 2 | 0.0000e+00 | 1.1498e+13 | 0.0000e+00 | 1.1705e+13 |
| 1 | -4.3714e+11 | -4.3714e+11 | 4.3718e+11 | 4.3718e+11 |
| sum | 1.3770e+16 | 2.2289e+16 | 1.3771e+16 | 2.2290e+16 |

Integrated Dopant

| layer | PHOSPHORUS | | ARSENIC | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 3 | 8.9661e+15 | 1.7376e+16 | 4.8040e+15 | 4.9019e+15 |
| 2 | 0.0000e+00 | 1.0926e+13 | 0.0000e+00 | 6.7499e+11 |
| 1 | 2.0359e+07 | 2.0359e+07 | 1.4714e-16 | 1.4714e-16 |
| sum | 8.9661e+15 | 1.7387e+16 | 4.8040e+15 | 4.9026e+15 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 |
| 3 | 3.3427e+08 | 3.3427e+08 |
| 2 | 0.0000e+00 | 1.0345e+11 |
| 1 | 4.3716e+11 | 4.3716e+11 |
| sum | 4.3749e+11 | 5.4094e+11 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 4 | 1 | n | 0.0000 | 0.0000e+00 | 0.0000e+00 |
| 3 | 1 | n | 0.0000 | 1.3770e+16 | 2.2278e+16 |
| 2 | 2 | n | 0.0000 | 0.0000e+00 | 1.1631e+13 |
| 2 | 1 | p | 0.0465 | 0.0000e+00 | 3.6428e+10 |
| 1 | 1 | p | 0.0000 | 4.3714e+11 | 4.3718e+11 |

Save the structure.

End Suprem-III

Suprem-III simulation through the gate region following all processing steps.

```
               ********************************
               ***       Suprem-III        ***
               ***   version 1B  rev. 8628   ***
               ********************************

                 Tue Oct 27 15:53:35 1987



       Commands input from file: s3ex1c.in

  1... Title        SUPREM-III Example 1.  NMOS Silicon Gate
  2... Comment       Source/drain regions.
  3... $            File s3ex1c

  4... Comment       Initialize silicon substrate.
  5... Initialize    Structure=s3e1as

  6... Comment       Etch polysilicon and oxide over source/drain regions.
  7... Etch          Polysilicon
  8... Etch          Oxide

  9... Comment       Implant Arsenic for source/drain regions.
 10... Implant       Arsenic  Dose=5E15  Energy=150

 11... Comment       Drive-in Arsenic and re-oxidize source/drain regions.
 12... Diffusion     Temperature=1000  Time=30  DryO2

 13... Comment       Etch contact holes to gate, source, and drain regions.
 14... Etch          oxide

 15... Comment       Deposit Phosphorus doped SiO2 using CVD.
 16... Deposit       Oxide  Thickness=.7500  Phosphorus Concentration=1e21

 17... Comment       Increase the diffusivity of phosphorus in oxide by
 18... $             two orders of magnitude.
 19... Phosphorus    Oxide  Dix.0=4.56E7

 20... Comment       Reflow glass to smooth surface and dope contact holes.
 21... Diffusion     Temperature=1000  Time=30
 22... Print         Layer

 23... Comment       Reopen contact holes.
 24... Etch          Oxide

 25... Comment       Deposit Aluminum.
 26... Deposit       Aluminum  Thickness=1.2  Spaces=10

 27... Comment       Plot the chemical impurity distributions at this point.
 28... Print         Layer
 29... Plot          Chemical Boron       Xmax=2.5   Clear ^Axis Linetype=2
 30... Plot          Chemical Arsenic     Xmax=2.5  ^Clear ^Axis Linetype=3
 31... Plot          Chemical Phosphorus  Xmax=2.5  ^Clear ^Axis Linetype=6
 32... Plot          Chemical Net         Xmax=2.5  ^Clear  Axis

 33... Comment       Save the structure.
 34... Save          Structure  File=s3e1cs

 35... Stop          End of SUPREM-III Example 1.
```

SUPREM-III Example 1. NMOS Silicon Gate
Source/drain regions.
File s3ex1c
Initialize silicon substrate.

Etch polysilicon and oxide over source/drain regions.

Implant Arsenic for source/drain regions.

Drive-in Arsenic and re-oxidize source/drain regions.

Etch contact holes to gate, source, and drain regions.

Deposit Phosphorus doped SiO2 using CVD.

Increase the diffusivity of phosphorus in oxide by
two orders of magnitude.

Reflow glass to smooth surface and dope contact holes.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 2 | OXIDE | 0.7500 | 0.0100 | 0.0010 | 287 | 362 | |
| 1 | SILICON | 1.4282 | 0.0050 | 0.0010 | 363 | 500 | <100> |

Integrated Dopant

| layer no. | Net active | Net chemical | Total active | Total chemical |
|---|---|---|---|---|
| 2 | 0.0000e+00 | 7.3653e+16 | 0.0000e+00 | 7.3654e+16 |
| 1 | 5.4178e+15 | 5.5214e+15 | 5.4184e+15 | 5.5221e+15 |
| sum | 5.4178e+15 | 7.9175e+16 | 5.4184e+15 | 7.9176e+16 |

Integrated Dopant

| layer no. | PHOSPHORUS active | PHOSPHORUS chemical | ARSENIC active | ARSENIC chemical |
|---|---|---|---|---|
| 2 | 0.0000e+00 | 7.3653e+16 | 0.0000e+00 | 9.5986e+11 |
| 1 | 6.2501e+14 | 6.7332e+14 | 4.7931e+15 | 4.8484e+15 |
| sum | 6.2501e+14 | 7.4326e+16 | 4.7931e+15 | 4.8494e+15 |

Integrated Dopant

| layer no. | BORON active | BORON chemical |
|---|---|---|
| 2 | 0.0000e+00 | 2.1491e+10 |
| 1 | 3.2537e+11 | 3.2537e+11 |
| sum | 3.2537e+11 | 3.4686e+11 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 2 | 1 | n | 0.0000 | 0.0000e+00 | 7.3653e+16 |
| 1 | 2 | n | 0.0000 | 5.4178e+15 | 5.5220e+15 |
| 1 | 1 | p | 1.2072 | 1.8688e+10 | 3.0137e+10 |

Reopen contact holes.

Deposit Aluminum.

Plot the chemical impurity distributions at this point.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 2 | ALUMINUM | 1.2000 | 0.0100 | 0.0010 | 352 | 362 | |
| 1 | SILICON | 1.4282 | 0.0050 | 0.0010 | 363 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 2 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 1 | 5.4178e+15 | 5.5214e+15 | 5.4184e+15 | 5.5221e+15 |
| sum | 5.4178e+15 | 5.5214e+15 | 5.4184e+15 | 5.5221e+15 |

Integrated Dopant

| layer | PHOSPHORUS | | ARSENIC | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 2 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 1 | 6.2501e+14 | 6.7332e+14 | 4.7931e+15 | 4.8484e+15 |
| sum | 6.2501e+14 | 6.7332e+14 | 4.7931e+15 | 4.8484e+15 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 2 | 0.0000e+00 | 0.0000e+00 |
| 1 | 3.2537e+11 | 3.2537e+11 |
| sum | 3.2537e+11 | 3.2537e+11 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 2 | 1 | n | 0.0000 | 0.0000e+00 | 0.0000e+00 |
| 1 | 2 | n | 0.0000 | 5.4178e+15 | 5.5220e+15 |
| 1 | 1 | p | 1.2072 | 1.8688e+10 | 3.0137e+10 |

Save the structure.

End Suprem-III

Suprem-III simulation through the source-drain region following all processing steps.

```
                ********************************
                ***       Suprem-III        ***
                ***   version 1B  rev. 8628   ***
                ********************************

                  Tue Oct 27 15:55:28 1987



  Commands input from file: s3ex1d.in

 1... Title         SUPREM-III Example 1.  NMOS Silicon Gate
 2... Comment       Gate region electrical simulation.
 3... $             File s3ex1d

 4... Comment       Initialize using gate region result.
 5... Initialize    Structure=s3e1bs

 6... Comment       Solve Poisson's equation with the gate biased from
 7... $             0. volts to 3. volts in .2 volt steps.
 8... Electrical    Steps=16
 9... Bias          Layer=3  Diffusion=1  V.Majority=0.  dV.Majority=.2
10... End

11... Stop          End of SUPREM-III Example 1.
```

SUPREM-III Example 1. NMOS Silicon Gate
Gate region electrical simulation.
File s3ex1d
Initialize using gate region result.

Solve Poisson's equation with the gate biased from
0. volts to 3. volts in .2 volt steps.

Required Iterations = 6

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 1 | 3 | 1 | 0.000e+00 | 2.059e+16 | 0.000e+00 | 9.840e-21 | 2.187e+24 |
| 1 | 1 | 1 | 2.378e+11 | 1.393e+06 | 1.263e-01 | 1.393e-06 | 5.444e+04 |

Required Iterations = 7

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 2 | 3 | 1 | 0.000e+00 | 2.059e+16 | 0.000e+00 | 9.839e-21 | 2.188e+24 |
| 2 | 1 | 1 | 2.127e+11 | 1.340e+08 | 1.136e-01 | 1.324e-04 | 6.048e+04 |

Required Iterations = 19

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 3 | 3 | 1 | 0.000e+00 | 2.058e+16 | 0.000e+00 | 9.838e-21 | 2.188e+24 |
| 3 | 1 | 1 | 1.925e+11 | 8.728e+09 | 1.032e-01 | 8.557e-03 | 6.156e+04 |

Required Iterations = 24

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 4 | 3 | 1 | 0.000e+00 | 2.058e+16 | 0.000e+00 | 9.837e-21 | 2.188e+24 |
| 4 | 1 | 1 | 1.851e+11 | 5.019e+10 | 9.928e-02 | 4.901e-02 | 4.638e+04 |

Required Iterations = 24

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 5 | 3 | 1 | 0.000e+00 | 2.058e+16 | 0.000e+00 | 9.836e-21 | 2.188e+24 |
| 5 | 1 | 1 | 1.823e+11 | 1.048e+11 | 9.783e-02 | 1.021e-01 | 3.440e+04 |

Required Iterations = 24

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 6 | 3 | 1 | 0.000e+00 | 2.058e+16 | 0.000e+00 | 9.835e-21 | 2.189e+24 |
| 6 | 1 | 1 | 1.808e+11 | 1.633e+11 | 9.704e-02 | 1.587e-01 | 2.690e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 7 | 3 | 1 | 0.000e+00 | 2.057e+16 | 0.000e+00 | 9.834e-21 | 2.189e+24 |
| 7 | 1 | 1 | 1.798e+11 | 2.234e+11 | 9.654e-02 | 2.168e-01 | 2.195e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 8 | 3 | 1 | 0.000e+00 | 2.057e+16 | 0.000e+00 | 9.833e-21 | 2.189e+24 |
| 8 | 1 | 1 | 1.791e+11 | 2.845e+11 | 9.618e-02 | 2.757e-01 | 1.850e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 9 | 3 | 1 | 0.000e+00 | 2.057e+16 | 0.000e+00 | 9.832e-21 | 2.189e+24 |
| 9 | 1 | 1 | 1.786e+11 | 3.461e+11 | 9.591e-02 | 3.351e-01 | 1.596e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 10 | 3 | 1 | 0.000e+00 | 2.056e+16 | 0.000e+00 | 9.831e-21 | 2.189e+24 |
| 10 | 1 | 1 | 1.782e+11 | 4.082e+11 | 9.570e-02 | 3.948e-01 | 1.402e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 11 | 3 | 1 | 0.000e+00 | 2.056e+16 | 0.000e+00 | 9.830e-21 | 2.190e+24 |
| 11 | 1 | 1 | 1.779e+11 | 4.706e+11 | 9.552e-02 | 4.547e-01 | 1.250e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 12 | 3 | 1 | 0.000e+00 | 2.056e+16 | 0.000e+00 | 9.829e-21 | 2.190e+24 |
| 12 | 1 | 1 | 1.776e+11 | 5.332e+11 | 9.538e-02 | 5.149e-01 | 1.127e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 13 | 3 | 1 | 0.000e+00 | 2.056e+16 | 0.000e+00 | 9.828e-21 | 2.190e+24 |
| 13 | 1 | 1 | 1.774e+11 | 5.960e+11 | 9.526e-02 | 5.751e-01 | 1.026e+04 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 14 | 3 | 1 | 0.000e+00 | 2.055e+16 | 0.000e+00 | 9.827e-21 | 2.190e+24 |
| 14 | 1 | 1 | 1.772e+11 | 6.589e+11 | 9.516e-02 | 6.355e-01 | 9.413e+03 |

Required Iterations = 24

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 15 | 3 | 1 | 0.000e+00 | 2.055e+16 | 0.000e+00 | 9.826e-21 | 2.191e+24 |
| 15 | 1 | 1 | 1.770e+11 | 7.219e+11 | 9.506e-02 | 6.960e-01 | 8.695e+03 |

Required Iterations = 23

| Step | Layer | Region | Concentration Holes | Electrons | Conductivity Holes | Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 16 | 3 | 1 | 0.000e+00 | 2.055e+16 | 0.000e+00 | 9.825e-21 | 2.191e+24 |
| 16 | 1 | 1 | 1.768e+11 | 7.851e+11 | 9.498e-02 | 7.565e-01 | 8.078e+03 |

End Suprem-III

Plot of channel region conductivity vs. applied gate potential generated from Suprem-III Poisson solution. From such a plot, the threshold voltage can be easily calculated.

```
*********************************
***        Suprem-III        ***
***   version 1B  rev. 8628   ***
*********************************

    Tue Oct 27 15:56:36 1987



  Commands input from file: s3ex1e.in

 1... Title        SUPREM-III Example 1.  NMOS Silicon Gate
 2... Comment      Isolation region initial processing.
 3... $            File s3ex1e

 4... Comment      Initialize silicon substrate.
 5... Initialize   <100> Silicon, Boron Concentration=1e15
  ... +            Thickness=3.0  dX=.01  Spaces=150

 6... Comment      Grow pad oxide, 400A.
 7... Diffusion    Temperature=1000  Time=40  DryO2

 8... Comment      Implant boron to increase field region doping.
 9... Implant      Boron  dose=1e13  energy=150

10... Comment      Grow field oxide.
11... Diffusion    Temperature=1000  Time=180  WetO2
12... Print        Layer

13... Comment      Implant boron to shift the enhancement threshold voltage.
14... Implant      Boron  Dose=4e11  Energy=50

15... Comment      Grow gate oxide
16... Diffusion    Temperature=1050  Time=30  DryO2  HCL%=3

17... Comment      Deposit polysilicon
18... Deposit      Polysilicon  Thickness=0.5  Temperature=600

19... Comment      Heavily dope the polysilicon using POCl3
20... Diffusion    Temperature=1000  Time=25  dTmin=.3
  ...   +          Phosphorus  Solidsolubility

21... Print        Layer
22... Plot         Chemical Boron        Clear ^Axis Linetype=2
23... Plot         Chemical Phosphorus  ^Clear ^Axis Linetype=3
24... Plot         Chemical Net         ^Clear  Axis

25... Comment      Save the structure at this point.
26... Save         Structure  File=s3e1es

27... Stop         End of SUPREM-III Example 1.
```

SUPREM-III Example 1. NMOS Silicon Gate
Isolation region initial processing.
File s3ex1e
Initialize silicon substrate.

Grow pad oxide, 400A.

Implant boron to increase field region doping.

Grow field oxide.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 2 | OXIDE | 0.7604 | 0.0100 | 0.0010 | 348 | 377 | |
| 1 | SILICON | 2.6654 | 0.0100 | 0.0010 | 378 | 500 | <100> |

Integrated Dopant

| layer no. | Net active | Net chemical | Total active | Total chemical |
|---|---|---|---|---|
| 2 | 0.0000e+00 | -6.1674e+12 | 0.0000e+00 | 6.1674e+12 |
| 1 | -4.1330e+12 | -4.1330e+12 | 4.1330e+12 | 4.1330e+12 |
| sum | -4.1330e+12 | -1.0300e+13 | 4.1330e+12 | 1.0300e+13 |

Integrated Dopant

| layer no. | BORON active | BORON chemical |
|---|---|---|
| 2 | 0.0000e+00 | 6.1674e+12 |
| 1 | 4.1330e+12 | 4.1330e+12 |
| sum | 4.1330e+12 | 1.0300e+13 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 2 | 1 | p | 0.0000 | 0.0000e+00 | 6.1674e+12 |
| 1 | 1 | p | 0.0000 | 4.1330e+12 | 4.1330e+12 |

Implant boron to shift the enhancement threshold voltage.

Grow gate oxide

Deposit polysilicon

Heavily dope the polysilicon using POCl3

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 3 | POLYSILICON | 0.5000 | 0.0100 | 0.0010 | 297 | 347 | 0.6130 |
| 2 | OXIDE | 0.7683 | 0.0100 | 0.0010 | 348 | 377 | |
| 1 | SILICON | 2.6620 | 0.0100 | 0.0010 | 378 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 9.6452e+15 | 1.7004e+16 | 9.6452e+15 | 1.7004e+16 |
| 2 | 0.0000e+00 | 3.6407e+12 | 0.0000e+00 | 1.6968e+13 |
| 1 | -4.0361e+12 | -4.0361e+12 | 4.0361e+12 | 4.0361e+12 |
| sum | 9.6411e+15 | 1.7004e+16 | 9.6492e+15 | 1.7025e+16 |

Integrated Dopant

| layer | BORON | | PHOSPHORUS | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 1.2793e+07 | 1.2793e+07 | 9.6452e+15 | 1.7004e+16 |
| 2 | 0.0000e+00 | 6.6638e+12 | 0.0000e+00 | 1.0305e+13 |
| 1 | 4.0361e+12 | 4.0361e+12 | 0.0000e+00 | 0.0000e+00 |
| sum | 4.0361e+12 | 1.0700e+13 | 9.6452e+15 | 1.7014e+16 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 3 | 1 | n | 0.0000 | 9.6452e+15 | 1.7004e+16 |
| 2 | 2 | n | 0.0000 | 0.0000e+00 | 9.7384e+12 |
| 2 | 1 | p | 0.0430 | 0.0000e+00 | 6.6450e+12 |
| 1 | 1 | p | 0.0000 | 4.0361e+12 | 4.0361e+12 |

Save the structure at this point.

End Suprem-III

Suprem-III simulation through the field oxide region after polysilicon deposition and doping.

```
********************************
***       Suprem-III        ***
***   version 1B  rev. 8628   ***
********************************

    Tue Oct 27 15:57:39 1987



 Commands input from file: s3ex1f.in

 1... Title         SUPREM-III Example 1.  NMOS Silicon Gate
 2... Comment       Final isolation region processing.
 3... $             File s3ex1f

 4... Comment       Initialize silicon substrate.
 5... Initialize    Structure=s3e1es

 6... Comment       Etch polysilicon and oxide over source/drain regions.
 7... Etch          Polysilicon
 8... Etch          Oxide  Amount=.0700

 9... Comment       Implant Arsenic for source/drain regions.
10... Implant       Arsenic  Dose=5E15  Energy=150

11... Comment       Drive-in Arsenic and re-oxidize source/drain regions.
12... Diffusion     Temperature=1000  Time=30  DryO2

13... Comment       Deposit Phosphorus doped SiO2 using CVD.
14... Deposit       Oxide  Thickness=.7500  Phosphorus Concentration=1e21

15... Comment       Reflow glass to smooth surface and dope contact holes.
16... Diffusion     Temperature=1000  Time=30

17... Comment       Deposit Aluminum.
18... Deposit       Aluminum  Thickness=1.2  Spaces=10

19... Comment       Plot the chemical impurity distributions at this point.
20... Print         Layer
21... Plot          Chemical Boron       Clear ^Axis Linetype=2
22... Plot          Chemical Arsenic    ^Clear ^Axis Linetype=3
23... Plot          Chemical Phosphorus  ^Clear ^Axis Linetype=6
24... Plot          Chemical Net        ^Clear  Axis

25... Comment       Save the structure.
26... Save          Structure  File=s3e1fs

27... Stop          End of SUPREM-III Example 1.
```

SUPREM-III Example 1. NMOS Silicon Gate
Final isolation region processing.
File s3ex1f
Initialize silicon substrate.

Etch polysilicon and oxide over source/drain regions.

Implant Arsenic for source/drain regions.

Drive-in Arsenic and re-oxidize source/drain regions.

Deposit Phosphorus doped SiO2 using CVD.

Reflow glass to smooth surface and dope contact holes.

Deposit Aluminum.

Plot the chemical impurity distributions at this point.

```
layer   material type     thickness   dx    dxmin  top  bottom  orientation
 no.                      (microns)  (microns)     node  node  or grain size
  3   ALUMINUM              1.2000  0.0100 0.0010  221   231
  2   OXIDE                 1.4515  0.0100 0.0010  232   377
  1   SILICON               2.6606  0.0100 0.0010  378   500      <100>

                  Integrated Dopant
layer          Net                   Total
 no.     active      chemical     active      chemical
  3    0.0000e+00   0.0000e+00   0.0000e+00   0.0000e+00
  2    0.0000e+00   7.9316e+16   0.0000e+00   7.9329e+16
  1   -3.9898e+12  -3.9898e+12   3.9898e+12   3.9898e+12
 sum  -3.9898e+12   7.9312e+16   3.9898e+12   7.9333e+16

                  Integrated Dopant
layer       PHOSPHORUS               ARSENIC
 no.     active      chemical     active      chemical
  3    0.0000e+00   0.0000e+00   0.0000e+00   0.0000e+00
  2    0.0000e+00   7.4323e+16   0.0000e+00   5.0000e+15
  1    0.0000e+00   0.0000e+00   0.0000e+00   0.0000e+00
 sum   0.0000e+00   7.4323e+16   0.0000e+00   5.0000e+15

                  Integrated Dopant
layer         BORON
 no.     active      chemical
  3    0.0000e+00   0.0000e+00
  2    0.0000e+00   6.6191e+12
  1    3.9898e+12   3.9898e+12
 sum   3.9898e+12   1.0609e+13

          Junction Depths and Integrated Dopant
         Concentrations for Each Diffused Region
layer  region  type  junction depth     net          total
 no.    no.          (microns)      active Qd    chemical Qd
  3      1      n      0.0000      0.0000e+00    0.0000e+00
  2      2      n      0.0000      0.0000e+00    7.9325e+16
  2      1      p      0.9899      0.0000e+00    3.8242e+12
  1      1      p      0.0000      3.9898e+12    3.9898e+12
```

Save the structure.

End Suprem-III

Suprem-III simulation through the field oxide region following all processing steps.

## 50. Example 2: Bipolar Polysilicon Doped Emitter.

Presented here is an example of the simulation of a bipolar process with a polysilicon doped emitter. Two vertical cross-sections are simulated, one through the emitter region, and other through the isolation region.

The structure was simulated using five input files. The first file simulates the processing in the active region of the device up to the point of the isolation oxidation. The second file starts with the result of this first file and completes the processing in the active region. The third file performs an electrical parameter calculation on the resulting structure. As in the first example, the fourth file is similar to the first one, except that the processing in the isolation region is simulated. The fifth file completes the isolation region processing.

The processing sequence used is listed below.

1. The process begins with a high resistivity, <100>, p-type substrate.

2. Thermally oxidize the substrate, growing approximately one micron of silicon dioxide.

3. Remove the oxide layer from the areas where the buried layers are to be placed.

4. Ion implant antimony at a dose of 10ˆ15/cmˆ2. Drive in the buried layer for five hours at 1150 degrees Centigrade.

5. Etch the silicon dioxide from the surface.

6. Epitaxial growth of 1.6 microns of arsenic doped silicon.

7. Thermally grow a 400 Angstrom pad oxide.

8. Deposit 800 Angstroms of silicon nitride.

9. Etch the nitride and oxide from the isolation regions.

10. Etch the silicon halfway through the epi-layer.

11. Ion implant boron in the field regions to increase the surface p doping. Use a dose of 10ˆ13/cmˆ2 and an implant energy of 50 KeV.

12. Thermally oxidize the field regions to an oxide thickness equal to approximately one-half that of the epi-layer.

13. Strip the nitride layer.

14. Using a photoresist mask, implant the base region. Use boron at a dose of 10ˆ14/cmˆ2 and an energy of 50KeV.

15. Etch the oxide from the emitter region.

16. Deposit arsenic doped polysilicon.

17. Remove the polysilicon from the non-emitter regions.

18. Anneal to drive-in the emitter and activate the base diffusion.

Cross-section of locally oxidized bipolar structure simulated in this example. Simulations through the active (emitter-base) region and through the field oxide are shown. In addition, a Poisson solution through the active region is used to calculate the base region sheet resistance as a function of collector-base voltage.

```
                   ********************************
                   ***      Suprem-III       ***
                   ***   version 1B  rev. 8628   ***
                   ********************************

                      Tue Oct 27 16:24:46 1987



  Commands input from file: s3ex2a.in

 1... Title       Suprem-III Example 2.  Bipolar Poly doped emitter.
 2... $           Initial active region formation.
 3... $           File s3ex2a

 4... $ Comment     Initialize the silicon substrate.
 5... Initialize  <100> Silicon,  Boron  Concentration=5e14
  ... +           Thickness=5.  dX=.01  XdX=.05  Spaces=100

 6... Comment     Grow masking oxide for non-active regions.
 7... Diffusion   Temperature=1150  Time=100  WetO2

 8... Comment     Etch the oxide over the buried layer regions.
 9... Etch        Oxide

10... Comment     Implant and drive-in the antimony buried layer.
11... Implant     Antimony  Dose=5E14  Energy=120
12... Diffusion   Temperature=1150  Time=15  DryO2
13... Diffusion   Temperature=1150  Time=300
14... Print       Layer
15... Plot        Net Chemical  Xmax=5

16... Comment     Etch off the oxide.
17... Etch        Oxide

18... Comment     Grow 1.6 micron of arsenic doped epi.
19... Epitaxy     Temperature=1050  Time=4  Growth.Rate=.4
  ...  +          Arsenic Gas.Conc=5E15

20... Comment     Grow a 400A pad oxide.
21... Diffusion   Temperature=1060  Time=20  DryO2

22... Comment     Deposit nitride to mask the field oxidation.
23... Deposit     Nitride  Thickness=.08

24... Comment     Plot the chemical impurity distributions at this point.
25... Print       Layer
26... Plot        Chemical Boron     Xmax=5   Clear  ^Axis  Linetype=2
27... Plot        Chemical Arsenic   Xmax=5  ^Clear  ^Axis  Linetype=4
28... Plot        Chemical Antimony  Xmax=5  ^Clear  ^Axis  Linetype=5
29... Plot        Chemical Net       Xmax=5  ^Clear   Axis  Linetype=1

30... Comment     Save the simulation structure at this point for use in
31... $           subsequent processing.
32... Savefile    Structure  File=s3e2as

33... Stop
```

Suprem-III Example 2. Bipolar Poly doped emitter.
Initial active region formation.
File s3ex2a
Comment Initialize the silicon substrate.

Grow masking oxide for non-active regions.

Etch the oxide over the buried layer regions.

Implant and drive-in the antimony buried layer.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 2 | OXIDE | 0.0694 | 0.0100 | 0.0010 | 422 | 424 | |
| 1 | SILICON | 4.5443 | 0.0100 | 0.0010 | 425 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 2 | 0.0000e+00 | 7.8487e+11 | 0.0000e+00 | 7.9134e+11 |
| 1 | 4.9032e+14 | 4.9032e+14 | 4.9074e+14 | 4.9074e+14 |
| sum | 4.9032e+14 | 4.9110e+14 | 4.9074e+14 | 4.9153e+14 |

Integrated Dopant

| layer | BORON | | ANTIMONY | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 2 | 0.0000e+00 | 3.2381e+09 | 0.0000e+00 | 7.8810e+11 |
| 1 | 2.1107e+11 | 2.1107e+11 | 4.9053e+14 | 4.9053e+14 |
| sum | 2.1107e+11 | 2.1430e+11 | 4.9053e+14 | 4.9131e+14 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 2 | 1 | n | 0.0000 | 0.0000e+00 | 7.9134e+11 |
| 1 | 2 | n | 0.0000 | 4.9041e+14 | 4.9062e+14 |
| 1 | 1 | p | 2.4736 | 9.6534e+10 | 1.0662e+11 |

Etch off the oxide.

Grow 1.6 micron of arsenic doped epi.

Grow a 400A pad oxide.

Deposit nitride to mask the field oxidation.

Plot the chemical impurity distributions at this point.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 3 | NITRIDE | 0.0800 | 0.0100 | 0.0010 | 254 | 262 | |
| 2 | OXIDE | 0.0406 | 0.0100 | 0.0010 | 263 | 266 | |
| 1 | SILICON | 6.1265 | 0.0100 | 0.0010 | 267 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 2 | 0.0000e+00 | 2.4201e+09 | 0.0000e+00 | 2.4201e+09 |
| 1 | 4.8995e+14 | 4.8995e+14 | 4.9037e+14 | 4.9037e+14 |
| sum | 4.8995e+14 | 4.8995e+14 | 4.9037e+14 | 4.9037e+14 |

Integrated Dopant

| layer | ARSENIC | | ANTIMONY | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 2 | 0.0000e+00 | 2.4201e+09 | 0.0000e+00 | 0.0000e+00 |
| 1 | 7.9866e+11 | 7.9866e+11 | 4.8936e+14 | 4.8936e+14 |
| sum | 7.9866e+11 | 8.0108e+11 | 4.8936e+14 | 4.8936e+14 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 3 | 0.0000e+00 | 0.0000e+00 |
| 2 | 0.0000e+00 | 7.3250e-01 |
| 1 | 2.1099e+11 | 2.1099e+11 |
| sum | 2.1099e+11 | 2.1099e+11 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 3 | 1 | n | 0.0000 | 0.0000e+00 | 0.0000e+00 |
| 2 | 1 | n | 0.0000 | 0.0000e+00 | 2.4201e+09 |
| 1 | 2 | n | 0.0000 | 4.9004e+14 | 4.9025e+14 |
| 1 | 1 | p | 4.0558 | 9.6256e+10 | 1.0673e+11 |

Save the simulation structure at this point for use in subsequent processing.

End Suprem-III

Suprem-III simulation of the active device region after drive-in of the buried layer.

Suprem-III simulation of the active device region after drive-in of the buried layer, epi growth, and oxide/nitride deposition.

```
                ********************************
                ***       Suprem-III        ***
                ***   version 1B  rev. 8628   ***
                ********************************

                  Tue Oct 27 16:31:39 1987



  Commands input from file: s3ex2b.in

 1... Title       Suprem-III Example 2.  Bipolar Poly doped emitter.
 2... $           Final active device region formation.
 3... $           File s3ex2b

 4... Comment     Start from the result of s3ex2a.
 5... Initialize  Structure=s3e2as

 6... Comment     Field oxide growth.  Oxidation is masked by nitride.
 7... Diffusion   Temperature=800   Time=30         t.rate=10
 8... Diffusion   Temperature=1000  Time=15  DryO2
 9... Diffusion   Temperature=1100  Time=210 WetO2
10... Diffusion   Temperature=1100  Time=15  DryO2
11... Diffusion   Temperature=1100  Time=10         t.rate=-30
12... Print       Layer
13... Plot        Net Chemical  Xmax=5

14... Comment     Etch the oxide and nitride layers.
15... Etch        Oxide
16... Etch        Nitride
17... Etch        Oxide

18... Comment     Move the fine grid to the surface.
19... Grid        Layer.1  Xdx=0.

20... Comment     Implant the boron base.
21... Implant     Boron  Dose=1E14  Energy=50

22... Comment     Remove oxide from emitter region.
23... Etch        Oxide

24... Comment     Deposit arsenic doped polysilicon for emitter contacts.
25... Deposit     Polysilicon,  Thickness=.5  Temperature=620
 ...  +           Arsenic  Concentration=1e20

26... Comment     Anneal to activate base and drive-in emitter.
27... Diffusion   Temperature=1000  Time=20  WetO2

28... Comment     Plot the electrically Active impurity distributions.
29... Print       Layer
30... Plot        Active  Boron      Xmax=6   Clear ^Axis  Linetype=2
31... Plot        Active  Arsenic    Xmax=6  ^Clear ^Axis  Linetype=4
32... Plot        Active  Antimony   Xmax=6  ^Clear ^Axis  Linetype=5
33... Plot        Active  Net        Xmax=6  ^Clear  Axis  Linetype=1

34... Comment     Save the resulting active region.
35... Savefile    Structure  File=s3e2bs

36... Stop
```

Suprem-III Example 2. Bipolar Poly doped emitter.
Final active device region formation.
File s3ex2b
Start from the result of s3ex2a.

Field oxide growth. Oxidation is masked by nitride.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 4 | OXIDE | 0.0694 | 0.0100 | 0.0010 | 252 | 257 | |
| 3 | NITRIDE | 0.0380 | 0.0100 | 0.0010 | 258 | 262 | |
| 2 | OXIDE | 0.0406 | 0.0100 | 0.0010 | 263 | 266 | |
| 1 | SILICON | 6.1265 | 0.0100 | 0.0010 | 267 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 3 | 0.0000e+00 | 1.1100e+07 | 0.0000e+00 | 1.1104e+07 |
| 2 | 0.0000e+00 | 2.3360e+09 | 0.0000e+00 | 2.3824e+09 |
| 1 | 4.8995e+14 | 4.8995e+14 | 4.9037e+14 | 4.9037e+14 |
| sum | 4.8995e+14 | 4.8995e+14 | 4.9037e+14 | 4.9037e+14 |

Integrated Dopant

| layer | ARSENIC | | ANTIMONY | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 3 | 0.0000e+00 | 1.1102e+07 | 0.0000e+00 | 1.7540e-02 |
| 2 | 0.0000e+00 | 2.3592e+09 | 0.0000e+00 | 2.9405e+02 |
| 1 | 7.9871e+11 | 7.9871e+11 | 4.8936e+14 | 4.8936e+14 |
| sum | 7.9871e+11 | 8.0108e+11 | 4.8936e+14 | 4.8936e+14 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 4 | 0.0000e+00 | 0.0000e+00 |
| 3 | 0.0000e+00 | 1.9123e+03 |
| 2 | 0.0000e+00 | 2.3213e+07 |
| 1 | 2.1096e+11 | 2.1096e+11 |
| sum | 2.1096e+11 | 2.1099e+11 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 4 | 1 | n | 0.0000 | 0.0000e+00 | 0.0000e+00 |
| 3 | 1 | n | 0.0000 | 0.0000e+00 | 1.1104e+07 |
| 2 | 1 | n | 0.0000 | 0.0000e+00 | 2.3824e+09 |
| 1 | 2 | n | 0.0000 | 4.9003e+14 | 4.9027e+14 |
| 1 | 1 | p | 4.3502 | 8.2717e+10 | 9.1007e+10 |

Etch the oxide and nitride layers.

Move the fine grid to the surface.

Implant the boron base.

Remove oxide from emitter region.

Error number 210 detected in line number 23
The material to be etched did not match the top material.
No etching occured.

Deposit arsenic doped polysilicon for emitter contacts.

Anneal to activate base and drive-in emitter.

Plot the electrically Active impurity distributions.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 3 | OXIDE | 0.2924 | 0.0100 | 0.0010 | 214 | 228 | |
| 2 | POLYSILICON | 0.3714 | 0.0100 | 0.0010 | 229 | 266 | 0.5465 |
| 1 | SILICON | 6.1265 | 0.0100 | 0.0010 | 267 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 0.0000e+00 | 5.0738e+14 | 0.0000e+00 | 5.0772e+14 |
| 2 | 3.8821e+15 | 3.9912e+15 | 3.8948e+15 | 4.0039e+15 |
| 1 | 8.7747e+14 | 8.8244e+14 | 1.0649e+15 | 1.0699e+15 |
| sum | 4.7596e+15 | 5.3811e+15 | 4.9597e+15 | 5.5815e+15 |

Integrated Dopant

| layer | ARSENIC | | ANTIMONY | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 0.0000e+00 | 5.0755e+14 | 0.0000e+00 | 1.6316e+03 |
| 2 | 3.8884e+15 | 3.9976e+15 | 4.3948e+04 | 4.3948e+04 |
| 1 | 4.8182e+14 | 4.8680e+14 | 4.8936e+14 | 4.8936e+14 |
| sum | 4.3703e+15 | 4.9919e+15 | 4.8936e+14 | 4.8936e+14 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 3 | 0.0000e+00 | 1.7080e+11 |
| 2 | 6.3257e+12 | 6.3257e+12 |
| 1 | 9.3716e+13 | 9.3716e+13 |
| sum | 1.0004e+14 | 1.0021e+14 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 3 | 1 | n | 0.0000 | 0.0000e+00 | 5.0772e+14 |
| 2 | 1 | n | 0.0000 | 3.8821e+15 | 4.0039e+15 |
| 1 | 4 | n | 0.0000 | 4.6016e+14 | 5.0284e+14 |
| 1 | 3 | p | 0.1051 | 7.1342e+13 | 7.2380e+13 |
| 1 | 2 | n | 0.4744 | 4.8978e+14 | 4.9003e+14 |
| 1 | 1 | p | 4.3076 | 8.3108e+10 | 9.4636e+10 |

Save the resulting active region.

End Suprem-III

Suprem-III simulation of the active device region following field oxidation. The Si3N4 has masked the oxidation in this region, although it has been partially oxidized itself. The Antimony buried layer has diffused upward during the local oxidation process.

Suprem-III simulation of the active device region following all processing steps. The original N epi layer has almost disappeared because of buried layer and base diffusion

```
               ********************************
               ***      Suprem-III        ***
               ***   version 1B  rev. 8628   ***
               ********************************

                 Tue Oct 27 16:36:05 1987



  Commands input from file: s3ex2c.in

 1... Title      Suprem-III Example 2.  Bipolar Poly doped emitter.
 2... $          Electrical simulation of the active device region.
 3... $          File s3ex2c.

 4... Comment    Start with the result of the active device region simulation.
 5... Initialize  Structure=s3e2bs

 6... Comment    Solve Poisson's equation with the collector ramped
 7... $          from 0 volts to 6 volts in 2 volt steps.
 8... Electrical  Extent=3  Steps=4
 9... Bias       Layer=1   Diffusion=3  V.Minority=0  DV.Minority=2
10... Bias       Layer=1   Diffusion=2  V.Majority=0  DV.Majority=2
11... Bias       Layer=1   Diffusion=1  V.Minority=0  DV.Minority=2
12... End

13... Stop
```

Suprem-III Example 2. Bipolar Poly doped emitter.
Electrical simulation of the active device region.
File s3ex2c.
Start with the result of the active device region simulation.

Solve Poisson’s equation with the collector ramped
from 0 volts to 6 volts in 2 volt steps.

Required Iterations = 6

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 1 | 2 | 1 | 0.000e+00 | 3.991e+15 | 0.000e+00 | 9.835e-21 | 2.738e+24 |
| 1 | 1 | 4 | 4.795e+02 | 4.629e+14 | 7.216e-10 | 4.164e+02 | 2.413e+02 |
| 1 | 1 | 3 | 6.950e+13 | 0.000e+00 | 3.456e+01 | 0.000e+00 | 7.879e+02 |
| 1 | 1 | 2 | 6.533e+07 | 4.895e+14 | 1.245e-05 | 3.752e+01 | 6.973e+01 |
| 1 | 1 | 1 | 1.886e+11 | 1.265e+07 | 8.058e-02 | 1.573e-05 | 6.755e+04 |

Required Iterations = 8

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 2 | 2 | 1 | 0.000e+00 | 3.991e+15 | 0.000e+00 | 9.835e-21 | 2.738e+24 |
| 2 | 1 | 4 | 4.795e+02 | 4.629e+14 | 7.216e-10 | 4.164e+02 | 2.413e+02 |
| 2 | 1 | 3 | 6.921e+13 | 0.000e+00 | 3.416e+01 | 0.000e+00 | 7.970e+02 |
| 2 | 1 | 2 | 2.844e+01 | 4.892e+14 | 5.391e-12 | 3.735e+01 | 7.003e+01 |
| 2 | 1 | 1 | 1.251e+11 | 0.000e+00 | 5.355e-02 | 0.000e+00 | 1.017e+05 |

Required Iterations = 11

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 3 | 2 | 1 | 0.000e+00 | 3.991e+15 | 0.000e+00 | 9.835e-21 | 2.738e+24 |
| 3 | 1 | 4 | 4.795e+02 | 4.629e+14 | 7.216e-10 | 4.164e+02 | 2.413e+02 |
| 3 | 1 | 3 | 6.898e+13 | 0.000e+00 | 3.388e+01 | 0.000e+00 | 8.037e+02 |
| 3 | 1 | 2 | 0.000e+00 | 4.889e+14 | 0.000e+00 | 3.725e+01 | 7.024e+01 |
| 3 | 1 | 1 | 8.433e+10 | 0.000e+00 | 3.609e-02 | 0.000e+00 | 1.508e+05 |

Required Iterations = 17

| Step | Layer | Region | Concentration Holes | Concentration Electrons | Conductivity Holes | Conductivity Electrons | Sheet Resistivity |
|---|---|---|---|---|---|---|---|
| 4 | 2 | 1 | 0.000e+00 | 3.991e+15 | 0.000e+00 | 9.835e-21 | 2.738e+24 |
| 4 | 1 | 4 | 4.795e+02 | 4.629e+14 | 7.216e-10 | 4.164e+02 | 2.413e+02 |
| 4 | 1 | 3 | 6.876e+13 | 0.000e+00 | 3.363e+01 | 0.000e+00 | 8.095e+02 |
| 4 | 1 | 2 | 0.000e+00 | 4.887e+14 | 0.000e+00 | 3.716e+01 | 7.040e+01 |
| 4 | 1 | 1 | 5.164e+10 | 0.000e+00 | 2.210e-02 | 0.000e+00 | 2.463e+05 |

End Suprem-III

Plot of base region sheet resistance vs. collector base voltage based upon a Suprem-III Poisson solution through the active device region.

```
                *********************************
                ***       Suprem-III        ***
                ***   version 1B  rev. 8628   ***
                *********************************

                  Tue Oct 27 16:36:45 1987



  Commands input from file: s3ex2d.in

 1... Title       Suprem-III Example 2.  Bipolar Poly Doped Emitter
 2... $           Initial isolation region formation.
 3... $           File s3ex2d.

 4... Comment     Initialize the silicon substrate.
 5... Initialize  <100> Silicon, Boron  Concentration=5E14
  ... +           Thickness=3  dX=.03  Spaces=75

 6... Comment     Grow masking oxide for the non-active regions.
 7... Diffusion   Temperature=1150  Time=100  WetO2

 8... Comment     Implant and drive in the antimony buried layer.
 9... Implant     Antimony  Dose=1E15  Energy=80
10... Diffusion   Temperature=1150  Time=15   DryO2
11... Diffusion   Temperature=1150  Time=300
12... Print       Layer
13... Plot        Net Chemical  Xmax=4.5

14... Comment     Etch off the oxide.
15... Etch        Oxide

16... Comment     Add 1.6 microns of arsenic doped epi.
17... Epitaxy     Temperature=1050  Time=4  Growth.Rate=.4
  ... +           Arsenic  Gas.Conc=5E15

18... Comment     Grow a 400A pad oxide.
19... Diffusion   Temperature=1060  Time=20  DryO2

20... Comment     Deposit a 800A layer of silicon-nitride.
21... Deposit     Nitride  Thickness=.08

22... Comment     Plot the chemical impurity distributions at this point.
23... Print       Layer
24... Plot        Chemical  Boron     Xmax=5   Clear  ^Axis  Linetype=2
25... Plot        Chemical  Arsenic   Xmax=5  ^Clear  ^Axis  Linetype=4
26... Plot        Chemical  Antimony  Xmax=5  ^Clear  ^Axis  Linetype=5
27... Plot        Chemical  Net       Xmax=5  ^Clear   Axis  Linetype=1

28... Comment     Save the initial part of the isolation simulation.
29... Savefile    Structure  File=s3e2ds

30... Stop
```

Suprem-III Example 2. Bipolar Poly Doped Emitter
Initial isolation region formation.
File s3ex2d.
Initialize the silicon substrate.

Grow masking oxide for the non-active regions.

Implant and drive in the antimony buried layer.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 2 | OXIDE | 0.9756 | 0.0100 | 0.0010 | 423 | 437 | |
| 1 | SILICON | 2.5708 | 0.0300 | 0.0010 | 438 | 500 | <100> |

Integrated Dopant

| layer no. | Net active | Net chemical | Total active | Total chemical |
|---|---|---|---|---|
| 2 | 0.0000e+00 | 4.6861e+14 | 0.0000e+00 | 4.6868e+14 |
| 1 | -1.1331e+11 | -1.1331e+11 | 1.1331e+11 | 1.1331e+11 |
| sum | -1.1331e+11 | 4.6850e+14 | 1.1331e+11 | 4.6879e+14 |

Integrated Dopant

| layer no. | BORON active | BORON chemical | ANTIMONY active | ANTIMONY chemical |
|---|---|---|---|---|
| 2 | 0.0000e+00 | 3.5514e+10 | 0.0000e+00 | 4.6864e+14 |
| 1 | 1.1331e+11 | 1.1331e+11 | 2.0222e+01 | 2.0222e+01 |
| sum | 1.1331e+11 | 1.4883e+11 | 2.0222e+01 | 4.6864e+14 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 2 | 2 | n | 0.0000 | 0.0000e+00 | 4.6866e+14 |
| 2 | 1 | p | 0.5489 | 0.0000e+00 | 1.7370e+10 |
| 1 | 1 | p | 0.0000 | 1.1331e+11 | 1.1331e+11 |

Etch off the oxide.

Add 1.6 microns of arsenic doped epi.

Grow a 400A pad oxide.

Deposit a 800A layer of silicon-nitride.

Plot the chemical impurity distributions at this point.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 3 | NITRIDE | 0.0800 | 0.0100 | 0.0010 | 374 | 382 | |
| 2 | OXIDE | 0.0415 | 0.0100 | 0.0010 | 383 | 384 | |
| 1 | SILICON | 4.1525 | 0.0300 | 0.0010 | 385 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 2 | 0.0000e+00 | 5.3688e+08 | 0.0000e+00 | 5.3688e+08 |
| 1 | 6.8806e+11 | 6.8806e+11 | 9.1451e+11 | 9.1451e+11 |
| sum | 6.8806e+11 | 6.8860e+11 | 9.1451e+11 | 9.1505e+11 |

Integrated Dopant

| layer | ARSENIC | | ANTIMONY | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 3 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 |
| 2 | 0.0000e+00 | 5.3688e+08 | 0.0000e+00 | 0.0000e+00 |
| 1 | 8.0129e+11 | 8.0129e+11 | 1.9762e+01 | 1.9762e+01 |
| sum | 8.0129e+11 | 8.0182e+11 | 1.9762e+01 | 1.9762e+01 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 3 | 0.0000e+00 | 0.0000e+00 |
| 2 | 0.0000e+00 | 6.1677e+00 |
| 1 | 1.1323e+11 | 1.1323e+11 |
| sum | 1.1323e+11 | 1.1323e+11 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 3 | 1 | n | 0.0000 | 0.0000e+00 | 0.0000e+00 |
| 2 | 1 | n | 0.0000 | 0.0000e+00 | 5.3688e+08 |
| 1 | 2 | n | 0.0000 | 7.9334e+11 | 8.0685e+11 |
| 1 | 1 | p | 1.7303 | 1.0504e+11 | 1.0587e+11 |

Save the initial part of the isolation simulation.

End Suprem-III

Suprem-III simulation of the field oxide isolation region after drive-in of the buried layer.

Suprem-III simulation of the field oxide isolation region after epi growth and oxide/nitride deposition.

```
*********************************
***       Suprem-III        ***
***   version 1B  rev. 8628   ***
*********************************

   Tue Oct 27 16:38:59 1987



Commands input from file: s3ex2e.in

 1... Title       Suprem-III Example 2.  Bipolar Poly doped emitter.
 2... $           Final isolation region formation.
 3... $           File s3ex2e.

 4... Comment     Start with the result of S3EX2D.
 5... Initialize  Structure=s3e2ds  Thickness=6

 6... Comment     Etch the nitride and oxide layers.
 7... Etch        Nitride
 8... Etch        Oxide

 9... Comment     Etch half the silicon epi layer.
10... Etch        Silicon  Amount=.8

11... Comment     Implant boron in the field region.
12... Implant     Boron  Dose=2E13  Energy=100

13... Comment     Grow the field oxide.
14... Diffusion   Temperature=800   Time=30         T.Rate=10
15... Diffusion   Temperature=1100  Time=15   DryO2
16... Diffusion   Temperature=1100  Time=210  WetO2
17... Diffusion   Temperature=1100  Time=15   DryO2
18... Diffusion   Temperature=1100  Time=10         T.Rate=-30
19... Print       Layer

20... Comment     Implant the boron base.
21... Implant     Boron  Dose=1E14  Energy=80

22... Comment     Deposit arsenic doped polysilicon for the emitter contact.
23... Deposit     Polysilicon,  Thickness=.5  Temperature=620.
 ...  +           Arsenic  Concentration=1E20

24... Comment     Remove the polysilicon.
25... Etch        Polysilicon

26... Comment     Anneal to activate base and emitter regions.
27... Diffusion   Temperature=1000  Time=20  WetO2

28... Comment     Plot the electrically active impurity distributions.
29... Print       Layer
30... Plot        Active  Boron      Xmax=5   Clear  ^Axis  Linetype=2
31... Plot        Active  Arsenic    Xmax=5  ^Clear  ^Axis  Linetype=4
32... Plot        Active  Antimony   Xmax=5  ^Clear  ^Axis  Linetype=5
33... Plot        Active  Net        Xmax=5  ^Clear   Axis  Linetype=1

34... Comment     Save the final isolation region simulation.
35... Savefile    Structure  File=s3e2es
```

36... Stop

Suprem-III Example 2. Bipolar Poly doped emitter.
Final isolation region formation.
File s3ex2e.
Start with the result of S3EX2D.

Etch the nitride and oxide layers.

Etch half the silicon epi layer.

Implant boron in the field region.

Grow the field oxide.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 2 | OXIDE | 1.2354 | 0.0100 | 0.0010 | 407 | 424 | |
| 1 | SILICON | 4.6564 | 0.0300 | 0.0010 | 425 | 500 | <100> |

Integrated Dopant

| layer no. | Net active | Net chemical | Total active | Total chemical |
|---|---|---|---|---|
| 2 | 0.0000e+00 | -1.3720e+13 | 0.0000e+00 | 1.3992e+13 |
| 1 | -4.8603e+12 | -4.8603e+12 | 5.3040e+12 | 5.3040e+12 |
| sum | -4.8603e+12 | -1.8580e+13 | 5.3040e+12 | 1.9296e+13 |

Integrated Dopant

| layer no. | ARSENIC active | ARSENIC chemical | ANTIMONY active | ANTIMONY chemical |
|---|---|---|---|---|
| 2 | 0.0000e+00 | 1.3628e+11 | 0.0000e+00 | 3.3793e-01 |
| 1 | 2.2189e+11 | 2.2189e+11 | 1.9424e+01 | 1.9424e+01 |
| sum | 2.2189e+11 | 3.5816e+11 | 1.9424e+01 | 1.9762e+01 |

Integrated Dopant

| layer no. | BORON active | BORON chemical |
|---|---|---|
| 2 | 0.0000e+00 | 1.3856e+13 |
| 1 | 5.0822e+12 | 5.0822e+12 |
| sum | 5.0822e+12 | 1.8938e+13 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 2 | 1 | p | 0.0000 | 0.0000e+00 | 1.3992e+13 |
| 1 | 2 | n | 0.0000 | 5.9448e+09 | 5.1887e+10 |
| 1 | 1 | p | 0.0404 | 4.8305e+12 | 5.2176e+12 |

Implant the boron base.

Deposit arsenic doped polysilicon for the emitter contact.

Remove the polysilicon.

Anneal to activate base and emitter regions.

Plot the electrically active impurity distributions.

| layer no. | material type | thickness (microns) | dx (microns) | dxmin | top node | bottom node | orientation or grain size |
|---|---|---|---|---|---|---|---|
| 2 | OXIDE | 1.2687 | 0.0100 | 0.0010 | 407 | 424 | |
| 1 | SILICON | 4.6418 | 0.0300 | 0.0010 | 425 | 500 | <100> |

Integrated Dopant

| layer | Net | | Total | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 2 | 0.0000e+00 | -1.1853e+14 | 0.0000e+00 | 1.1880e+14 |
| 1 | -4.7368e+12 | -4.7368e+12 | 5.1778e+12 | 5.1778e+12 |
| sum | -4.7368e+12 | -1.2326e+14 | 5.1778e+12 | 1.2398e+14 |

Integrated Dopant

| layer | ARSENIC | | ANTIMONY | |
|---|---|---|---|---|
| no. | active | chemical | active | chemical |
| 2 | 0.0000e+00 | 1.3770e+11 | 0.0000e+00 | 3.9708e-01 |
| 1 | 2.2046e+11 | 2.2046e+11 | 1.9365e+01 | 1.9365e+01 |
| sum | 2.2046e+11 | 3.5816e+11 | 1.9365e+01 | 1.9762e+01 |

Integrated Dopant

| layer | BORON | |
|---|---|---|
| no. | active | chemical |
| 2 | 0.0000e+00 | 1.1866e+14 |
| 1 | 4.9573e+12 | 4.9573e+12 |
| sum | 4.9573e+12 | 1.2362e+14 |

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

| layer no. | region no. | type | junction depth (microns) | net active Qd | total chemical Qd |
|---|---|---|---|---|---|
| 2 | 1 | p | 0.0000 | 0.0000e+00 | 1.1880e+14 |
| 1 | 1 | p | 0.0000 | 4.7368e+12 | 5.1778e+12 |

Save the final isolation region simulation.

End Suprem-III

Suprem-III simulation through the field oxide isolation region after all processing steps. Isolation has been achieved since the substrate is all p type, although barely. The base implant is also seen in the field oxide.

## 51. Suggestions and Bug Reports

In any program of the size of Suprem-III there is bound to be at least one bug (Do I hear some laughter?). And even if everything works as claimed, there will always be room for improvement. Therefore, I am listing both an electronic and U.S. mail address for such things as bug reports, suggestions, complaints, and compliments (if any).

Please send as much detail as possible about the problem and especially indicate which version of the program you are using and what system you are working on.


Electronic Mail U.S Mail

via INTERNET: Suprem-III
sup3bugs@Oasis.Stanford.Edu c/o Stephen E. Hansen
Applied Electronics Labs
via BITNET: Stanford University
SUP3BUGS%OASIS@STANFORD Stanford, California
94305
via USENET (UUCP):
{ucbvax,hplabs,decwrl,ihnp4}!{glacier,shasta}!oasis!sup3bugs

via CSNET:
sup3bugs%Oasis.Stanford.Edu@csnet-relay.arpa


If you can manage it I really prefer electronic mail as it makes response easier. In either case the response time will depend on a number of factors, primarily the severity of the problem.

Your feedback is crucial and appreciated!

Thanks,

Stephen E. Hansen