Aquarius TCAD User Manual

Pre-Release DRAFT

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General Introduction

Aquarius is a mixed mode 2D semiconductor process, device and circuit simulator for the desktop PC. With Aquarius you can create complex physical models of semiconductor devices and build sophisticated circuits with the minimum of effort in a powerful, yet easy to use TCAD environment. With access to the full range of device physics (including electro-thermal modelling), Aquarius provides a reliable and cost effective way to evaluate the performance and characteristics of most semiconductor devices before committing to fabrication.

Aquarius is composed of three highly integrated modules:

Device Simulator: Used to define the physical attributes of a two-dimensional semiconductor device structure. The definition of the device may be imported from a fabrication process model or defined directly without reference to a process model. The device model is then conveyed to the circuit simulator module for electrothermal simulation in the context of a circuit.

Circuit Simulator: Used to define the circuit and bias conditions for the device, it also solves the device and circuit equations, saving the results to a disk file.

Post Processor: Used to view the results of a simulation and to obtain hard copies.

Device Modelling

The definition of a physical device model consists of several steps. This includes the definition of the device geometry, doping and physical properties of the device, as well as the finite element mesh used in the analysis and the models employed to simulate the device.

To define the device geometry directly, a user friendly CAD interface is provided that enables the user to rapidly construct complex device structures and to define the material regions. The user can also define ancillary items and properties such as electrical and thermal contacts and interface states.

The doping profile of the device is normally defined in the fabrication process model. However, the doping profile can also be defined directly without reference to a process model. Functions are provided to allow the user to apply uniform doping concentrations to device regions and the definition of more complex profiles specified through windows which can be placed on any horizontal surface in the geometry. Standard functions (Guassian and error function) or a use defined profile can be specified though each window. The user defined data can come from measurements or from a process simulation package such as SUPREM. All the different doping steps are summed to give a total doping concentration. The shape of the lateral doping profile can also be specified.

The finite element mesh generator is based on the Delaunay triangulation method for connecting up a given set of points into an optimum set of triangles. Using this technique, any set of points can be triangulated to give a set of triangles with positive pipe-widths along triangle edges. This is a very important consideration when solving the current continuity equations in the main solver. The difficulty is thus defining the location of a set of nodes for the analysis. The user has the task of defining a set of orthogonal lines in the x any y directions. The intersection of these lines gives a set of nodes that will be used in the mesh definition. Lines need not extend the entire span of the device in the x or y directions. The termination of the lines in this way allows regions of localised refinement to be defined, allowing the nodes to be placed in the place they are needed. An existing mesh may also be refined in the X or Y direction to refine a mesh in a given region.

Finally, a range of physical models are available to be used in the simulation of the device being defined and can be configured by the user. The available models include:

- **Mobility**
  - Constant
  - Impurity
  - Carrier-Scattering
  - Surface
  - Field Dependent
- **Generation Recombination**
  - Shockley-Read-Hall
  - Direct
  - Auger
  - Impact Ionisation
- **Optical**
- **Band-gap Narrowing**
- **Fermi-Dirac Statistics**
- **Temperature**
- **Surface Recombination Effects**

The physical models employed by the simulator are described in more detail in the reference section at the end of this document.

Circuit Simulation

The previous section described the definition of a two-dimensional device model. The next step involves the definition of a circuit to drive the device model. Principally, this involves loading the device model into the circuit environment and defining a complete circuit around it. The mixed mode capabilities of the simulator mean that the circuit may contain passive and active components as well as other two-dimensional devices or predefined circuit models. Once a suitable circuit has been defined, the device structure can be simulated in any one of three modes of operation:

1. **Steady State** - Define a set of steady state (DC) bias points.
2. **Transient** - Define a transient waveform and perform a temporal simulation.
3. **IV Curve Tracer** - Perform a steady state curve trace.

Simulations can also be re-started from existing simulations as a continuation run from an initial condition. Sometimes re-starting a simulation from an initial condition is desirable when the numerical complexity of a model is such that the solver will fail to converge on a solution and an indirect approach is required.

The solver employed in the simulation of the circuit and solution of the device physics equations is fully configurable. In many cases, the default settings of the solver will be appropriate for most simulations. However, for highly non-linear problems the user can adjust the search parameters to achieve optimum convergence on a solution.

Simulation Results

The post processor module is used to view the results of the numerical calculations and to export the relevant data. The module enables the following results to be extracted from the simulation:

- **Cut Line** - For producing line plots on "cuts" through the 2D cross-section of device models.
- **Contour** - For producing contour plots at device level.
- **Isometric** (coming soon) - For producing 3-D isometric plots at device level.
- **I-V Plot** for producing terminal I/V characteristics at circuit level.
- **Transient** (coming soon) - For plotting transient terminal and circuit waveforms at circuit level.

The first three modes are used to plot the internal distributions in the device, and the last two are for looking at the terminal quantities of the device.

The philosophy for viewing the internal distributions is to define what you want to plot. This will include the selection of the required plot variable (e.g. Electrostatic Potential, Electron Concentration, Net Doping Concentration etc.), the required result case number(s) and the type of plot (i.e. Cut Line, Isometric or Contour Plot). Terminal quantities are extracted directy at circuit level.

The following results are available at device level:

- Electrostatic Potential
- Hole and Electron Quasi-Fermi Levels
- Electron and Lattice Temperatures
- Acceptor and Donor Concentrations

- Valence and Conduction Band Energies
- Intrinsic Fermi-Energy
- Hole and Electron Quasi-Fermi Energies
- Hole and Electron Concentrations
- Intrinsic Carrier Concentration
- Valence and Conduction Band Off-set Parameters
- Net Doping Concentration
- Net Charge Concentration
- Recombination Rate
- Hole and Electron Mobilities
- E-Field Magnitude (or X and Y components of)
- Hole Current Magnitude (or X and Y components of)
- Electron Current Magnitude (or X and Y components of)
- Total Current Magnitude (or X and Y components of)

Release History

Current Release : Version 0.0.1

Release History: v0.0.1 : (December 09, 2024)

- Initial Release.

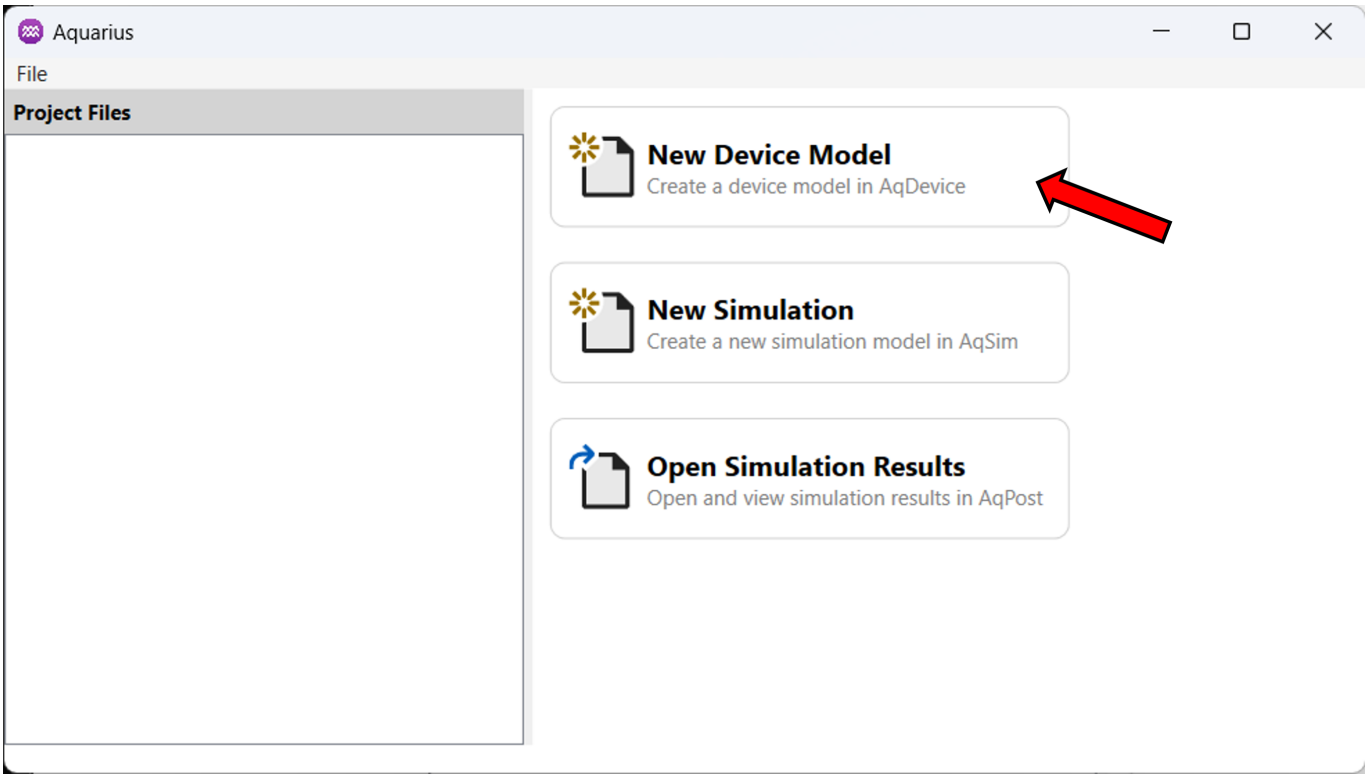
Device Modelling

Introduction to Device Modelling

The definition of a physical device model consists of several steps. This includes the definition of the geometry, doping and physical properties of the device, as well as the finite element mesh used in the analysis and the models employed to simulate the device. The geometry, doping profile and meshing of a device may be (*imported from a fabrication process simulation - coming soon*) or defined directly without reference to a process model.

To create a new device model directly without reference to process model data:

1. From the Main Window, Select New Device Model.
2. When prompted *Do you want to create a new Device Model (.sdm) file?*, click OK.



The definition of a physical device model consists of several steps. This includes the definition of the device geometry, doping and physical properties of the device, as well as the finite element mesh used in the analysis and the models employed to simulate the device.

To define the device geometry directly, a user friendly CAD interface is provided that enables the user to rapidly construct complex device structures and to define the material regions. The user can also define ancillary items and properties such as electrical and thermal contacts and interface states.

The doping profile of the device is normally defined in the fabrication process model. However, the doping profile can also be defined directly without reference to a process model. Functions are provided to allow the user to apply uniform doping concentrations to device regions and the definition of more complex profiles specified through windows which can be placed on any horizontal surface in the geometry. Standard functions (Guassian and error function) or a use defined profile can be specified though each window. The user defined

data can come from measurements or from a process simulation package such as SUPREM. All the different doping steps are summed to give a total doping concentration. The shape of the lateral doping profile can also be specified.

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  - Auger
  - Impact Ionisation
- **Optical**
- **Band-gap Narrowing**
- **Fermi-Dirac Statistics**
- **Temperature**
- **Surface Recombination Effects**

The physical models employed by the simulator are described in more detail in the reference section at the end of this document.

2.2 Device Shape (Not sure if this is right? - I think this is now defined in the circuit simulator)

Device Shape

The shape of a device can be defined as either linear or cylindrical. The z axis depth of the device (into the screen) can also be specified.

To edit the global shape properties of the device:

1. From the main menu, select Device..Shape.

 alt text

Parameters

Depth Scale Factor: The device is assumed to be 1cm deep in the z-direction by default if a linear device is used, and the area if a cylindrical device is chosen is calculated by rotating the device around the specified origin. This parameter allows the device depth / effective area to be increased by a scaling factor.

Device Shape: Either linear or cylindrical. Selects how device is represented in the 3rd spatial dimension. If cylindrical is selected the device is solved in cylindrical co-ordinates and is swept around the x values specified by the parameter x axis rotation origin.

X Axis Rotation Origin: Origin around which the device is rotated if cylindrical type is chosen.

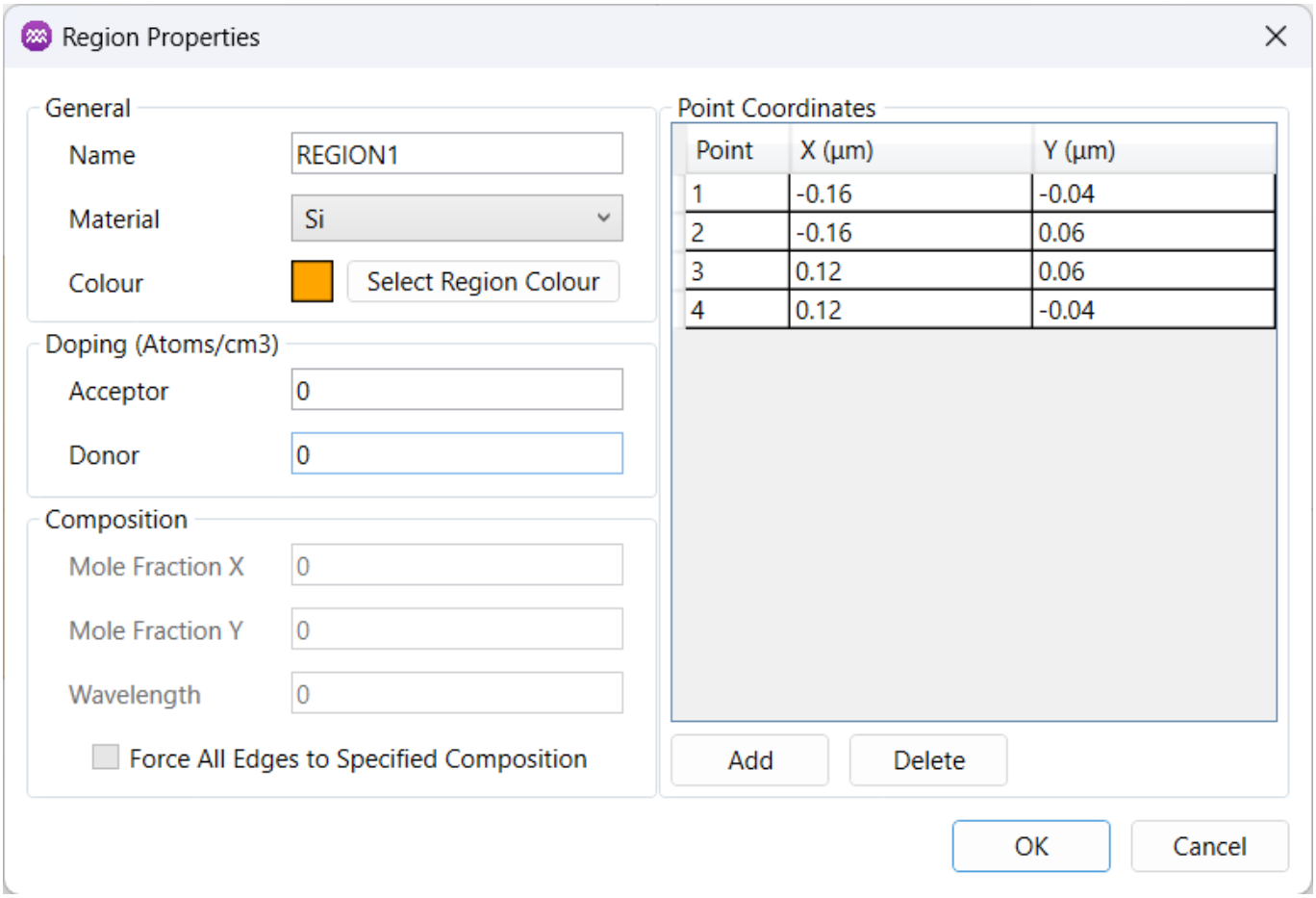
2.4 Device Regions

One of the most important features of the Aquarius's device modelling capabilities is the ability to define the geometry of a device's regions using the Rectangle, Rounded Rectangle, Polygon and Import from CSV drawing functions.

After the outline geometry of a device has been drawn, the regions properties can be defined and material properties assigned to them.

To define a region:

1. From the Menu, select Define..Region and select the type of geometry you would like to define (Rectangle, Polygon etc.).
2. Once the region's shape has been defined, it will be filled with colour to denote that it is a defined region and the region properties dialog box will appear.



Region Properties

General

demo
demo

demo

- Name: A unique idemtifier for the region. Note: No two regions may share the same name.
- Material: Used to define the material properties of the region. Available materials include Si, SiC, Oxide, Air (more coming soon). The properties of these materials can be fully customised by the user during setup of the device model. Note: There are two general types of semiconductor can be defined, namely:

1. Single Composition (e.g. Si, GaAs)
2. Variable Composition (e.g. AlGaN).

Doping

Parameters:

- Acceptor Doping: Used to define the acceptor doping concentration in the region. (Units = Atoms/cm3).
- Donor Doping: Used to define the donor doping concentration in the region. (Units = Atoms/cm3).

Composition (Coming soon)

After a region has been defined, the user can specify a constant compositional profile over the region. The mole fraction X for a ternary compound and both X and Y mole fractions for quaternary materials can be specified. This command sets a constant values in a specified region.

Parameters:

- Mole Fractions X and Y: Used define the mole fractions X and Y. Value range between 0 and 1.
- Wavelength: Re-calculates X and Y from the cut-off wavelength of the specific material.
- Force All Edges to Specified Composition: Forces all the lines (edges) of a defined region to have the compositions defined by X and Y in the Mole-fraction parameter.
- InGaAsP Lattice Match: Uses the value of the Y mole fraction to re-calculate the X mole fraction in order give the correct compositions for the specified lattice matching (Only applies to InGaAsP structures). Options to specify Off, GaAs or InP.

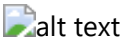
2.6 Graded Composition (Coming Soon)

Graded Composition Windows allow a user to specify a rectangular window where a graded compositional profile can set up for hetero-junction structures.

To draw a graded composition window:

1. From the main menu, select Define..Window..Composition.
2. Drag the cursor to define a rectangular graded composition window.

Once a graded composition window has been defined, the graded composition window properties dialog box will appear. In this dialog, a graded mole fraction profile can be specified. Double-click the cursor on the window to edit its properties at any time.

 alt text

Parameters

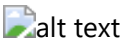
Mole Fractions: Used define the mole fraction grading across the window. If a horizontal gradient direction is specified then the user can input the left and right mole fractions to correspond with the left and right sides of the graded composition window. If a vertical gradient direction is specified then the user can input the top and bottom mole fractions to correspond with the top and bottom sides of the graded composition window.
Gradient profile: Used select the type of grading of the composition. Options are linear or hyperbolic tangent (tanh) functions.
Gradient direction: Used select the direction of the gradient. Options are vertical (top to bottom) grading of the mole fraction or horizontal (left to right) grading of the mole fraction.
Layout parameters: Used the specifiy the position of the graded composition window.

2.7 Material Properties

Material Properties

Aquarius contains a library of materials for the commonly used semiconductor and non-semiconductor materials. To edit material properties:

1. From the main menu, select Device..Materials.
2. Select the Properties tab. In the materials library the user can edit the properties associated with each individual material and even define completely new materials.



Parameters

General Properties:

Semcn: Semiconductor material (1=yes, -1=no)
Fixsc: Fixed semiconductor (1=single composition material e.g. silicon, -1=variable composition material e.g. AlGaAs). Used in heterojunction module.
Epslr: Relative dielectric constant Eg: Band gap (eV)
Affin: Electron Affinity (eV)
Mass_p: Relative hole and electron effective masses
Mass_n: Relative hole and electron effective masses
Lat_const: Lattice constant (Angstroms)

Mobility Properties:

Mu_0_p: Constant mobilities for holes and electrons (cm2/Vs)
Mu_0_n: Constant mobilities for holes and electrons (cm2/Vs)
Mu_AlpT_p: Temperature coefficients for lattice scattering mobility
Mu_AlpT_n: Temperature coefficients for lattice scattering mobility
Mu_max_p: Maximum mobilities, also used in lattice scattering mobility which reduces maximum mobility with increasing lattice temperature (cm2/Vs)
Mu_min_p: Minimum mobilities, used in the impurity and carrier scattering mobility expression (cm2/Vs)
Mu_nref_p: Reference doping used in the impurity and carrier scattering mobility expression (cm-3)
Mu_alpD_p: Coefficients used in the impurity and carrier scattering mobility expression (units)
Mu_max_n: Maximum mobilities, also used in lattice scattering mobility which reduces maximum mobility with increasing lattice temperature (cm2/Vs)
Mu_min_n: Minimum mobilities, used in the impurity and carrier scattering mobility expression (cm2/Vs)
Mu_nref_n: Reference doping used in the impurity and carrier scattering mobility expression (cm-3)
Mu_alpD_n: Coefficients used in the impurity and carrier scattering mobility expression
Mu_vsat_p: Carrier saturation velocities at 300K (cm s-1)
Mu_beta_p: Coefficients for field dependent mobility
Mu_vsat_n: Carrier saturation velocities at 300K (cm s-1)
Mu_beta_n: Coefficients for field dependent mobility
Mu_gsur_p: Oxide interface mobility reduction factor

Mu_gsur_n: Oxide interface mobility reduction factor
Mu_S_Ec_p: Critical electric fields for electron and hole oxide interface mobility model: (V cm-1)
Mu_S_Ec_n: Critical electric fields for electron and hole oxide interface mobility model: (V cm-1)
E_trap: Trap energy relative to the intrinsic Fermi-level (eV)

Recombination Properties:

SRH_TAU_p: Minority carrier lifetimesunits (secs)
SRH_Ap: Coefficients used in doping dependent lifetime models
SRH_Bp: Coefficients used in doping dependent lifetime models
SRH_Cp: Coefficients used in doping dependent lifetime models
SRH_Dp: Coefficients used in doping dependent lifetime models
SRH_Nrefp: Reference doping concentrations for lifetime models (cm-3)
SRH_TAU_n: Minority carrier lifetimesunits (secs)
SRH_An: Coefficients used in doping dependent lifetime models
SRH_Bn: Coefficients used in doping dependent lifetime models
SRH_Cn: Coefficients used in doping dependent lifetime models
SRH_Dn: Coefficients used in doping dependent lifetime models
SRH_Nrefn: Reference doping concentrations for lifetime models (cm-3)
Auger_Cp: Auger coefficients (cm6 s-1)
Auger_Cn: Auger coefficients: (cm6 s-1)
Direct_C: Direct recombination coefficient (cm3 s-1)
Av_alph_p: Avalanche prefactor coefficients (cm-1)
Av_beta_p: Avalanche exponential coefficients (V/cm)
Av_alph_n: Avalanche prefactor coefficients (cm-1)
Av_beta_n: Avalanche exponential coefficients (V/cm)

Optical Properties:

Abscoeff: Optical absorption coefficient (cm-1)

Thermal Properties:

Ther_cond: Thermal conductivity
Heat_Capa: Thermal heat capacity
Ther_coef: Coefficient for thermal conductivity
Vs_coefTp: Coefficients for temperature dependent saturation velocity
Vs_coefTn: Coefficients for temperature dependent saturation velocity

2.8 Material Models

Material Models

The physical models implemented in the simulator are fully configurable. To configure the physical models:

1. From the main menu, select Device..Materials.
2. Select the Models tab.

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Parameters

General Parameters:

Reference Material: Used to select reference material to calculate reference energy levels to. Used mainly in heterojunction devices.
Temperature: Ambient temperature for the simulation. Kelvin

Mobility Models:

Low Field Mobility: Option to set as constant, lattice, impurity or carrier_carrier. If the constant model is selected then mobility is set to the value supplied in the properties command. If the lattice model is selected then the reduction in mobility due to increased collision with the lattice with increased temperature will be taken into account. If the impurity model is selected then the reduction in mobility due to extra collisions with the lattice is taken into account. If the carrier_carrier model is selected then the reduction in mobility due to extra collisions with the lattice is taken into account, except that the carrier concentration is taken into account (very important at high injection levels). Note: If the high field model is selected then the low-field mobility model will feed into the high field-mobility model. Otherwise it will be the mobility used in the simulation.
High Field Mobility: Option to set as none, e_field or j_field. The e_field or j_field models are used to select the high-field mobility model, which can be based on either the electric field magnitude or the magnitude of the field in the direction of the current.
High Field Calculation: Option to set as edge or element. Used to choode how the highfield mobility field is calculated. This will either use the values along an element edge or calculate the field based on the whole element.
Surface Mobility: Option to set as yes or no. Used to select surface mobility along oxide semiconductor interfaces. This model only affects those edges that actually lie along the interface.

Recombination Models:

SRH: Option to set as yes or no. Used to select Shockley Read Hall recombination model.
Auger: Option to set as yes or no. Used to select Auger recombination model. *Direct*: Option to set as yes or no. Used to select direct band-to-band recombination model.
Avalanche: Option to set as none, II_ELEM or II_EDGE. II_ELEM is used to select an impact-ionisation model

based on a discretisation that uses the full elemental information. II_EDGE is used to select an impact-ionisation model based on a discretisation along an edge of an element only.

Other Models:

Band Gap Narrowing: Option to set as none, Slotboom, Gaur. Used to select the bandgap narrowing model used in regions of heavy doping. Both Slotboom and Gaur models are empirical and are descibed in the reference section of this manual.
Transport: Option to set as drift-diffusion or energy. Used to select drift-diffusion or energy transport model (not fully implemented)
Statistics: Option to set as boltz or fermi. Used to select Boltzmann or Fermi-Dirac carrier statistics. Using Fermi-direct is slightly slower than the Boltzmann approximation.
Heat Source: Option to set as element or edge. Used to select how to calculate the heat source term in an electro-thermal simulation.

2.9 Contacts

Electrical and Thermal Contacts

Electrical and/or thermal contacts can be added to any edge or combination of edges on the perimeter of a region. Individual contacts can be made up of several different edges. Contacts can also be split across different regions and can occur at the junction between two different regions. In order to successfully model a device, the model requires a minimum of two contacts to be specified. The maximum number of contacts than can be added to a device model is eight.

To define a contact:

1. From the main toolbar, click on the Select Edge button.
2. With the cursor, select all the geometric edges which comprise the contact.
3. Select Device..Define..Contact from the main menu to create a contact.

Once a contact has been defined, the contact properties dialog box will appear allowing its properties to be edited. Double-click the cursor on the contact to activate the contact properties dialog box at any time.

 alt text

Parameters

Contact Type: Option to set as Ohmic or Schottky. Selects how contact will interact with the semiconductor.
Work Function: Work function of the metal. Used to calculate the barrier height for a Schottky diode or the Flat-band voltage for an oxide contact.
P Richardson: If set to a non-zero value is used as the Richardson constant to calculate the thermionic emission current for holes.
N Richardson: If set to a non-zero value is used as the Richardson constant to calculate the thermionic emission current for electrons.
Barrier Lowering: Option to set on or off. Select if image force barrier lowering is included at a Schottky contact.
Dipole Alpha: Coefficient for calculating dipole lowering of Schottky barrier height.
Resistance: Thermal resistance at ambient temperature. Kelvin / Watt
Capacitance: Thermal capacitance at ambient temperature. Joules / Kelvin.
Ambient Temperature: Ambient temperature used in the simulation. Kelvin

2.10 Surface States

Surface States

A surface state can be added to any edge or combination of edges on the perimeter of a region. This allows the user to specify interface/surface properties, including recombination velocities, fixed charges and fast surface states. Individual surface states can be composed of several different edges. Surface states can also be split across different regions and can occur at the junction between two different regions.

To define a surface state:

1. From the main toolbar, click on the Select Edge button.
2. With the cursor, select all the geometric edges which comprise the contact.
3. Select Device..Define..Surface from the main menu to create a surface state.

Once a surface state has been defined, the properties dialog box will appear allowing its properties to be edited. Double-click the cursor on the surface state to activate the properties dialog box at any time.

 alt text

Parameters

NSurface: Electron surface recombination velocity. cm s-1
PSurface: Hole surface recombination velocity. cm s-1
QFixed: Fixed interface charge. cm-2
NAcceptor: Electron acceptor trapped charge density. cm s-1
PAcceptor: Hole acceptor trapped charge density. cm s-1
NDonor: Electron donor trapped charge density. cm s-1
PDonor: Hole donor trapped charge density. cm s-1
QInsulator: Insulator trapped charge density. cm s-1
QDistribution: Specification of charge density in insulator. No units

2.11 Doping Windows

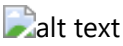
Doping Windows

Doping windows are used to specify an implant/diffusion doping profile through a window. The vertical profile maybe a Gaussian, a complementary Error function or a user specified profile. Doping windows can also be projected in the upward or downward directions or even in both directions simultaneously. The doping profile of a device is built-up using region doping and horizontal doping windows, which are summed to give a total doping concentration.

To draw a horizontal doping window:

1. From the main menu, select Device..Window..Doping.
2. Drag the cursor to define a rectangular doping window.
3. Click on the screen to finish.

Once a doping window has been defined, the doping windows properties dialog box will appear. In this dialog, the properties and profile of the doping window can be edited. Double-click the pointer on the doping window to activate the doping window dialog box at any time.

 alt text

Parameters

Window and Layout:

Type: Option to set as normal, left symetric, right symetric or double symetric. Used to select the shape of the diffusion.
Direction: Option to set as upwards, downwards or both. Used to select the direction of the implant. *Doping*: Option to set as acceptor or donor. Used to specify the type of doping implant. *Left*: X coordinate of left hand side of the window. Microns.
Top: Y coordinate of top of the window. Microns.
Width: Width of the window. Microns.
Depth: Height of the window. Microns.

Vertical Parameters:

Doping Type: Option to set as Gaussian, erfc, user. Used to specify the functiont that controls the scaling of the diffusion in the vertical direction.
Peak Concentration: Used to specify the peak doping concentration. For a diffusion implanted in the downwards direction, the peak concentration will occur at the top of the window.
Junction Doping: Used to specify the doping concentration. For a diffusion implanted in the downwards direction, the junction concentration will occur at the bottom of the window.
Straddle: Not used.
*User Doping Profil*e: Used to specify a user defined doping profile. The profiles is defined using a data table that is formatted into two columns, the first value gives the depth (co-ordinate in microns) the second gives the doping concentration (in cm-3). The data table can be applied through a non-uniform window. Interpolation is used to calculate the doping profile at the points below the window.

Lateral Parameters:

Type: Option to set as rotate or erfc. Used to specify the lateral profile type. The rotate option causes the doping profile to rotate around the end window point. The erfc option provides a lateral erfc type profile with a lateral set in LPARAMS.
Reduction: The lateral reduction factor is used to reduce the lateral spread can be reduced. If the 'rotate' option is chosen then this parameter specifies the lateral reduction factor. If the option chosen is 'erfc' then the lateral spread length is specified.

Calculation of Vertical and Lateral Diffusions

Vertical Gaussian scaling factor

$$ y_{\text{fact}} = N_0 , \text{erfc} \left(\frac{y}{\sigma_v} \right) $$

1 Introduction

Welcome to Aquarius Semiconductor Device Modelling..

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Aquarius is composed of four highly integrated modules:

*Process Simulator** : used to simulate fabrication processes, including the simulation of implantation and multiparticle diffusion steps, including one dimensional thermal oxidation. Once simulated, fabrication process models are conveyed to the device simulator module for further development.

*MUSIC Multigrid Process Simulator. Copyright (C) 1991-2006 Prof. Dr. S. Mijalkovic

Device Simulator: used to define the physical attributes of a two-dimensional semiconductor device structure. The definition of the device may be imported from a fabrication process model or defined directly without reference to a process model. The device model is then conveyed to the circuit simulator module for electrothermal simulation in the context of a circuit.

Circuit Simulator: used to define the circuit and bias conditions for the device, it also solves the device and circuit equations, saving the results to a disk file.

Simulation Results: used to view the results of a simulation and to obtain hard copies.

Process Simulation

The process simulator* module is used to model the device fabrication processes, including the implantation of impurities (phosphorus, boron, arsenic and/or antimony), multiparticle diffusions and one dimensional thermal oxidation. The module is based on a multigrid adaptive strategy which is characterized by a highly efficient convergence rate in the solution of multiparticle diffusion equations, robustness and natural parallelization of all simulation procedures. This approach enables rapid simulation of manufacturing processes, eliminating the bottlenecks present in the existing two dimensional process simulation programs.

Typically, the simulation of a fabrication process will involve the definition of the substrate geometry and impurity concentration and the definition of a sequence of implants, diffusions and thermal oxidations to form a process 'recipe'. Once simulated, fabrication process models are conveyed to the device simulator module for further development.

Device Modelling

The definition of a physical device model consists of several steps. This includes the definition of the device geometry, doping and physical properties of the device, as well as the finite element mesh used in the analysis

and the models employed to simulate the device. The geometry, doping profile and meshing of a device may be imported from a fabrication process simulation or defined directly without reference to a process model.

To define the device geometry directly (without reference to a process model), a user friendly CAD interface is provided that enables the user to rapidly construct complex device structures and to define the material regions. The user can also define ancillary items and properties such as electrical and thermal contacts and interface states.

The doping profile of the device is normally defined in the fabrication process model. However, the doping profile can also be defined directly without reference to a process model. Functions are provided to allow the user to apply uniform doping concentrations to device regions and the definition of more complex profiles specified through windows which can be placed on any horizontal surface in the geometry. Standard functions (Guassian and error function) or a use defined profile can be specified though each window. The user defined data can come from measurements or from a process simulation package such as SUPREM. All the different doping steps are summed to give a total doping concentration. The shape of the lateral doping profile can also be specified.

The finite element mesh generator is based on the Delaunay triangulation method for connecting up a given set of points into an optimum set of triangles. Using this technique, any set of points can be triangulated to give a set of triangles with positive pipe-widths along triangle edges. This is a very important consideration when solving the current continuity equations in the main solver. The difficulty is thus defining the location of a set of nodes for the analysis. The user has the task of defining a set of orthogonal lines in the x any y directions. The intersection of these lines gives a set of nodes that will be used in the mesh definition. Lines need not extend the entire span of the device in the x or y directions. The termination of the lines in this way allows regions of localised refinement to be defined, allowing the nodes to be placed in the place they are needed. An existing mesh may also be refined in the x or y direction to refine a mesh in a given region.

Finally, a range of physical models are available to be used in the simulation of the device being defined and can be configured by the user. The available models include:

- Mobility: Constant, Impurity, Carrier-scattering, Surface, Field dependent
- Generation Recombination: Shockley-Read-Hall, Direct, Auger, Impact Ionisation, User
- Defined
- Band-gap narrowing
- Fermi-Dirac statistics
- Temperature
- Surface recombination effects

The physical models employed by the simulator are described in more detail in the reference section at the end of this document.

Circuit Simulation

The previous section described the definition of a two-dimensional device model. The next step involves the definition of a circuit to drive the device model. Principally, this involves loading the device model into the circuit environment and defining a complete circuit around it. The mixed mode capabilities of the simulator mean that the circuit may contain passive and active components as well as other two-dimensional devices or

predefined circuit models. Once a suitable circuit has been defined, the device structure can be simulated in any one of three modes of operation:

1. Steady state - define a set of steady state (dc) bias points.
2. Transient - define a transient waveform and perform a temporal simulation.
3. IV Curve Tracer - perform a steady state curve trace.

Simulations can also be re-started from existing simulations as a continuation run from an initial condition. Sometimes re-starting a simulation from an initial condition is desirable when the numerical complexity of a model is such that the solver will fail to converge on a solution and an indirect approach is required.

The solver employed in the simulation of the circuit and solution of the device physics equations is fully configurable. In many cases, the default settings of the solver will be appropriate for most simulations. However, for highly non-linear problems the user can adjust the search parameters to achieve optimum convergence on a solution.

Simulation Results The results query module is used to view the results of the numerical calculations on the screen and to produce hardcopies. The results query modules enables the following results to be extracted from the simulation:

Line: for producing line plots on "cuts" through the 2D cross-section of device models. Isometric: for producing 3-D isometric plots at device level Contour: for producing contour plots at device level Ivplot: for producing terminal I/V characteristics at circuit level Transient: for plotting transient terminal and circuit waveforms at circuit level

The first three modes are used to plot the internal distributions in the device, and the last two are for looking at their terminal quantities of the device. The philosophy for viewing the internal distributions is to define what you want to plot. This will include the selection of the required plot variable (e.g. potential, electron concentration, net doping concentration etc), the required result cases and the manner of presentation (i.e. line, isometric or contour plot). Terminal quantities are extracted directy at circuit level.

The following device level results are available at device level: Electrostatic Potential Hole and Electron Quasi-Fermi Levels Electron and Lattice Temperatures Acceptor and Donor Concentrations Aquarius User Manual | 6 Valence and Conduction Band Energies Intrinsic Fermi-Energy Hole and Electron Quasi-Fermi Energies Hole and Electron Concentrations Intrinsic Carrier Concentration Valence and Conduction Band Off-set Parameters Net Doping Concentration Net Charge Concentration Recombination Rate Hole and Electron Mobilities E-Field Magnitude (or X and Y components of) Hole Current Magnitude (or X and Y components of) Electron Current Magnitude (or X and Y components of) Total Current Magnitude (or X and Y components of)

2 Device Modelling

2.1 Introduction

Introduction to Device Modelling

The definition of a physical device model consists of several steps. This includes the definition of the device geometry, doping and physical properties of the device, as well as the finite element mesh used in the analysis and the models employed to simulate the device. The geometry, doping profile and meshing of a device may be imported from a fabrication process simulation or defined directly without reference to a process model.

To create a new device model using data derived from a process simulation:

1. Refer to the 'Process Simulation' section of this document.

To create a new device model directly without reference to process model data:

1. From the main menu, select **File..New**.
2. Select the 'Device Model' option and click **OK**.

 alt text

To define the device geometry directly (without reference to a process model), a user friendly CAD interface is provided that enables the user to rapidly construct complex device structures and to define the material regions. The user can also define ancillary items and properties such as electrical and thermal contacts and interface states.

The doping profile of the device is normally defined in the fabrication process model. However, the doping profile can also be defined directly without reference to a process modlel. Functions are provided to allow the user to apply uniform doping concentrations to device regions and the definition of more complex profiles specified through windows which can be placed on any horizontal surface in the geometry. Standard functions (Guassian and error function) or a use defined profile can be specified though each window. The user defined data can come from measurements or from a process simulation package such as SUPREM. All the different doping steps are summed to give a total doping concentration. The shape of the lateral doping profile can also be specified.

The finite element mesh generator is based on the Delaunay triangulation method for connecting up a given set of points into an optimum set of triangles. Using this technique, any set of points can be triangulated to give a set of triangles with positive pipe-widths along triangle edges. This is a very important consideration when solving the current continuity equations in the main solver. The difficulty is thus defining the location of a set of nodes for the analysis. The user has the task of defining a set of orthogonal lines in the x any y directions. The intersection of these lines gives a set of nodes that will be used in the mesh definition. Lines need not extend the entire span of the device in the x or y directions. The termination of the lines in this way allows regions of localised refinement to be defined, allowing the nodes to be placed in the place they are needed. An existing mesh may also be refined in the x or y direction to refine a mesh in a given region.

Finally, a range of physical models are available to be used in the simulation of the device being defined and can be configured by the user. The available models include:

Mobility: Constant, Impurity, Carrier-scattering, Surface, Field dependent
Generation Recombination: Shockley-Read-Hall, Direct, Auger, Impact Ionisation, User Defined
Band-gap narrowing

Fermi-Dirac statistics
Temperature
Surface recombination effects

The physical models employed by the simulator are described in more detail in the reference section at the end of this document.

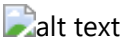
2.2 Device Shape

Device Shape

The shape of a device can be defined as either linear or cylindrical. The z axis depth of the device (into the screen) can also be specified.

To edit the global shape properties of the device:

1. From the main menu, select Device..Shape.


alt text

Parameters

Depth Scale Factor: The device is assumed to be 1cm deep in the z-direction by default if a linear device is used, and the area if a cylindrical device is chosen is calculated by rotating the device around the specified origin. This parameter allows the device depth / effective area to be increased by a scaling factor.

Device Shape: Either linear or cylindrical. Selects how device is represented in the 3rd spatial dimension. If cylindrical is selected the device is solved in cylindrical co-ordinates and is swept around the x values specified by the parameter x axis rotation origin.

X Axis Rotation Origin: Origin around which the device is rotated if cylindrical type is chosen.

2.3 Device Geometry

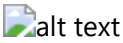
Device Geometry

One of the most important features of the Aquarius's device modelling capabilities is the ability to define the geometry of a device using the point, line, polyline, spline, rectangle, arc, circle and ellipse drawing functions. At this stage, it is only necessary to draw the outline geometry that defines the perimeter of each device region.

To draw a polyline:

1. From the main menu, select **Draw..Polyline**.
2. Click the cursor down and drag to draw the first line segment.
3. Move to the next point and click the cursor to draw the next line segment.
4. Repeat step 3 until the required shape is drawn.
5. Right click the cursor on the main view and select **End Polyline** from the popup menu.

All drawing functions can be accessed through Draw on the main menu or from the main toolbar. Polylines can be terminated by right clicking on the main view and selecting End Polyline from the popup menu. Splines are terminated in a similar manner.



2.4 Device Regions

Device Regions

After the outline geometry of a device has been drawn, the material regions that comprise the device can be defined and material properties assigned to them.

To define a region:

1. From the main menu, select Device..D**efine..Region**.
2. Click the cursor on a point inside the boundary of the region to be defined

Once a region has been defined, it will be filled with colour to denote that it is a defined region and the region properties dialog box will appear. Double-click the cursor on the region to activate the region properties dialog box

 alt text

Parameters

Material: Use to define the material properties of the region. Available materials include Silicon, AlGaAs, Oxide, Air, AlAs, GaAs, GaP, GaAsP, InP, InGaAsP. Note that there are two general types of semiconductor can be defined, namely (i) single composition (e.g. silicon, GaAs) and, (ii) variable composition (e.g. AlGaAs).
Acceptor Doping: Used to define the acceptor doping concentration in the region. Atoms/cm3
Donor Doping: Used to define the donor doping concentration in the region. Atoms/cm3

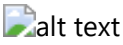
2.5 Region Composition

Device Regions

After a region has been defined, the user can specify a constant compositional profile over the region. The mole fraction x for a ternary compound and both x and y mole fractions for quaternary materials can be specified. This command sets a constant values in a specified region.

To edit region composition:

1. Double-click the cursor on the region to activate the region properties dialog box.
2. Select the composition tab and edit the constant composition parameter.

 alt text

Parameters

Mole Fractions X and Y: Used define the mole fractions x and y. Value range between 0 and 1.
Wavelength: Re-calculates x and y from the cut-off wavelength of the specific material.
Force All Edges to Specified Composition: Forces all the lines of a defined region to have the compositions defined by x and y in the Mole-fraction parameter.
InGaAsP Lattice Match: Uses the value of the y mole fraction to re-calculate the x mole fraction in order give the correct compositions for the specified lattice matching (Only applies to InGaAsP structures). Options to specify OFF, GaAs or InP.

2.6 Graded Composition

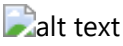
Graded Composition Windows

Allows user to specify a rectangular window where a graded compositional profile can set up for hetero-junction structures.

To draw a graded composition window:

1. From the main menu, select **Device**..**Window**..**Composition**.
2. Drag the pointer to define a rectangular graded composition window.

Once a graded composition window has been defined, the graded composition window properties dialog box will appear. In this dialog, a graded mole fraction profile can be specified. Double-click the cursor on the window to edit its properties at any time.

 alt text

Parameters

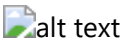
Mole Fractions: Used define the mole fraction grading across the window. If a horizontal gradient direction is specified then the user can input the left and right mole fractions to correspond with the left and right sides of the graded composition window. If a vertical gradient direction is specified then the user can input the top and bottom mole fractions to correspond with the top and bottom sides of the graded composition window.
Gradient profile: Used select the type of grading of the composition. Options are linear or hyperbolic tangent (tanh) functions.
Gradient direction: Used select the direction of the gradient. Options are vertical (top to bottom) grading of the mole fraction or horizontal (left to right) grading of the mole fraction.
Layout parameters: Used the specifiy the position of the graded composition window.

2.7 Material Properties

Material Properties

Aquarius contains a library of materials for the commonly used semiconductor and non-semiconductor materials. To edit material properties:

1. From the main menu, select Device..Materials.
2. Select the Properties tab. In the materials library the user can edit the properties associated with each individual material and even define completely new materials.



Parameters

General Properties:

Semcn: Semiconductor material (1=yes, -1=no)
Fixsc: Fixed semiconductor (1=single composition material e.g. silicon, -1=variable composition material e.g. AlGaAs). Used in heterojunction module.
Epslr: Relative dielectric constant *Eg*: Band gap (eV)
Affin: Electron Affinity (eV)
Mass_p: Relative hole and electron effective masses
Mass_n: Relative hole and electron effective masses
Lat_const: Lattice constant (Angstroms)

Mobility Properties:

Mu_0_p: Constant mobilities for holes and electrons (cm2/Vs)
Mu_0_n: Constant mobilities for holes and electrons (cm2/Vs)
Mu_AlpT_p: Temperature coefficients for lattice scattering mobility
Mu_AlpT_n: Temperature coefficients for lattice scattering mobility
Mu_max_p: Maximum mobilities, also used in lattice scattering mobility which reduces maximum mobility with increasing lattice temperature (cm2/Vs)
Mu_min_p: Minimum mobilities, used in the impurity and carrier scattering mobility expression (cm2/Vs)
Mu_nref_p: Reference doping used in the impurity and carrier scattering mobility expression (cm-3)
Mu_alpD_p: Coefficients used in the impurity and carrier scattering mobility expression (units)
Mu_max_n: Maximum mobilities, also used in lattice scattering mobility which reduces maximum mobility with increasing lattice temperature (cm2/Vs)
Mu_min_n: Minimum mobilities, used in the impurity and carrier scattering mobility expression (cm2/Vs)
Mu_nref_n: Reference doping used in the impurity and carrier scattering mobility expression (cm-3)
Mu_alpD_n: Coefficients used in the impurity and carrier scattering mobility expression
Mu_vsat_p: Carrier saturation velocities at 300K (cm s-1)
Mu_beta_p: Coefficients for field dependent mobility
Mu_vsat_n: Carrier saturation velocities at 300K (cm s-1)
Mu_beta_n: Coefficients for field dependent mobility
Mu_gsur_p: Oxide interface mobility reduction factor

Mu_gsur_n: Oxide interface mobility reduction factor
Mu_S_Ec_p: Critical electric fields for electron and hole oxide interface mobility model: (V cm-1)
Mu_S_Ec_n: Critical electric fields for electron and hole oxide interface mobility model: (V cm-1)
E_trap: Trap energy relative to the intrinsic Fermi-level (eV)

Recombination Properties:

SRH_TAU_p: Minority carrier lifetimesunits (secs)
SRH_Ap: Coefficients used in doping dependent lifetime models
SRH_Bp: Coefficients used in doping dependent lifetime models
SRH_Cp: Coefficients used in doping dependent lifetime models
SRH_Dp: Coefficients used in doping dependent lifetime models
SRH_Nrefp: Reference doping concentrations for lifetime models (cm-3)
SRH_TAU_n: Minority carrier lifetimesunits (secs)
SRH_An: Coefficients used in doping dependent lifetime models
SRH_Bn: Coefficients used in doping dependent lifetime models
SRH_Cn: Coefficients used in doping dependent lifetime models
SRH_Dn: Coefficients used in doping dependent lifetime models
SRH_Nrefn: Reference doping concentrations for lifetime models (cm-3)
Auger_Cp: Auger coefficients (cm6 s-1)
Auger_Cn: Auger coefficients: (cm6 s-1)
Direct_C: Direct recombination coefficient (cm3 s-1)
Av_alph_p: Avalanche prefactor coefficients (cm-1)
Av_beta_p: Avalanche exponential coefficients (V/cm)
Av_alph_n: Avalanche prefactor coefficients (cm-1)
Av_beta_n: Avalanche exponential coefficients (V/cm)

Optical Properties:

Abscoeff: Optical absorption coefficient (cm-1)

Thermal Properties:

Ther_cond: Thermal conductivity
Heat_Capa: Thermal heat capacity
Ther_coef: Coefficient for thermal conductivity
Vs_coefTp: Coefficients for temperature dependent saturation velocity
Vs_coefTn: Coefficients for temperature dependent saturation velocity

2.8 Material Models

Material Models

The physical models implemented in the simulator are fully configurable. To configure the physical models:

1. From the main menu, select **Device**..**Materials**.
2. Select the **Models** tab.


alt text

Parameters

General Parameters:

Reference Material: Used to select reference material to calculate reference energy levels to. Used mainly in heterojunction devices.
Temperature: Ambient temperature for the simulation. Kelvin

Mobility Models:

Low Field Mobility: Option to set as constant, lattice, impurity or carrier_carrier. If the constant model is selected then mobility is set to the value supplied in the properties command. If the lattice model is selected then the reduction in mobility due to increased collision with the lattice with increased temperature will be taken into account. If the impurity model is selected then the reduction in mobility due to extra collisions with the lattice is taken into account. If the carrier_carrier model is selected then the reduction in mobility due to extra collisions with the lattice is taken into account, except that the carrier concentration is taken into account (very important at high injection levels). Note: If the high field model is selected then the low-field mobility model will feed into the high field-mobility model. Otherwise it will be the mobility used in the simulation.
High Field Mobility: Option to set as none, e_field or j_field. The e_field or j_field models are used to select the high-field mobility model, which can be based on either the electric field magnitude or the magnitude of the field in the direction of the current.
High Field Calculation: Option to set as edge or element. Used to choode how the highfield mobility field is calculated. This will either use the values along an element edge or calculate the field based on the whole element.
Surface Mobility: Option to set as yes or no. Used to select surface mobility along oxide semiconductor interfaces. This model only affects those edges that actually lie along the interface.

Recombination Models:

SRH: Option to set as yes or no. Used to select Shockley Read Hall recombination model.
Auger: Option to set as yes or no. Used to select Auger recombination model. *Direct*: Option to set as yes or no. Used to select direct band-to-band recombination model.
Avalanche: Option to set as none, II_ELEM or II_EDGE. II_ELEM is used to select an impact-ionisation model

based on a discretisation that uses the full elemental information. II_EDGE is used to select an impact-ionisation model based on a discretisation along an edge of an element only.

Other Models:

Band Gap Narrowing: Option to set as none, Slotboom, Gaur. Used to select the bandgap narrowing model used in regions of heavy doping. Both Slotboom and Gaur models are empirical and are descibed in the reference section of this manual.
Transport: Option to set as drift-diffusion or energy. Used to select drift-diffusion or energy transport model (not fully implemented)
Statistics: Option to set as boltz or fermi. Used to select Boltzmann or Fermi-Dirac carrier statistics. Using Fermi-direct is slightly slower than the Boltzmann approximation.
Heat Source: Option to set as element or edge. Used to select how to calculate the heat source term in an electro-thermal simulation.

2.9 Contacts

Electrical and Thermal Contacts

Electrical and/or thermal contacts can be added to any edge or combination of edges on the perimeter of a region. Individual contacts can be made up of several different edges. Contacts can also be split across different regions and can occur at the junction between two different regions. In order to successfully model a device, the model requires a minimum of two contacts to be specified. The maximum number of contacts than can be added to a device model is eight.

To define a contact:

1. From the main toolbar, click on the **Select Edge** button.
2. With the cursor, select all the geometric edges which comprise the contact.
3. Select **Device**..**Define**..Contact from the main menu to create a contact.

Once a contact has been defined, the contact properties dialog box will appear allowing its properties to be edited. Double-click the cursor on the contact to activate the contact properties dialog box at any time.

 alt text

Parameters

Contact Type: Option to set as Ohmic or Schottky. Selects how contact will interact with the semiconductor.
Work Function: Work function of the metal. Used to calculate the barrier height for a Schottky diode or the Flat-band voltage for an oxide contact.
P Richardson: If set to a non-zero value is used as the Richardson constant to calculate the thermionic emission current for holes.
N Richardson: If set to a non-zero value is used as the Richardson constant to calculate the thermionic emission current for electrons.
Barrier Lowering: Option to set on or off. Select if image force barrier lowering is included at a Schottky contact.
Dipole Alpha: Coefficient for calculating dipole lowering of Schottky barrier height.
Resistance: Thermal resistance at ambient temperature. Kelvin / Watt
Capacitance: Thermal capacitance at ambient temperature. Joules / Kelvin.
Ambient Temperature: Ambient temperature used in the simulation. Kelvin

2.10 Surface States

Surface States

A surface state can be added to any edge or combination of edges on the perimeter of a region. This allows the user to specify interface/surface properties, including recombination velocities, fixed charges and fast surface states. Individual surface states can be composed of several different edges. Surface states can also be split across different regions and can occur at the junction between two different regions.

To define a surface state:

1. From the main toolbar, click on the **Select Edge** button.
2. With the cursor, select all the geometric edges which comprise the contact.
3. Select **Device**..**Define**..**Surface** from the main menu to create a surface state.

Once a surface state has been defined, the properties dialog box will appear allowing its properties to be edited. Double-click the cursor on the surface state to activate the properties dialog box at any time.

 alt text

Parameters

NSurface: Electron surface recombination velocity. cm s-1
PSurface: Hole surface recombination velocity. cm s-1
QFixed: Fixed interface charge. cm-2
NAcceptor: Electron acceptor trapped charge density. cm s-1
PAcceptor: Hole acceptor trapped charge density. cm s-1
NDonor: Electron donor trapped charge density. cm s-1
PDonor: Hole donor trapped charge density. cm s-1
QInsulator: Insulator trapped charge density. cm s-1
QDistribution: Specification of charge density in insulator. No units

2.11 Doping Windows

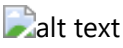
Doping Windows

Doping windows are used to specify an implant/diffusion doping profile through a window. The vertical profile maybe a Gaussian, a complementary Error function or a user specified profile. Doping windows can also be projected in the upward or downward directions or even in both directions simultaneously. The doping profile of a device is built-up using region doping and horizontal doping windows, which are summed to give a total doping concentration.

To draw a horizontal doping window:

1. From the main menu, select **Device**..**Window**..**Doping**.
2. Drag the cursor to define a rectangular doping window.
3. Click on the screen to finish.

Once a doping window has been defined, the doping windows properties dialog box will appear. In this dialog, the properties and profile of the doping window can be edited. Double-click the pointer on the doping window to activate the doping window dialog box at any time.

 alt text

Parameters

Window and Layout:

Type: Option to set as normal, left symetric, right symetric or double symetric. Used to select the shape of the diffusion.
Direction: Option to set as upwards, downwards or both. Used to select the direction of the implant. *Doping*: Option to set as acceptor or donor. Used to specify the type of doping implant. *Left*: X coordinate of left hand side of the window. Microns.
Top: Y coordinate of top of the window. Microns.
Width: Width of the window. Microns.
Depth: Height of the window. Microns.

Vertical Parameters:

Doping Type: Option to set as Gaussian, erfc, user. Used to specify the functiont that controls the scaling of the diffusion in the vertical direction.
Peak Concentration: Used to specify the peak doping concentration. For a diffusion implanted in the downwards direction, the peak concentration will occur at the top of the window.
Junction Doping: Used to specify the doping concentration. For a diffusion implanted in the downwards direction, the junction concentration will occur at the bottom of the window.
Straddle: Not used.
*User Doping Profil*e: Used to specify a user defined doping profile. The profiles is defined using a data table that is formatted into two columns, the first value gives the depth (co-ordinate in microns) the second gives the doping concentration (in cm-3). The data table can be applied through a non-uniform window. Interpolation is used to calculate the doping profile at the points below the window.

Lateral Parameters:

Type: Option to set as rotate or erfc. Used to specify the lateral profile type. The rotate option causes the doping profile to rotate around the end window point. The erfc option provides a lateral erfc type profile with a lateral set in LPARAMS.
Reduction: The lateral reduction factor is used to reduce the lateral spread can be reduced. If the 'rotate' option is chosen then this parameter specifies the lateral reduction factor. If the option chosen is 'erfc' then the lateral spread length is specified.

Calculation of Vertical and Lateral Diffusions

Vertical Gaussian scaling factor

$$ y_{\text{fact}} = N_0 \exp \left(-\left(\frac{y - y_{\text{offset}}}{\sigma_y} \right) \right) $$

N_0 is the Peak doping concentration, given as 1st vertical parameter
y is the distance in y direction below/above window
σ_ν is the vertical straddle, given as 2nd vertical parameter
y $offset$ is the offset of vertical peak below window, given as 3rd vertical parameter.

Vertical ERFC Scaling Factor $$y_{\text {fact }}=N_0 \operatorname{erfc}\left(\frac{y}{\sigma_\nu}\right)$$

y is the distance in y direction below/above window
N_0 is the peak doping concentration, fiven as 1st vertical parameter
σ_ν is the vertical straddle, given as 2nd vertical parameter

Vertical user defined scaling factor
$y_{\text {fact }}=y_{\text {user }}(y)$ y is the distance in y direction below/above window
$\mathrm{y}_{\mathrm{user}}(y)$ is the user profile The lateral extent of the profile is controlled by the point types, and the lateral choice.

Lateral rotation scaling factor
The lateral rotation scaling factor defines a set of elliptical contours for lateral profile (circular if r=1), typically used in the range 0.5 to 0.8.


alt text
y is the distance in y direction below/above window
r is the Radial reducation factor, given as 1st parameter

Lateral ERFC scaling factor

 alt text

y is the distance in y direction below/above window.

σ_l is the lateral straddle, given as 1st lateral parameter.

Total doping

$N(x, y)=x_{\text {fact }} \cdot y_{\text {fact }}$

2.14 SRH Windows

SRH (Shockley Reed Hall) Windows

Allows user to specify a rectangular window where the default value of the SRH carrier lifetimes can be altered by multiplying them by a constant scale factor within the window.

To draw a SRH window:

1. From the main menu, select Device..Window..SRH.
2. Drag the pointer to define a rectangular SRH window. Once a SRH window has been defined, the SRH window properties dialog box will appear. In this dialog, the SRH lifetime can be specified. Double-click the cursor on the window to edit its properties at any time.

 alt text

Parameters

Left: X coordinate of left hand side of the window. Microns.
Top: Y coordinate of top of the window. Microns.
Width: Width of the window. Microns.
Depth: Height of the window. Microns.
Scale Factor: Scale factor for carrier lifetime Units : none

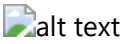
2.13 Optical Illumination Windows

Optical Illumination Windows

Optically illuminated windows are used to set up an optical illumination in a specified region of a device. In steady state simulations, the photon flux density list specifies the flux that will be used at each separate bias point in the simulation. In the case of a transient simulation the photon flux can be modulated with time.

To draw an optically illuminated window:

1. From the main menu, select **Device**..**Window**..**Illumination**.
2. Drag the pointer to define a rectangular optically illuminated window. Once an optically illuminated window has been defined, the illuminated window properties dialog box will appear. Double-click the cursor on the window to activate the properties dialog box at any time.



Parameters

Xmin: Minimum x co-ordinate of the window. Microns.
Xmax: Maximum x co-ordinate of the window. Microns.
Ymin: Minimum y co-ordinate of the window. Microns.
Ymax. Maximum y co-ordinate of the window. Microns.
Photon Flux: List of photon flux densities. In the dc case it specifies a flux that will be used on each separate bias point. If there are more bias points than specified values then the late value will be used. Units of photon flux density are cm-2 s-1.
Time: List of times which combine with the Photon Flux list to give an optical modulation of the optical generation. Not functional at present.

Calculations

If the window defines a surface (aligned with either the x or y axis) then it will be assumed to be a window and the following expressions for absorption will be used:

$U_{O P T}(x)=\alpha \Phi \exp (-\alpha x)$

where G is the generation rate due to optical illumination, is the absorption coefficient (specified for the material by Abscoeff in the properties command of Mprep), is the photon flux and x is the distance of the point below the window. Otherwise it us assumed it is a region in which case all the points inside the window will have the following generation rate:
$U_{O P T}(x)=\Phi$

2.14 Meshing Grid

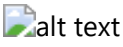
Meshing Grid

In order to create a triangulated finite element model of a device, the user must define the form and layout of the mesh required. A mesh is defined from a set of triangles which are created by triangulation of a set of nodes in 2D space. The meshing grid is used to define the positioning of this set of nodes. The nodes are located at the intersection of these mesh lines which are either aligned in the x-direction or the ydirection. The user has the task of defining groups of orthogonal lines in both the horizontal and vertical directions to form a template for the construction of the mesh. The intersections of these orthogonal lines with each other and with the region boundaries defines a set of geometric node points that are used to construct the finite element mesh.

To define a rectangular meshing grid:

1. From the main menu, select **Device**..**Mesh Grid** to display the meshing grid dialog.
2. Select the **Vertical Lines** at **Regular Intervals** option from the combo box.
3. Click on the **Add** button and a dialog box will appear.
4. Define a rectangular area in terms of X and Y coordinates e.g. (0,0) to (5,5)
5. Specify the spacing between the each line.
6. Click on **OK** and a series of regularly spaced vertical lines will appear over the defined area.
7. Repeat the above procedure, but this time select the **Horizontal Lines** at **Regular Intervals** option from the dropdown combo box in the meshing grid dialog.

This process of generating line groups in the x and y directions is repeated until a suitable meshing grid of intersecting lines is achieved.



2.15 Finite Element Mesh

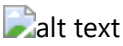
Finite Element Mesh

Having defined a mesh in terms of a set of mesh lines, this command will generate the nodes at the intersection of the mesh lines and triangulate them into a mesh. The Delauney algorithm is used to triangulate the nodes. In order to create a finite element (FE) device model, at least one region and two contacts must be defined and a suitable meshing grid specified.

To generate a FE device model:

1. From the main menu, select **Device**..**FE Mesh Model**. To exit the FE model at any time
2. From the device model window, select **Exit Mesh**.

Depending on the complexity of the device geometry and the meshing grid, it may take some time for the system to generate a fully triangulated finite element model. The progress of the mesh generator will be displayed in the status bar at the bottom of the screen and when complete, the finished FE model will be dispayed in the main view. The p and n regions in the device will also be plotted, thus defining the position of the metallurgical junction i.e. the position where net doping is zero atoms/cm3.



2.16 Mesh Refinement

Mesh Refinement

The quality of an FE device model is largely governed by the quality of the initial meshing grid defined by the user. However, three methods are provided for improving the quality of the mesh and the refinement the triangular elements.

Junction refinement

The junction refinement function enables the user to refine a band of triangular elements that fall within within a specified distance of the metallurgical junction. In fact, facilities are provided to enable a number of successive refinements in order to derive the best possible quality mesh around the junction

To refine the mesh around a metallurgical junction:

1. From the main menu, select **Device**..**Refine** and a dialog will appear.
2. Choose the **Junction** tab.
3. Specify the distance to refine around the junction.
4. Specify the number of successive refinements required.
5. Click the **Apply** button to initiate the refinement.

 alt text

Selective Refinement

The selective refinement function enables the user to interactively select and refine individual or groups of mesh elements. To selectively refine groups of mesh elements:

1. From the main toolbar, choose the **Select Object** button
2. Drag a rectangular selection window over the model to select a group of mesh elements.
3. From the main menu, select **Device**..**Refine** and a dialog will appear.
4. Choose the **Selected** tab.
5. Choose the direction of the refinement required
6. Click the **Apply** button the initiate the refinement.

Set meshing tolerances

As noted at the start of this topic, the initial quality of a mesh is governed by the quality of the mesh points defined by the user. During the mesh generation process however, the triangulation of these mesh points is largely undertaken with only minimal consideration to the shape and size of the triangular elements that will be generated. As a result, poor quality triangular elements may sometimes be created.

The quality of most meshes can be improved by setting a tolerance value for the minimum allowable spacing between adjacent node points on the boundary of a region and for the minimum allowable spacing between

points inside a region and those on a region boundary. By setting these tolerance values to an appropriate value, unwanted nodes can be eliminated from the mesh and the quality of the triangles will often be improved.

To set the meshing tolerances:

1. From the main menu, select **Device**..**Refine** and a dialog will appear.
2. Choose the **Tolerances** tab.
3. Specify suitable tolerance values.
4. Click the **Apply** button the initiate the refinement.

3 Circuit Simulation

5.1 Circuit Components

Circuit Components

The following components can be added to the circuit: Resistor, Capacitor, Linear Inductor, Non-Linear Inductor, DC Voltage Source, DC Current Source, Transient Voltage Source, Transient Current Source, Ground, Diode, Zener Diode, Dependant Source, Initial Voltage, Comparator, Switch, 2 Coil Transformer, 3 Coil Transformer and circuit Models for NPN, PNP, MOSFET, Npt IGBT (Non punch through IGBT), Pt IGBT (Punch Through IGBT), Thyristor and PIN Diode devices.

To add a component to the circuit:

1. From the main toolbar, click on the required component toolbar button.
2. Click the cursor on the main view to add the component to the circuit.

2D Physical Device Models can also be added to the circuit. The process of creating a 2D physical device model is described in detail in the previous chapter.

To add a 2D device model to a circuit:

1. From the main menu, select **Circuit**..**Device Model**.
2. Click the cursor on the main window to add a device model to the circuit.
3. Double click on the device model component and a file dialog will appear.
4. Browse for the previously saved FE model file. e.g. '\TCADStudio\Projects\PiN.sdm'.
5. Click **OK**to load the model

The properties of all components can be edited by double clicking them with the cursor. The position of all components can be changed by dragging them to a new position with the cursor and the orientation of components by selecting the component and then selecting **Edit**..**R**otate Left** or **Edit**..**Rotate Right** from the main menu.

Parameters

The operation of most components is self explanatory, however some additional notes are given below:

Ground: There must be at least one ground in any circuit.

Initial Voltage: Used to specify an initial voltage to a network node. This is done in order to aid the solution process, by giving it a good initial guess. It is not part of the circuit.

Diodes: There are two ideal diodes available, the standard diode and a zener diode. In the forward bias case they are identical and need the same parameters specified. As the forward bias voltage increases, so the resistance of the diode decreases very rapidly. The minimum forward bias resistance should be entered. In the case of the Zener diode the extra parameters required are the breakdown voltage and the resistance of the diode in breakdown.

Comparator: The Comparator has the following model V4 = V3 + Output Voltage HIGH if V1 - V2 > Threshold Voltage V4 = V3 + Output Voltage LOW if V1 - V2 < Threshold Voltage
Switch The Switch has the following model Rout = Output Resistance OFF if Vin < Lower Threshold Voltage Rout = Output Resistance ON if Vin > Upper Threshold Voltage For Vin between Lower Threshold Voltage and

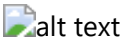
Upper Threshold Voltage the Output Resistance is linearly extrapolated between Output Resistance OFF and Output Resistance ON.

Steady State Current and Voltage Sources In steady state analysis mode, steady state current and voltage sources are used to specify a list of current or voltage values for steady state cases.

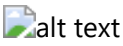
Transient Current and Voltage Sources: In transient analysis mode, transient current and voltage sources are used to define a current v time waveform or a voltage v time waveform. Four types of source are available, including the periodic source, sine wave source, triangle wave source and rectangle wave source. Periodic sources enable the user to define any shape of current v time or voltage v time waveforms. The waveform can be repeated with the period set at the longest time point programmed in the waveform.

The sine wave source is defined as:

The triangle wave source is defined as:



The rectangle wave source is defined as:



3.2 IV Curve Tracer Component

IV Curve Tracer Component

The current voltage (IV) tracing algorithm is used to automatically trace around awkward IV characteristics by specifying how to start off the trace and when to stop the trace. The algorithm will then fill in the points in-between. This is particularly useful when the curve becomes very steep (such as in the case of avalanche breakdown) in which case the voltage source driven device becomes very unstable and will not converge. This algorithm drives one of the device contacts with a variable impedance current source (a voltage source in series with a resistor), this allows the source to look more like a current source on vertical sections of the curve. Using this algorithm it is possible to trace round complete curves that would not ordinarily be possible, such as the forward break-over characteristics of a thyristor. The algorithm uses the number of Newton iterations to control the step size.

The IV Trace component is only valid for steady state simulation mode, and a 2D physical device model must also be present in the circuit. An IV trace should be directly connected to a device contact. Wires should not be used to connnect the IV trace to a device contact.

Parameters

Start Bias: Normally the sweep will start from the origin. If it is desired to solve from some other point then the starting bias must be specified. This may need to be used in conjunction with an appropriate initial solution from a previous run
Initial Step: Size of first voltage step in IV trace. The next step will be taken as half the first and the automatic curve tracing takes over.
Vmax: Maximum voltage allowed in curve tracing algorithm. When Vmax is reached the solver will stop.
Imax: Maximum current allowed in curve tracing algorithm. When Imax is reached the solver will stop.
Min Newton: If the number of Newton iterations falls below Min Newton the step length will be increased.
Max Newton: If the number of Newton iterations is greater than Max Newton the step length will be decreased. Simulation mode is automatically set to Curve Trace mode.

3.3 Wiring Circuits

Wiring Circuits

Connections should only be drawn between two component nodes - these points are marked clearly on the screen by a small blue cross. Individual wires cannot be connected together, except at common component nodes.

To connect circuit components together with wires:

1. From the main menu, select Circuit..Connection.
2. Click the cursor on a component node and drag the cursor to join it to the next node.
3. Double click the cursor to end the connection.
4. Repeat the above steps to complete the circuit wiring.

3.4 Performing a Simulation

Performing a Simulation

Aquarius can perform two main types of simulation namely, steady state (DC), Transient (time dependant) simulations. Simulations can also be re-started from existing simulations as a continuation run from an initial condition.

To perform a steady state simulation:

1. From the main menu, select Simulation..Steady State.
2. The simulation window will appear and the simulation will start.
3. When the simulation has finished, close the simulation window.

To perform a transient simulation:

1. From the main menu, select Simulation..Transient.
2. Set the simulation end time to the required value.
3. When the simulation has finished, close the simulation window

Simulations can also be re-started from existing simulations as a continuation run from an initial condition. Sometimes re-starting a simulation from an initial condition is desirable when the numerical complexity of a model is such that the solver will fail to converge on a solution and an indirect approach is required.

To restart an existing simulation:

1. From the main menu, select Simulation..Restart.
2. When prompted select the existing simulation you wish to restart from.
3. Select the restart case or simulation time.

If the file from which the initial condition is being read is a transient then the time parameter may be used to find the nearest case in the results files to the time specified. Otherwise the case parameter provides the case number to read in for the initial condition.

Parameters

Case: Used to select steady state or transient case number to used as initial condition to simulation. Care should be taken to ensure that the case chosen has a full internal solution saved in the case of a 2-D device simulation.
Time: Used to scan through the transient results file and find the nearest case with a full solution to use as the initial condition.

3.5 Solver Controls

Solver Options

The solver employed in the simulation of the circuit and solution of the device physics equations is fully configurable. In most cases, the default settings are appropriate for common simulations. However, users can configure the settings to their own requirements.

To edit the solver settings:

1. From the main menu, select Simulation..Solver Options

Parameters

General
Monitor: Options are yes or no. Display more detailed monitor information as solution progresses.
Minimum Resistance: Used to specify the value of the linking resistor used to link a device into the circuit.

Solver Equations
Coupled Type: Options are Fully Decoupled, Decoupled Elec Therm and Fully Coupled. Used to select the coupling used in the solution process.
Poisson: Options are yes or no. Used to solve Poisson's equation.
Hole Continuity: Options are yes or no. Used to solve hole continuity equation.
Electron Continuity: Options are yes or no. Used to solve electron continuity equation
Heat Equation: Options are yes or no. Used to solve heat equation.
Elect Temp: Options are yes or no. Used to solve energy transport equation. Not active.

Linear Solver
*Solver Type: *Options are CGS, CGSTAB or DIRECT. Type of linear algebra to use.
Max Linear Loops: Maximum number of iterations allowed for ICCG, CGS and CGS-STAB solvers
Linear Tolerance: Tolerance for ICCG, CGS and CGS-STAB iterative linear solvers
Pivot Factor: Provides extra working space for direct solver. Large values are needed when the matrix becomes ill-conditioned.

Decoupled Solver
MAX_DECOUPLED_LOOPS: Maximum number of de-coupled (Gummel) loops allowed.
DECOUPLED_TOL: Tolerance for de-coupled (Gummel) solver.

Newton Search
MAX_NEWTON_LOOPS: Maximum number of Newton loops allowed
NETWORK_TOL: Tolerance for network voltage convergence
VOLTAGE_TOL: Tolerance for voltage convergence
MAX_VOLT_UPDATE: Maximum voltage update at any node in the mesh for a single Newton step
TEMPERATURE_TOL: Tolerance for temperature convergence
MAX_TEMP_UPDATE: Maximum temperature update at any node in the mesh for a single Newton step
DELTA_TEMP: Temperature step used in numerical calculations of derivatives with respect to temperature

Back Tracking
MAX_INCREASE: Maximum times solution update is allowed to increase before solution is assumed to have failed and back-tracking is used
MAX_BACK_STEP: Maximum times solution is allowed to back-track during a single Newton-process
BT_INC_FAC Real:: Multiplication factor for increasing bias after back-tracking is used
BT_DEC_FAC: Division factor for reducing bias when back-tracking is used
SAVE_BACK_TRACK: Options are yes or no. Save solution points when the process back-tracks.

Time Stepping (Transient Simulations)

This is used to control the time steps in a transient simulation. The simulator uses a backward Euler time stepping algorithm. The time steps can be supplied either manually or selected by the simulator in two ways.

When supplying the time steps manually, they are supplied as a sequence of break points. These are given as a pair of values; time and time step. The time specifies when the time step will start, which will be used until another break point is encountered. The times are given in a real list and the time step vales as another real list which means they are enclosed in parenthesis.

Automatic time stepping is controlled in two ways. Firstly, based on a predictor-corrector method, the error between the forward (explicit) and backward (implicit) solutions are compared. The time step may be rejected based on this comparison and recalculated with a new time step, or it may be selected and a suggested value for the next time step selected.

The second method for time step selection is based on monitoring the number of Newton-loops taken per non-linear solution step. The algorithm will expand the time step if the number of Newton iterations is small and reduce the time step if the number of iteration is large.

In all three cases above it is likely that at some point the Newton-process will fail. If this happens the simulator will 'back-track', this involves reducing the time step until the process converges. This will always happen since at very small time steps the difference between the solution at the last time step and that at this time step are sufficiently small that the solution must converge. Once convergence is achieved the process will continue on forward again.

Parameters
TIME: Provide a set of break points at which the time step will change. The number must match the number of time step values specified in the DELTA_T list of values.
DELTA_T: Provide a set time step values. The number must match the number of time step values specified in the TIME list of values
AUTO_TIME: Options are on, off or newton_loops. Used to select method of time step control. 'Off' uses manual time steps specified by the TIME and DELTA_T. 'On' uses automatic time stepping based on comparing difference in solutions between forward and backward difference methods. 'Newton_loops' adjusts the time step based on the number of Newton loops taken to converge in the non-linear process. The rate at which the step is increased and decreased is set by the MIN_NEWTON, MAX_NEWTON and STEP_INCREASE, STEP_DECREASE parameters.
MIN_DELTA_T: Minimum allowed time step.

MAX_DELTA_T: Maximum allowed time step.
EPSILON_R: Relative error tolerance for time automatic time-stepping algorithm.
EPSILON_A: Absolute error tolerance for time automatic time-stepping algorithm.
MIN_NEWTON: Specify number of Newton loops that will trigger an increase in the time step. NewTimeStep = OldTimeStep*STEP_INCREASE
MAX_NEWTON: Specify number of Newton loops that will trigger an decrease in the time step NewTimeStep = OldTimeStep/STEP_DECREASE
STEP_INCREASE: Specify how much a time step will increase by
STEP_DECREASE: Specify how much a time step will decrease by

Write Times (Transient Simulations)

This command controls when the full internal solution is written to disk for a transient simulation. For a steady state simulation the internal solution is written for each bias point. At every point in the transient solution and dc. Simulation, the terminal solution (Currents, voltages, network voltages) will always be written to the ASCII results file (*.res). However, the internal solution is written out separately into a file referenced by the results file but containing only one internal solution. If multiple devices are being simulated each device will be written to a separate file. There are three ways of selecting whether a full solution is written, these are selected by the WRITE_TYPE parameter.

Firstly, the results may be written out at equally spaced time intervals. Next, a set of specific times may be specified to write the full internal solution. Both these methods will force solutions to occur at the specified times. Finally, the solution may be written at an equi-spaced number of time steps.

Parameters

WRITE_TYPE: Options are equal_spacing, specified or time_steps. Used to select criteria for writing out a full internal device solution fir a transient simulation. The method is described above.

TIMES: Meaning of this parameter depends on the method selected by WRITE_TYPE above. equal_spacing : first value in list specifies time between writing out full device solutionsspecified : list of values specifying times for writing out full device solutionstime_steps : first value is converted to an integer and used as number of time steps between writing the full internal solution out

4 Simulation Results

4.1 Introduction

Introduction to Simulation Results

The results query module is used to view the results of the numerical calculations on the screen and to produce hardcopies. The results query modules enables the following results to be extracted from the simulation:

Line: for producing line plots on "cuts" through the 2D cross-section of device models.
Isometric: for producing 3-D isometric plots at device level
Contour: for producing contour plots at device level
Ivplot: for producing terminal I/V characteristics at circuit level
Transient: for plotting transient terminal and circuit waveforms at circuit level

The first three modes are used to plot the internal distributions in the device, and the last two are for looking at their terminal quantities of the device. The philosophy for viewing the internal distributions is to define what you want to plot. This will include the selection of the required plot variable (e.g. potential, electron concentration, net doping concentration etc), the required result cases and the manner of presentation (i.e. line, isometric or contour plot). Terminal quantities are extracted directy at circuit level.

4.2 Circuit Level Results

Circuit Level Results Simulation results can be obtained at circuit level using the Query Circuit function. The Query Circuit function provides the facility to generate 2D XY line plots of circuit level currents and voltages in both steady state and transient simulations.

To create a 2D XY line plot of circuit level results:

1. From the Results Manager window, select Query Circuit.
2. Click the pointer on a circuit component or contact and a popup menu will appear.
3. From the popup menu, select the required variable (the X graph variable).
4. Again, click the pointer on a circuit component or contact and a popup menu will appear.
5. From the popup menu, select the required variable (the Y graph variable).
6. A graph showing the IV characteristic will now appear.

To print or edit the graph, right click the cursor on the graph window and a pop-up menu with various options will appear.

4.3 Device Level Results

Device Level Results

Simulation results can be obtained at device level using the Query Device function. The Query Device function provides the facility to generate 2D XY line plots of results through a device and 3D isometric or contour plots of results for complete devices.

2D XY line plots at device level

In order to take a 2D line plot at device level, we need to specify the coordinates of a section (or a cut) through the device where we wish to obtain results from.

1. From the Results Manager window, select Query Device and the results wizard will appear.
2. In the wizard, select 2D Line Plot and then click Next.
3. Check the required variable in the variables window and then click Next.
4. Check the required case in the cases list and then click Next.
5. Add an X or Y cut position to the cut list and then click Next to finish.
6. A graph showing the required variable plot will now appear. To print or edit the graph, right click the cursor on the graph window and a pop-up menu with various options will appear.

3D isometric plots at device level

1. From the Results Manager window, select Query Device and the results wizard will appear.
2. In the wizard, select 3D Isometric Plot and then click Next.
3. Check the required variable the variables window and then click Next.
4. Check the required case in the cases list and then click Next.
5. A graph showing an isometric plot of the required variable will now appear.

To print or edit the graph, right click the cursor on the graph window and a pop-up menu with various options will appear.

The following device level results are available at device level:

Electrostatic Potential
Hole and Electron Quasi-Fermi Levels
Electron and Lattice Temperatures
Acceptor and Donor Concentrations
Valence and Conduction Band Energies
Intrinsic Fermi-Energy
Hole and Electron Quasi-Fermi Energies
Hole and Electron Concentrations
Intrinsic Carrier Concentration
Valence and Conduction Band Off-set Parameters
Net Doping Concentration
Net Charge Concentration

Recombination Rate
Hole and Electron Mobilities
E-Field Magnitude (or X and Y components of)
Hole Current Magnitude (or X and Y components of)
Electron Current Magnitude (or X and Y components of)
Total Current Magnitude (or X and Y components of)

5 Worked Examples

5.1 PiN Power Diode

Example 1 - Ivestigation of PiN Power Diode Characteristics

The aim of this example is to become familiar with the use of Aquarius software for the design and simulation of the PiN Power Diode structure and characteristics. The use of numerical TCAD is very powerful because it allows an insight into the device internal physics and enables the student to be able to develop a good understanding of the links between the device structure and its technology parameters. Brief Theory Of PiN Power Diode Operation Figure 1. shows the structure of fast switching epitaxial power diode. Here, the starting material is a wafer of heavily doped n+ substrate, onto which a lightly doped n-layer is deposited epitaxially. A p+ surface layer is diffused into this to form the junction. As well as being capable of blocking the required reverse voltage in the off-state, a power diode requires low forward voltage drop in the onstate. In many applications, a rapid transition from the forward conducting to the reverse blocking state is required.

 alt text

Figure 2. shows the dependence of the maximum breakdown voltage VBR on the doping N and the width wv of lightly doped i-layer. To obtain a higher VBR, either lower doped and/or wider I-layer is needed. In turn, the both increase diode forward voltage drop. When the PiN diode is subjected to an abrupt change of current or voltage, the carrier distribution in the device is very different from the steady-state conditions. In many power electronic circuits, a diode is called upon to switch quickly from forward conducting state to the blocking state.

Figure 2
The example of reverse recovery waveforms of power diode operating in a rectifying circuit with series inductance is illustrated in Fig. 3. At the beginning of turn-off process, the i-layer is flooded with excess carriers. Initially, it prevents the establishment of a space charge region, so the voltage across the diode remains small and, in the first part of the transition process, the current falls to zero and reverses at a rate determined by the external circuit. Only when sufficiently charge has recombined, or has diffused out as a reverse current, do the carrier concentrations at the p-n junction reach thermodynamically equilibrium, permitting the formation of space charge region. The reverse current comes gradually to a maximum (here 75A) then decays away as the residual carriers recombine or diffuse out. The reverse voltage across the diode passes through its steady-state value as the current reaches its maximum value. It continues rising to a peak whose magnitude (here 853V) is governed by the rate of fall of the reverse diode current and hence by rate at which the remaining carriers are swept out from the base region.

Figure 3
The reverse recovery phase of diode operation has many important implications for the circuit designers. The reverse recovery waveforms depend on previous forward current and its rate of fall, the circuit conditions (especially the series inductance) and the carrier life-time within a diode i-layer. As an example, Fig. 4 shows the influence of the decrease of carriers life-time value on the reverse recovery current waveforms.

Figure 4
Modelling PiN Power Diode Structure The Aquarius software should be ready to use on your pc. Follow these step-by-step instructions and refer to the screen shots on the opposite page to help you. Ask for assistance from one of the lecturers if you require help.

Process Simulation Steps

1. Select **File..New** from the pull-down menu at the top left of the screen. Select **Process Model** and then click **OK** to finish. A new window will appear titled process 1.
2. Click the **Define Substrate** button. Set the Substrate Length to 10 microns, the Impurity Type to Phosphorous, the Impurity Concentration to 3E16 and the Crystal Orientation to 100. Click **OK** to finish (refer to figure 1).
3. Click the **Add Implant** button. Change the Title to 'Global p- Implant'. Set the Impurity Type to Boron, the Ion Energy to 100keV, the impurity dose to 1E13cm-2, leave the mask material unchanged as this feature is irrelevant with setting a Mask Shape. As this is a global implant then a mask is not required here. Click **OK** finish. You will observe that an implant recipe is added in the process 1 window.
4. A diffusion step is now added to drive and activate the p- implant. Click the **Add Diffusion** button. Change the title to 'p- drive'. Set the Temperature to 1100C, the Time to 3600 seconds, leave the Model unchanged at Neutral. Click **OK** to finish. This recipe is now added beneath the previous implant in the process window.
5. A shallow p+ implant is now added to enable a good ohmic contact for the anode.Click the **Add Implant** button. Change the Title to 'p+ Implant'. Set the Impurity Type to Boron, the Ion Energy to 20keV, the impurity dose to 1E15cm-2 and the mask material to SiO2. Do not click ok yet, for this implant a mask is required so therefore click the **Mask Shape** button. Click the **Preview Mask Shape** button. A new window is opened that enables a preview of the mask to be observed to help prevent user error. Now click **Add Point** in the implant window. Enter values of Mask Position X = 2.5 microns, Mask Depth Y = 0 microns. Click **OK**. The first point P1 is added in both windows. Now enter another point with coordinates X = 2.5 microns, Y = 1 micron and click **OK**. A second point is added to both Windows and the mask is clearly shown (refer to figure 2.). Finally click **OK** in the implant window to finish the p+ implant step. This added to the process flow.
6. Another Diffusion step is now added to activate the p+ implant. Click the **Add Diffusion** button. Change the title to 'p+ rtp'. Set the Temperature to 1100C, the Time to 120 seconds, leave the Model unchanged at Neutral. Click **OK** to finish.
7. Select **File..SaveAs** in the pull-down menu. Save the file in the projects folder as 'pin.prm'.
8. Now click the **Simulation** button in the process window. After a few seconds a new window will appear called device 1. This window shows the 2-D cross-sectional image of the structure.
9. Select **View..Options** from the top pull-down menu and select the **Mesh** tab. Now click the Acceptor Profile and Donor Profile boxes and click **OK**. The device 1 structure should now show the p+ region. Refer to figure 3. to check.
10. Select **File..Save As** in the pull-down menu. Save the file in the projects folder as 'pin.sdm'. This saves the device structure.
11. This concludes the part of the worked example that makes use of the process simulator. The rest of the example makes use of the device and circuit simulation features in Aquarius.

Device Simulation Steps

1. The n+ cathode region is now added to the generated structure using the device simulation tools. First right click the mouse cursor on the simulated structure and select **Exit Mesh**. The structure reverts to a plain box shape.
2. From the main menu, select **Draw..Rectangle** (or click on the draw rectangle toolbar) buton button . Using the cross-hairs shown and the coordinates at the bottom left of the screen draw a 10 microns by 2 microns rectangle connected to the bottom of the structure (refer to figure 4. for position). Right

click the mouse cursor in the rectangle and select Define and then Region. The cross-hairs change to an arrow. Left click in the 10*2 microns rectangle. A new region window is opened on the screen. Use the Select Region Colour to change the region to a different colour and set the Donor doping to 1e19 Atoms/cm3. Click OK. A new n+ region is now added to the bottom of the structure (refer to figure 4.). Click the select object button to deselect the define rectangle function.

3. A point is now added to select the right edge of the anode contact. Click the define point icon. Using the cross-hairs add a point at coordinates (2.5,10) located on the top surface of the structure.
4. An oxide is now added to the right of the point on the top surface. Click the button. Add a 7.5 microns by 0.6 microns rectangle attached to the top of the structure (refer to figure 5. for position). Right click in the rectangle and select Define and then Region. The cross-hairs change to an arrow. Left click in the 7.5*0.6 microns rectangle. A new region window is opened on the screen. Use the **Select Region Colour** to change the region to a different colour. Change the Material to oxide. Click **OK**. An oxide is now added to the structure (Refer to figure 5).
5. A grid is now added to the new n+ and oxide regions to enable numerical solutions to be obtained for the device when it is placed in the circuit simulator. Click the **Mesh Grid** button. A window labelled Meshing Grid is opened. Select **Horizontal lines** at regular intervals in the window. Now using the cross-hairs click on the lower left and upper right corners of the p+ region at the bottom of the structure. A new window called Horizontal Lines is opened. Set the Spacing Between Lines to 0.4 microns and click **OK**. Some horizontal lines are now added to the n+ region in the structure. Select Vertical lines at regular intervals in the window. Click on **Add**. A new window called Vertical Lines is opened. Set the Spacing Between Lines to 0.25 microns and click **OK**. Vertical lines are now added. Close the Meshing Grid Window.
6. Repeat number 5. above but this time mesh the oxide layer. Use spacing between lines of 0.3 microns for horizontal line and 0.25 microns for vertical lines.
7. Click the **FE Mesh Model** to create the Finite Element mesh. Check the result against figure 6. If the mesh looks correct right click on the structure and select **Exit Mesh**. Otherwise delete the mesh and restart it.
8. The next steps are to add the ohmic anode and cathode contacts. Right click on the device and select **Define** and then **Contact**. Left click on the top line of the structure between the top left point and the point that was added earlier - refer to figure 7. for the correct position. A red line is drawn between the two points along the device surface to depict the position of the contact. Again right click on the device and select **Define** and then **Contact**. A new window called contact is opened. Change the Name to Anode and click **OK**. A new thicker red line is drawn .
9. Repeat the sep 8. but this time select the line between the bottom two points of the n+ region at the bottom of the device. Change the Name of this contact to Cathode and click **OK**. Refer to figure 8. for final device structure.
10. Finally select **File** then **Save As** in the pull-down menu. Save the file in the IGDS folder as pin_final_ini.sdm (where ini are your initials). This saves the final device structure.
11. This concludes the part of the lab that creates the PiN structure. The remainder of the lab uses the circuit simulation features to analyse the device characteristics.

Determination of Reverse Breakdown Voltage

1. Using the circuit simulator in Aquarius the characteristics of the PiN Power Diode can be explored. Select File then New from the Pull-down menu at the top left of the screen. Select **Circuit Simulation**

and then click **OK**. A new window will appear titled Circuit 1.

2. Select **Circuit** then **Device Model** from the Pull-down menu at the top left of the screen Left click the mouse in the circuit window. A two terminal unassigned device will appear. Double left click on the device and then select your device model pin_final_ini.sdm and click open. The PiN Diode will appear with the Anode and Cathode terminals displayed (alternatively the circuit simulation icons may be used - position the mouse arrow over each icon to display its function)..
3. Select **Circuit** then **IV Curve Tracer** from the Pull-down menu at the top left of the screen. Left click in the circuit and an IV Curve Tracer device is displayed. Position the IV Curve Tracer terminal (denoted by a cross) directly over the Cathode Terminal (refer to figure 9).
4. Select **Circuit** then **Ground**. Left click in the circuit and position the Ground symbol underneath the PiN Power Diode.
5. Click the **Connection Icon** (towards the left side of the screen). Using the mouse 'wire up' the circuit as shown in figure 9. Single left click the mouse on a terminal to start a wire. Single left click to change direction and double left click on a terminal to terminate the wire.
6. Finally select **File** then **Save As** in the pull-down menu. Save the file in the IGDS folder as pin_bv_ini.cim (where ini are your initials). This saves the circuit name.
7. Select **Simulation** then **Steady State**. A simulation window opens and the internal solver will calculate the Breakdown Voltage. This will take several minutes.

Plotting The Results

1. In the Results Manager window to the left of the screen click the **Query Circuit** button. Now move the mouse arrow back into the Circuit window. A question mark appears at the side of the arrow. Left click the cathode terminal and select Voltage. Left click the cathode terminal again and select Total Current. After a few seconds an XY plot of Cathode current against Cathode Voltage is displayed (see figure 10.). It is also possible to export data to an external software package such as Microsoft Excel by selecting the **Export Plot Data** button in the Results Manager window. Right clicking on the graph also provides options such as a Log scale for the Y axis.
2. Select **Query Device** in the Results Manager window. Click **2D Line Plot** in the Query Device window that opens and then select Next. Select **E-Field Magnitude** and click **Next**. Select the last Case and click **Next**. Change the Add X = value 1 micron and then click the Add X = button. Click **Finished**. A plot of the Electric Field in the device at Breakdown is shown. In this case the electric field has reached the critical value to cause avalanche breakdown (refer to figure 11.).

Reverse Recovery Characterisation

1. Using the same methodology as used for the Reverse Breakdown voltage experiment create the test circuit shown in figure 12.
2. Use values for the circuit components of: a. Resistor = 0.5? b. Inductor = 1?H c. Transient Voltage Source - referring to figure 12. Left double click the **Transient Voltage Source** symbol. A window will open titled Transient Voltage Source. Click the **S**elect Waveform** button. Select **Custom** and then **Add**. Add values in turn of: Voltage (V) Time (S) 3 0 3 1e-6 -40 3e-6 -40 1e-5 Left click **Apply** when completed and then Ok.
3. Save the circuit as PiN_rec_ini.crm.

4. Select **Simulation** from the pull down menu and then select **Transient**. Enter an End Time of 1e-5 Seconds. The simulation will and take several minutes to complete.
5. Using the Query Circuit function plot graphs of Anode Voltage versus Time and Anode Current Verses time. Check your results against figures 13. and 14.
6. This concludes the PiN Power Diode Laboratory.

6 Reference

6.1 Physical Models

This topic describes the various physical models implemented in the simulator.

1.0 Physical Models

1.1 Device Model

The program solves the following set of partial differential equations, namely Poisson's equation, along with the hole and electron continuity equations:

INSERT LATEX HERE !!

with the hole and electron currents being given by the drift-diffusion equations:

INSERT LATEX HERE !!

where and are the electron and hole mobilities respectively, and and are the electron and hole diffusivities (which are related to the mobilities by Einstein's relation). The quantities and are band-parameters associated with the conduction and valence bands. They represent the shift in the band edges due to either heavy doping effects in silicon, or to compositional variations in non-uniform materials, such as heterojunctions. Boltzmann-statistics are normally used to describe the carrier concentrations in most situations:

INSERT LATEX HERE !!

where is the intrinsic carrier concentration in the reference material, and the thermal voltage is given by

INSERT LATEX HERE !!

Alternatively, Fermi-Dirac statistics may also be used to correctly describe the situation where degeneracy is important.

INSERT LATEX HERE

where the degeneracy factors are

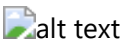
INSERT LATEX HERE

and

INSERT LATEX HERE

The band parameters are calculated with aid of the following band diagram, all the energies (potentials) are calculated with respect to a reference material. All the potentials used in Sundial are referenced to the intrinsic Fermi-level in the reference material (zero volts) and the reference potential is simply the energy difference (expressed in volts) between this reference potential to the vacuum level in the reference material:

INSERT LATEX HERE



One-dimensional representation of the energy-band diagram The band parameter for electrons calculated as the difference between the conduction band energy and the conduction-band energy in the reference material, due to changes in band structure (not due to changes in electrostatic field), a similar calculation exists for the valence band parameter. This leads to the following expressions:

INSERT LATEX HERE

where the effective valence and conduction band density of states are given by:

INSERT LATEX HERE

and the intrinsic carrier concentration is given by:

INSERT LATEX HERE

1.2 Band gap narrowing

Band gap narrowing occurs in heavily doped regions of the semiconductor, where the impurity bands merge into either the conduction band or valence band - effectively reducing the band-gap. This is accounted for using the following empirical models: Slotboom's Model

INSERT LATEX HERE

Gaur's Model

INSERT LATEX HERE

The band-gap reduction is attributed 50% to the conduction band and 50% to the valence band, via the band parameters.

1.3 Mobility models

The mobility is arrived at via a combination of different physical effects, to reflect the way that different scattering mechanisms cause the carrier mobilities to change. Basically the mobility selection process is split into two parts :

- Low field mobility

- High field mobility

with the resulting low-field mobility being used as an input to the high field mobility.

1.3.1 Low-field Mobility

The low-field mobility can be selected from a number of alternatives as listed below, these are :

1.3.1.1 Constant mobility

This is the simplest form of mobility and just sets the low-field mobility for each semiconductor material type to be constant.

INSERT LATEX HERE

which are settable for each material in the material properties box.

1.3.1.2 Lattice mobility

The lattice mobility uses an empirical model to take into account the scattering that occurs between the lattice and the carriers contained in it. This is simply a function of lattice temperature (T o C), increased temperature leads to a reduction in carrier mobility :

INSERT LATEX HERE

1.3.1.3. Impurity mobility

The impurity mobility implies that the lattice mobility is also used, to define the maximum mobility, and is due to collisions with impurity atoms, again, naturally the higher the doping the more likely a collision is resulting in a reduced mobility.

INSERT LATEX HERE

1.3.1.4. Carrier-carrier scattering mobility

This is similar to the model above, except it attempts to model in influence of carriers scattering from one another under levels of high injection. Thus the mobility is modified so as to depend on total carrier concentration. Again this model implies that the lattice mobility is used to define the maximum mobility:

INSERT LATEX HERE

2.3.1.5. Surface mobility reduction

In addition to the bulk mobility models described above, the interface between oxide and semiconductor will cause a reduction in the mobility along the interface due to surface roughness and usually depends on the perpendicular electric field. This mobility is only applied to those edges of elements that lie along the oxide/semiconductor interface. This is applied to the edge after all the other mechanisms (1-4) described above have been calculated.

INSERT LATEX HERE

INSERT LATEX IN BELOW SENTENCE

E perp is the electric field perpendicular to the edge along the interface.

1.3.2 High-field Mobility

The high-field mobility reduction describes the effect of velocity saturation at high fields. In Sundial this is applied after the low-field mobility has been calculated, thus implies the resultant value of low field mobility described above. The field dependency is implemented using the following expression for the saturation velocity:

INSERT LATEX HERE

and the mobility as:

INSERT LATEX HERE

here the magnitude of the electric field which can be calculated in different ways, either by using a method based on the electric field itself or on the electric field in the direction of current flow (), either of which may be based on the element edge or the full element.

1.4 Recombination models

The recombination models are independent of each other in their formulation obviously there will be some interplay between the different mechanisms and this is taken care of by the solver.

1.4.1 Shockley-Reed-Hall recombination process

This describes the process of trap-assisted recombination in the bulk of the semiconductor. The model provides for doping dependence of the minority carrier lifetime. The position of the trap in the band-gap is also adjustable.

INSERT LATEX HERE

Where the doping dependent lifetimes are defined by:

INSERT LATEX HERE

The default values are such that the lifetime is constant and equal to the values set in **SRH_TAU_P** and **SRH_TAU_N.** Additionally the lifetime can be made position dependent by defining a rectangular region and an multiplication factor inside that box. This is done using a rectangular SRH Window to define a box in which the values of **SRH_TAU_P** and **SRH_TAU_N** in the bulk of the device can be increased by a scaling factor.

1.4.2 Auger recombination process

The Auger mechanism becomes the dominant recombination method under levels of high bipolar injection. It is modelled using:

INSERT LATEX HERE

1.4.3 Direct recombination process

The Direct recombination mechanism models direct band-to-band recombination

INSERT LATEX HERE

1.4.4 Avalanche generation process

Avalanche generation is modelled using the following empirical law:

INSERT LATEX HERE

where the avalanche coefficients are determined using the following:

INSERT LATEX HERE

INSERT LATEX HERE

INSERT LATEX HERE

1.4.5 Total recombination rate

The total recombination rate is found by summing up all the different mechanisms:

INSERT LATEX HERE

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