

Device simulation



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Atlas overview

Atlas is a *physically-based* two and three dimensional device simulator that predicts the electrical behavior of semiconductor devices at specified bias conditions.

- The physical structures simulated with Athena are used as input by Atlas.
- The combination of Athena and Atlas makes possible to determine the impact of process parameters on device characteristics.

Atlas input file

- It is a *text file* that can be arranged by using Deckbuild or any text editor.
- It collects a sequence of commands (*statements*) corresponding to required bias conditions and control commands specified to select physical models and parameters.

Atlas simulation

- Generating Atlas *input file*
- Running Atlas *simulation*
- Analyzing Atlas *output file*

Simulation problem specification

The simulation problem must be specified in the *input file*, defining the following steps:

- The *physical structure* to be simulated.
- The *physical models* to be used.
- The *numerical methods* needed to solve the physical equations.
- The *bias conditions* for the electrical characteristics.

The present section describes how to perform these steps.

Running Atlas simulation

Running Atlas inside Deckbuild

To run Atlas inside Deckbuild use the following command line:

```
> go atlas
```

Running a given Atlas version

The syntax is:

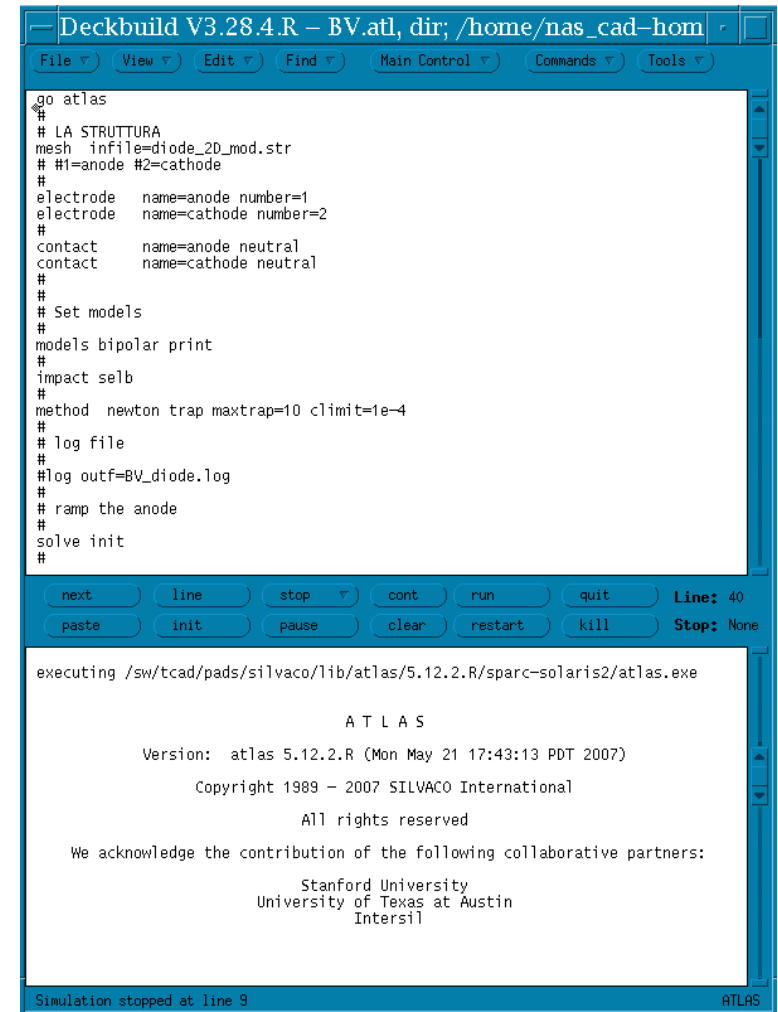
```
> go atlas simflags="-V 5.10.0.R"
```

Running Atlas without Deckbuild

To run Atlas directly under unix use the following command line:

```
> atlas <input filename>
```

```
> atlas -V 5.10.0.R <input filename>
```



```
Deckbuild V3.28.4.R - BV.atl, dir; /home/nas_cad-hom
File View Edit Find Main Control Commands Tools
go atlas
#
# LA STRUTTURA
mesh infile=diode_2D_mod.str
# #1=anode #2=cathode
#
electrode name=anode number=1
electrode name=cathode number=2
#
contact name=anode neutral
contact name=cathode neutral
#
# Set models
#
models bipolar print
#
!impact selb
#
method newton trap maxtrap=10 climit=1e-4
#
# log file
#
#log outf=BV_diode.log
#
# ramp the anode
#
solve init
#
next line stop cont run quit Line: 40
paste init pause clear restart kill Stop: None
executing /sw/tcad/pads/silvaco/lib/atlas/5.12.2.R/sparc-solaris2/atlas.exe
ATLAS
Version: atlas 5.12.2.R (Mon May 21 17:43:13 PDT 2007)
Copyright 1989 - 2007 SILVACO International
All rights reserved
We acknowledge the contribution of the following collaborative partners:
Stanford University
University of Texas at Austin
Intersil
Simulation stopped at line 9 ATLAS
```

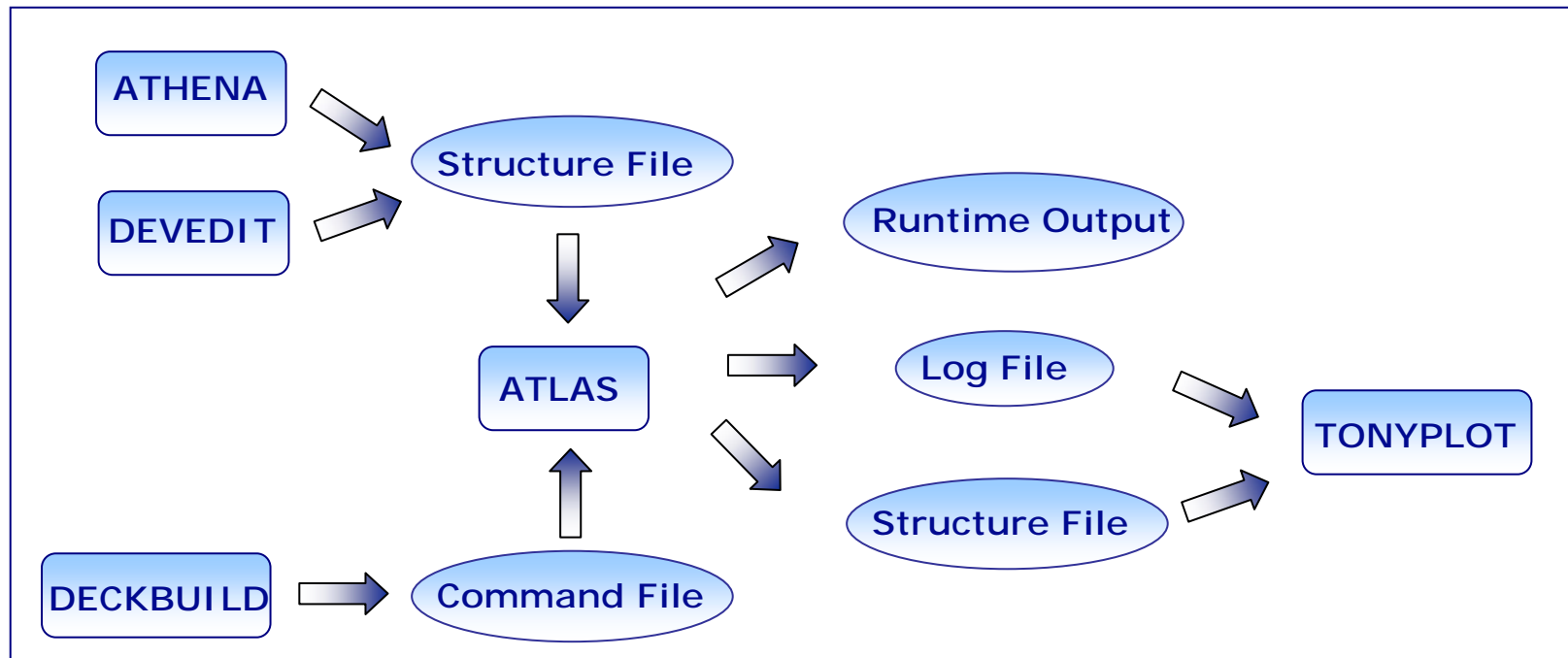
Atlas Inputs and Outputs

Atlas uses two types of input file

- A *text file* that contains Atlas commands.
- A *structure file* that defines the structure to be simulated

Atlas produces three types of output files

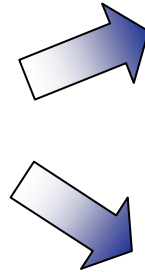
- The *runtime output* that gives error and warning messages as the simulation proceeds.
- The *log file* that stores voltages and currents.
- The *structure file* that stores 2D and 3D data relating to the values of solution variables



Atlas input structure

The physical structure built by Athena is used as input by Atlas to predict its electrical behavior. The grid of the input structure is crucial for the device simulation.

There is a trade-off between the requirements of accuracy and numerical efficiency



Accuracy requires a fine grid

Numerical efficiency is greater when fewer grid points are used

The most efficient way to work is to allocate a *fine grid only in critical areas* and a coarser grid elsewhere. Most critical areas tend to coincide with reverse biased metallurgical junctions.

Typical critical areas

- Transverse electric field under the MOSFET gate
- Areas of considerable recombination effects
- Areas of high impact ionization

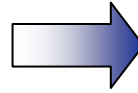
Question 1

An Atlas input file is:

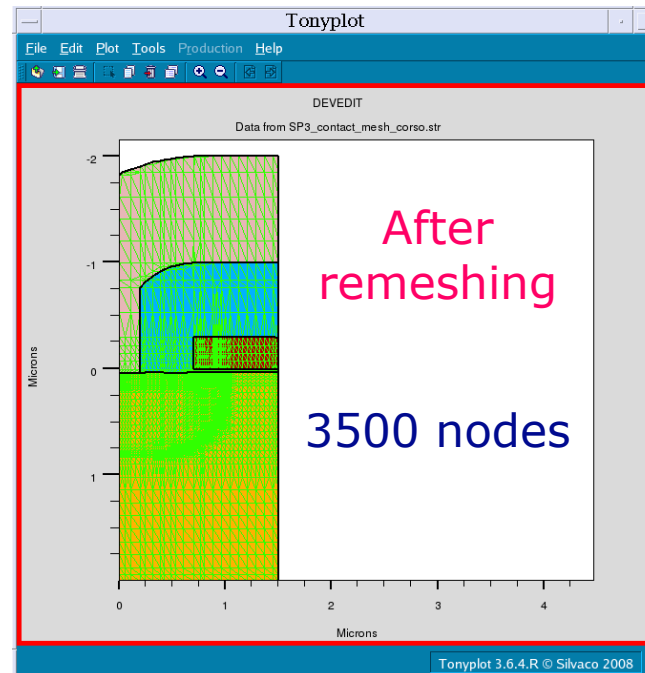
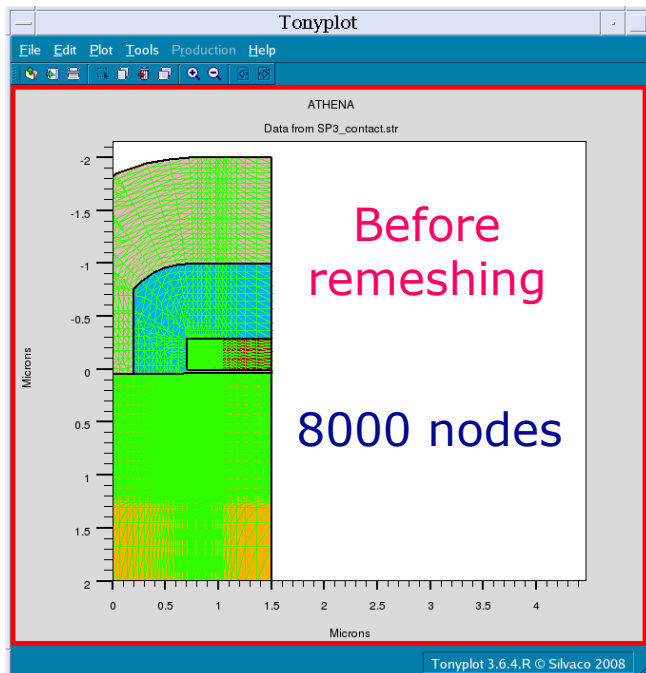
- a) a text file that contains Atlas commands
- b) a log file that stores voltages and currents
- c) a structure file that contains Atlas commands

Devedit

Usually, a grid that is appropriate for process simulation is not always appropriate for device simulation.



To remesh the process simulation output for device simulation, the structure editing and gridding tool *Devedit* can be used.



- The Standard Structure File can be read into Devedit.
- The mesh contained into the file can be replaced using the meshbuild algorithm.
- The mesh can be refined by setting parameters that describe critical areas or by simply pointing to the areas that require refinement.

Remeshing

When remeshing a structure for device simulation

- Ensure adequate mesh density in high field areas
- Avoid abrupt discontinuities in mesh density
- Avoid, or at least minimize, the number of obtuse triangles
- Avoid, or at least minimize, the number of long and thin triangles

Atlas sets some limits on the maximum number of grid nodes

- 2D Atlas simulations have a maximum node limit of 20,000. This limit is high enough for simulations of conventional devices.
- For most 2D simulations, you can obtain accurate results with somewhere between 6,000 and 10,000 node points properly located in the structure.

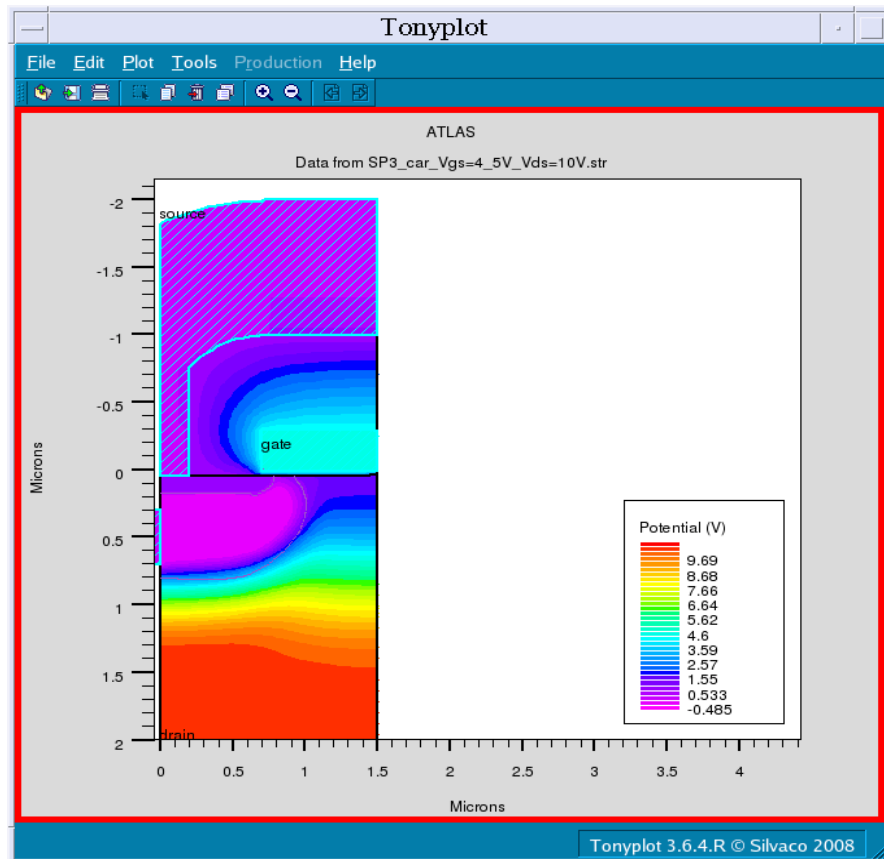
Question 2

When remeshing a structure for device simulation, ensure:

- a) an adequate number of obtuse triangles
- b) a number of nodes greater than 20,000
- c) an adequate mesh density in critical areas

Atlas output: structure files

Structure files (.str) provide an image of the device at a particular bias point. This allows to display any evaluated quantity within the device structure, from doping profiles and band parameters to electron concentrations and electric fields.

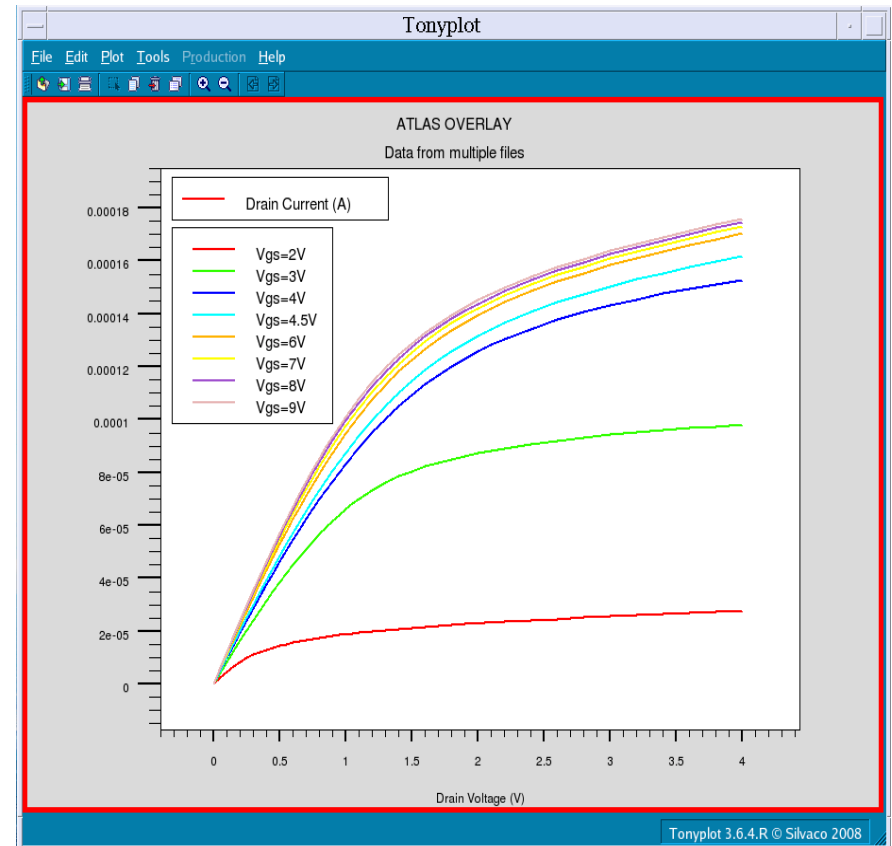


- Structure files can be plotted using Tonyplot.
- Several quantities are saved by default within the structure file (doping, electron concentration, potential, electric field).
- Additional quantities can be specified by using the `OUTPUT` statement.

Atlas output: log files

Log files (.log) store the terminal characteristics calculated by Atlas. These are current and voltages at electrodes in *DC* simulations. In transient simulations, the time is stored. In AC simulations, the small signal frequency, the conductances and capacitances are saved.

- Log files can be plotted using Tonyplot.
- The statement `LOG OUTF=<FILENAME>` is used to open a log file. Terminal characteristics from all `SOLVE` statements after the `LOG` statement are saved into this file. To not save the terminal characteristics to this file, use the `LOG OFF` statement.
- A separate log file should be used for each bias sweep. For example, *separate log files* are used for each gate bias in a MOS I_d/V_{ds} simulation or for each base current in a bipolar I_c/V_{ce} simulation. These files can be overlaid in Tonyplot.



Question 3

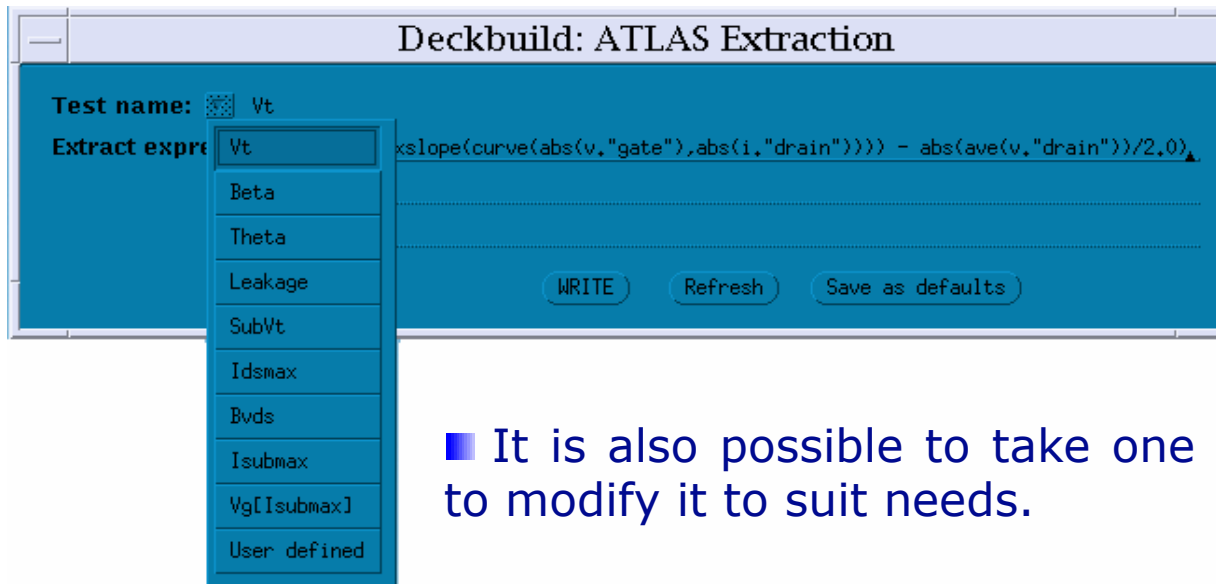
Atlas structure output:

- a) can be plotted using Tecplot
- b) stores currents and voltages at electrodes
- c) saves quantities as electron concentration, potential, electric field at a particular bias point

Extract function

The Extract command (provided within the Deckbuild environment) allows to extract device parameters, operating on the log file or the structure file. To generate the Extract statement:

Select *Extract* → *Device...* from the *Commands* menu



■ It is possible to create customized expressions or choose from a number of standard routines provided for the device simulators.

■ It is also possible to take one of the standard expressions and to modify it to suit needs.

■ In the Extraction popup a list of ready-made extract statements is provided

■ The User defined option allows to generate custom extracts

Atlas examples

Atlas examples are a good starting point for creating a device simulation. It is possible to access the examples through Deckbuild:

- *Click on the **Main Control** menu*

- *Select **Examples**:*

the examples are divided by technology or technology group

- *Choose the technology by double clicking over that item:*

a list of examples for that technology will appear

- *Choose a particular example by double clicking over that item in the list:*

a text description of the example will appear in the window

- *Press the **Load Example** button:*

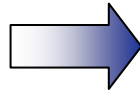
the input command file will be loaded into Deckbuild

- *Press the **Run** button to run the example*

Basic Semiconductor Equations

The mathematical model that describes semiconductor device physics consists of a set of fundamental equations (derived from Maxwell's laws), which link together electrostatic potential and carriers densities:

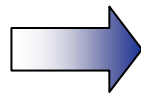
Poisson's equation



It relates variations in **electrostatic potential** to local charge densities.

Continuity equation

Constitutive equation



They describe the way **electron and hole densities** evolve as a result of transport, generation, and recombination processes.

Poisson's equation

It relates variations in electrostatic potential to space charge densities:

$$\text{div}(\epsilon \nabla \psi) = -\rho$$

where:

- ψ is the electrostatic potential
- ϵ is the local permittivity
- ρ is the local space charge density

The local space charge density is the sum of contributions from all mobile and fixed charges, including electrons, holes, and ionized impurities.

The electric field is obtained from the gradient of the potential:

$$\vec{E} = -\nabla \psi$$

Carrier continuity equation

The continuity equations for electrons and holes are defined by:

$$\frac{\partial n}{\partial t} - \frac{1}{q} \operatorname{div} \vec{J}_n = G_n - R_n$$
$$\frac{\partial p}{\partial t} + \frac{1}{q} \operatorname{div} \vec{J}_p = G_p - R_p$$

where:

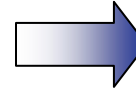
- n and p are the electron and hole concentration
- \vec{J}_n and \vec{J}_p are the electron and hole current densities
- G_n and G_p are the generation rates for electrons and holes
- R_n and R_p are the recombination rates for electrons and holes
- q is the the magnitude of electron charge.

It is sufficient in some cases solving only one carrier continuity equation.

Constitutive equations

Secondary equations are needed to specify physical models for J_n , J_p , G_n , R_n , G_p , R_p

The current density equations, usually obtained by applying *approximations* to the Boltzmann Transport Equation, define the Transport Model.



<i>Drift-Diffusion Model</i>
<i>Energy Balance Model</i>
<i>Hydrodynamic Model</i>

The simplest model of constitutive equations defines the *Drift-Diffusion Model*

$$\vec{J}_n = qn\mu_n\vec{E}_n + qD_n\nabla n$$

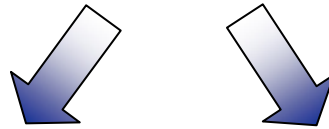
$$\vec{J}_p = qp\mu_p\vec{E}_p - qD_p\nabla p$$

where:

- μ_n and μ_p are the electron and hole mobilities
- $D_n = \frac{K_B T_L}{q} \mu_n$, $D_p = \frac{K_B T_L}{q} \mu_p$ are the Einstein relationships
- $\vec{E} = -\nabla\psi$ is the Electric Field

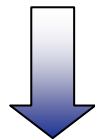
Drift-Diffusion model

Drift-Diffusion model

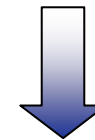


- Simplicity
- Immediate physical interpretation
- Efficient numerical methods

Limitation of not introducing the energy (carrier temperature) as independent variable



Adequate for nearly all devices



Less accurate for deep submicron devices and too high gradients



Energy Balance and Hydrodynamic Models
(higher order solutions to the general Boltzmann Transport Equation)

Question 4

The simplest transport model implemented in the device simulators is:

- a) the Hydrodynamic model
- b) the Energy Balance model
- c) the Drift-Diffusion model

Physical Models

Physical models implemented in Atlas can be grouped into five classes

- Mobility
- Recombination
- Carrier statistics
- Impact ionization
- Tunneling

All models with exception of impact ionization are specified on the `MODELS` statement. Impact ionization is specified in the `IMPACT` statement.

Next slides will give a summary description and recommendations on the use of the most important models.

Mobility model

Electrons and holes are accelerated by electric fields, but lose momentum as a result of *scattering processes*, which includes:

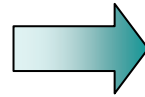
- *Lattice vibrations* (phonons)
- *Impurity ions*
- *Other carriers*
- *Material imperfections* (surface roughness, ...)

Model	Syntax	Notes
Concentration Dependent	conmob	It is a doping versus mobility table valid for 300K only.
Concentration and Temperature Dependent	analytic	Caughey - Thomas formula. Tuned for 77-450K.
Carrier-Carrier Scattering	ccsmob	Important when carrier concentration is high (e.g., forward bias power devices).
Parallel Electric Field Dependence	fldmob	Required to model any type of velocity saturation effect.
Lombardi (CVT) Model	cvt	Complete model including N, T, E// and E _⊥ effects. Good for non-planar devices.
Yamaguchi Model	yamaguchi	Includes N, E// and E _⊥ effects. Only for 300K.

Carrier Generation-recombination model

Carrier generation-recombination is the process through which the semiconductor material attempts to return to equilibrium after being disturbed from it.

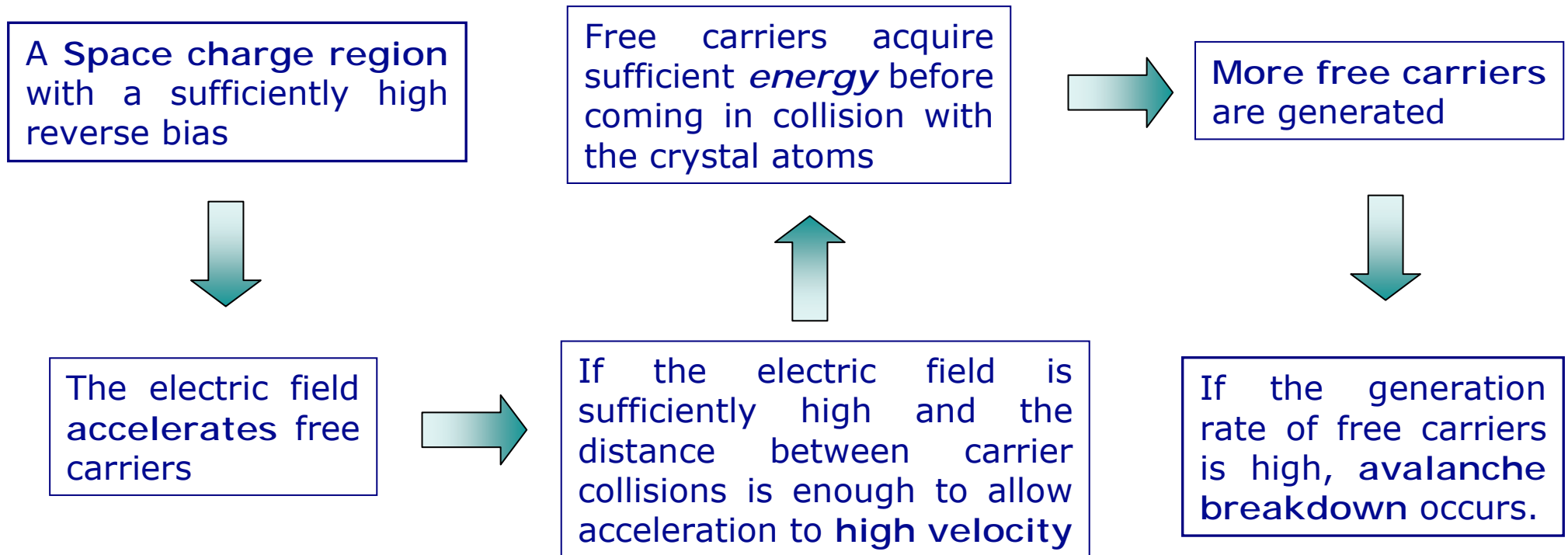
Processes responsible for generation-recombination



- Phonon transitions
- Photon transitions
- Auger transitions
- Surface recombination
- Impact ionization
- Tunneling

Model	Syntax	Notes
Shockley-Read-Hall	srh	Uses fixed minority carrier lifetimes. It Should be used in most simulations.
Concentration Dependent	consrh	Specifies Shockley-Read-Hall recombination using concentration dependent lifetimes.
Auger	auger	Specifies Auger recombination. Important at high current densities.

Impact ionization model



Model	Syntax	Notes
Selberherr	Impact selb	Recommended for most cases. Includes temperature dependent parameters.
Crowell-Size	Impact crowell	Uses dependence on carrier scattering length.

Model Macros

Atlas provides an easy method for selecting the correct models for various technologies. The `MOS` and `BIPOLAR` parameters for the `MODELS` statement configure a basic set of mobility, recombination, carrier statistics, and tunneling models for MOSFET and BIPOLAR devices.

MODELS MOS PRINT

Enables the `CVT`, `SRH`, and `FERMI` models

MODELS BIPOLAR PRINT

Enables the `CONMOB`, `FLDMOB`, `CONSRH`, `AUGER`, and `BGN` models

The `print` option in the `MODELS` statement displays the details of material parameters and mobility models at the start of the run-time output.

Question 5

Models specification in Atlas is:

- a) not necessary for impact ionization
- b) possible only for bipolar device
- c) possible through MODELS and IMPACT statements

Boundary Conditions (1)

Atlas supports several boundary conditions

- *Ohmic* contacts
- *Schottky* contacts
- *Current* boundary conditions
- *Lumped* elements between applied biases and device contacts
- *Distributed* contact resistance to take into account the finite resistivity of semiconductor contacts.

Ohmic Contacts

An electrode is assumed by default to be ohmic:

CONTACT NAME=ANODE NEUTRAL

Boundary Conditions (2)

Schottky Contacts

To set a Schottky contact, specify a workfunction (eV) using the WORKFUN parameter of the CONTACT statement:

```
CONTACT NAME=BODY WORKFUN=4.94
```

In practice, the workfunction is defined as

$$\text{WORKFUN} = \text{AFFINITY} + \Phi_B$$

where Φ_B is the barrier height at the metal-semiconductor interface in eV. For example, if the Schottky contact is aluminum with a workfunction difference to the silicon of 4.2eV and a barrier height of 0.7eV, then WORKFUN=4.9

Current boundary conditions

Calculation of current boundary conditions is activated by the CURRENT parameter in the CONTACT statement:

```
CONTACT NAME=BASE CURRENT
```

Current controlled electrodes are useful when the current is highly sensitive to voltage or is a multi-valued function of voltage (post-breakdown and snap-back).

Boundary Conditions (3)

External Resistor, Capacitors, Inductors

Resistance, capacitance and inductance connected to an electrode can be specified using the RESISTANCE, CAPACITANCE and INDUCTANCE parameters in the CONTACT statement:

```
CONTACT NAME=DRAIN CAPACITANCE=20e-12
```

Since contact materials have finite resistivities, the electrostatic potential is not always uniform along the metal-semiconductor surface. To account for this effect, a distributed contact resistance can be associated with any electrode using the CON.RESIST parameter:

```
CONTACT NAME=SOURCE CON.RESISTANCE=0.01
```

<i>Parameter</i>	<i>Units</i>
capacitance	F/ μm
inductance	H· μm
resistance	$\Omega\cdot\mu\text{m}$
con.resistance	$\Omega\cdot\text{cm}^2$

Floating Contacts

To specify a floating contact place a very large resistor at the electrode:

```
CONTACT NAME=SOURCE RESISTANCE=1e14
```

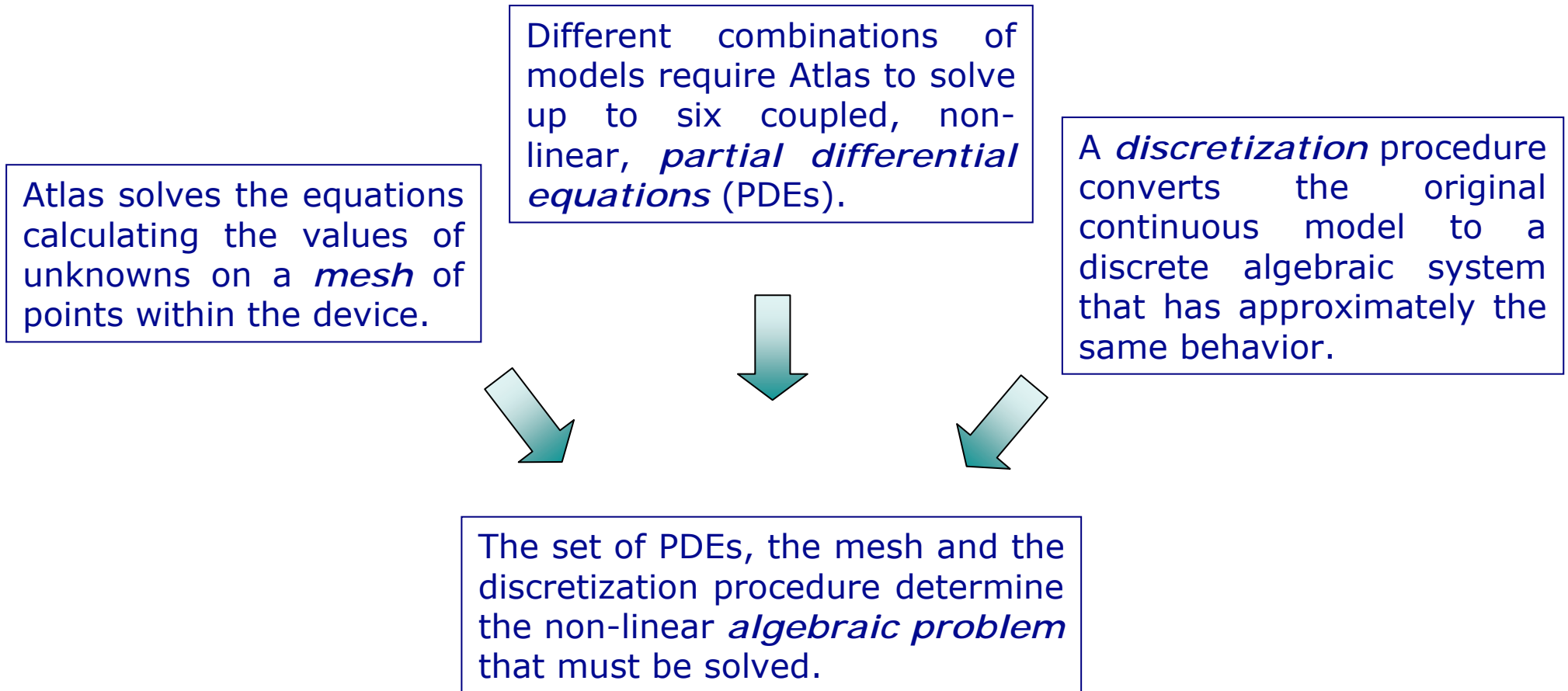
Question 6

For what concerns boundary conditions:

- a) it's possible to define only ohmic contacts
- b) it's possible to switch to current control
- c) it's not possible to specify floating contacts

Numerical Methods (1)

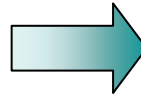
Different numerical methods can be used for calculating the solutions to semiconductor device problems.



Numerical Methods (2)

The non-linear *iteration procedure* starts from an initial guess and uses an iterative procedure that refines successive estimates of the solution.

Iteration continues until the corrections are small enough to satisfy convergence criteria, or until it is clear that the procedure is not going to converge.



When a solution fails to converge, a user normally tries a different grid, a different initial guess strategy, or a different non-linear iteration technique.

There are *three types of solution techniques*: *Gummel*, *Newton* and *Block*.

- Numerical methods are given in the `METHOD` statements of the input file.
- If more than one method is specified in the same `METHOD` statement, each solution method will be applied in succession until convergence is obtained.
- The order that the solution methods will be applied is Gummel then Block then Newton. If no solution methods are specified Newton is applied by default.

Gummel and Block Method

Gummel (decoupled)

The Gummel method solves for each unknown in turn, keeping the other variables constant and repeating the process until a stable solution is achieved.

- This method tolerates relatively poor initial guesses
- Generally, it is useful where the system of equations is weakly coupled but has only linear convergence.
- It cannot be used with lumped elements or current boundary conditions.

Block

The Block method solves some equations fully coupled while others are decoupled. It is useful when lattice heating or energy balance equations are included.

Newton Method

Newton (fully coupled)

The Newton method solves the total system of unknowns together.

- It is useful when the system of equations is strongly coupled and has quadratic convergence.
- It may spend extra time solving for quantities that are essentially constant or weakly coupled. However for almost all cases, this method is preferred and it is the default.
- The following cases require the Newton method to be set for isothermal drift-diffusion simulations:
 - Current boundary conditions
 - External elements
 - AC analysis
 - Impact ionization

Question 7

In Atlas three types of numerical methods are implemented:

- a) Shockley, Read, Hall
- b) Gummel, Newton, Crowell
- c) Block, Newton, Gummel

Obtaining Solutions

Obtaining solutions is similar to setting up test equipment for device tests.

- You usually define the voltages on each of the electrodes in the device.
- Atlas then calculates the current through each electrode.
- Atlas also calculates internal quantities, such as carrier concentrations and electric fields throughout the device. This information is difficult or impossible to measure.

Solution statements

- When no previous solutions exist, the initial guess for potential and carrier concentrations must be made from the doping profile. The initial solution (zero bias or thermal equilibrium) is specified by the statement:

```
SOLVE INIT
```

- Solutions are obtained by stepping the biases on electrodes from the initial equilibrium condition. The voltage on each electrode is specified by using the following statement:

```
SOLVE NAME=ANODE VANODE=0 VFINAL=-200 VSTEP =-5
```

Atlas Statements

Atlas input file contains a sequence of command lines. Each line consists of a keyword (*statement*) that identifies the command and a set of parameters. The general format is:

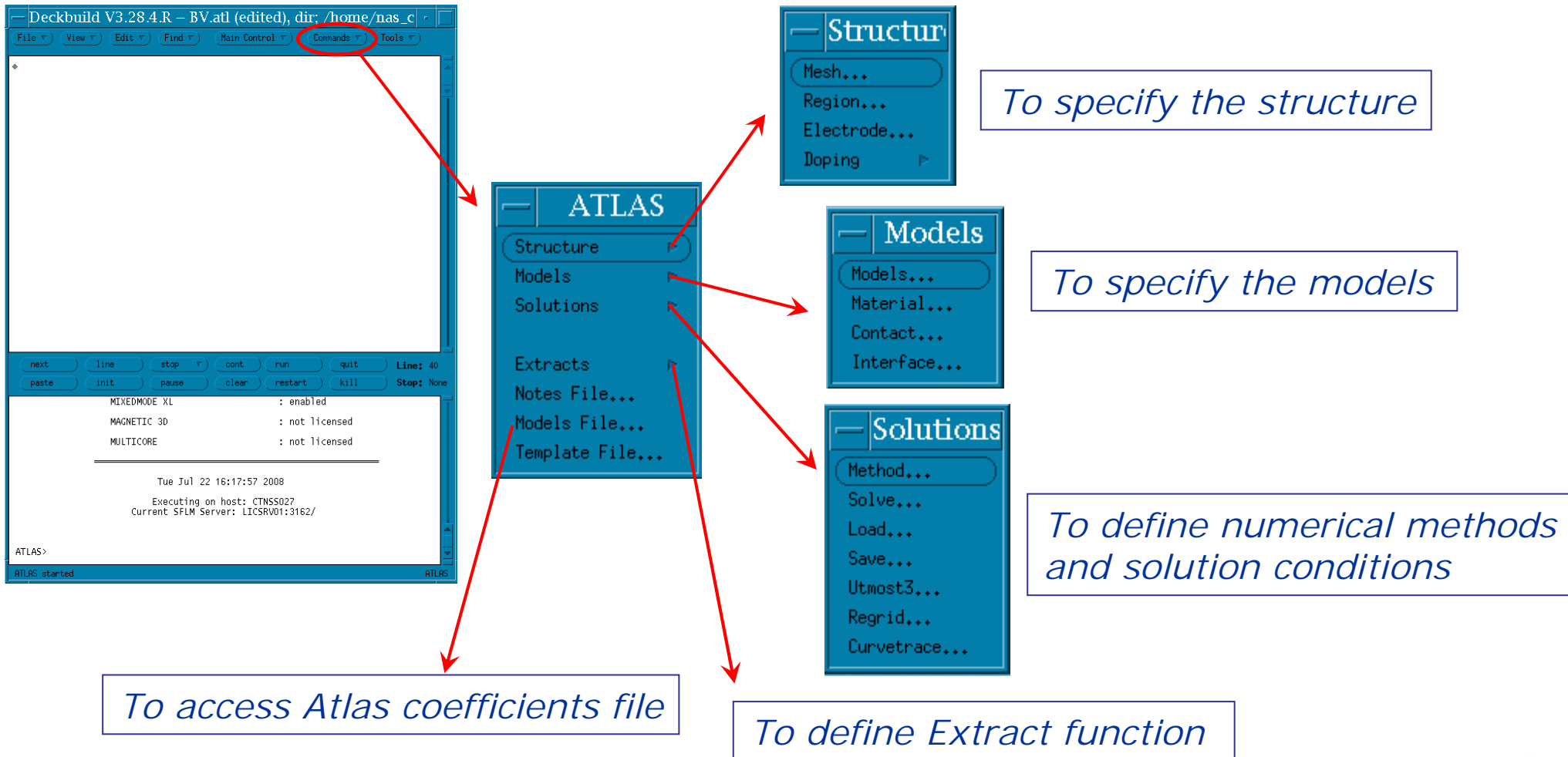
<STATEMENT> <PARAMETER> = <VALUE>

In Atlas input file there are four groups of statements that must occur in the correct order.

Group	Statements
1. Structure Specification	MESH
	ELECTRODE
	CONTACT
2. Models specification	MODELS
3. Numerical Method Selection	METHOD
4. Solution Specification	LOG
	SOLVE
	LOAD
	SAVE

Running Atlas inside Deckbuild

When Atlas is the active simulator in Deckbuild, the *Commands* menu is configured for Atlas *statements* and can help to create the input file.



Diode breakdown simulation

The following section provides a typical example of device simulation. The input file of a breakdown simulation of a simple pn diode is generated by using Deckbuild interface.

Basic operations to create the input file

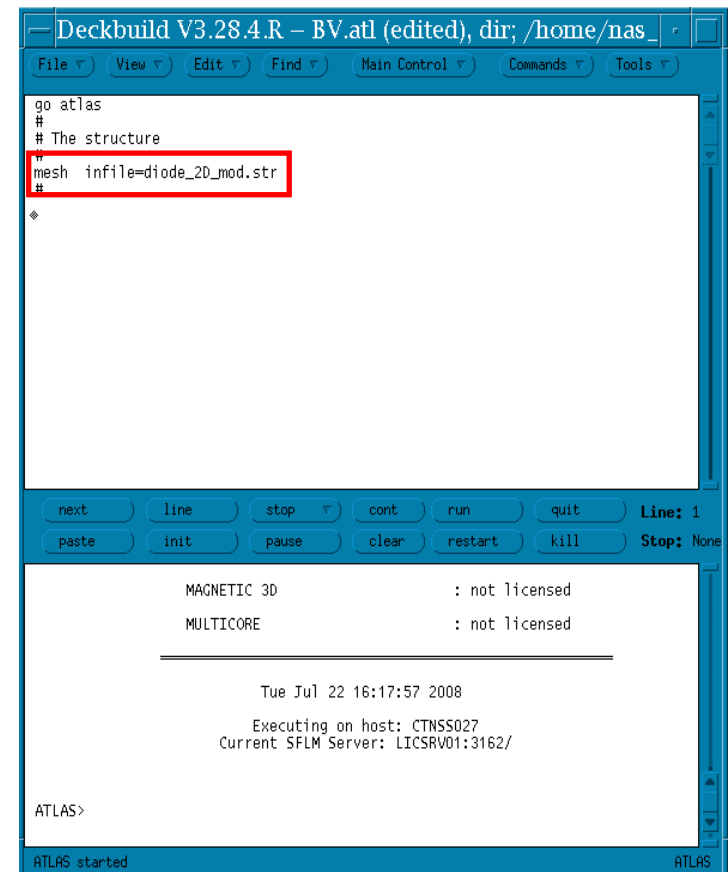
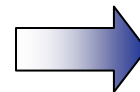
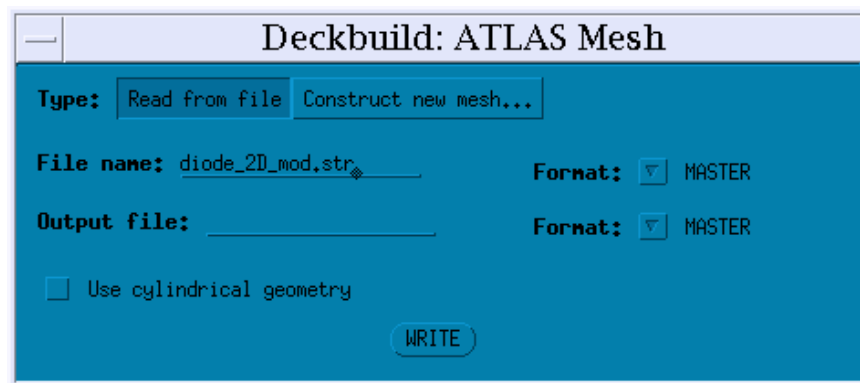
- Loading the diode structure
- Specifying the electrodes (anode and cathode)
- Selecting the bipolar models and the impact ionization model
- Specifying the numerical method
- Reverse biasing the diode to obtain the breakdown curve
- Saving the log and the structure files

Structure Specification: the MESH statement

A 2D or 3D structure created by Athena or Devedit can be read into Atlas using the statement `MESH INFILE`, which loads in mesh, geometry, electrode positions, and doping of the structure. To generate the `MESH` statement:

Select *Structure* → *Mesh...* from the *Commands* menu

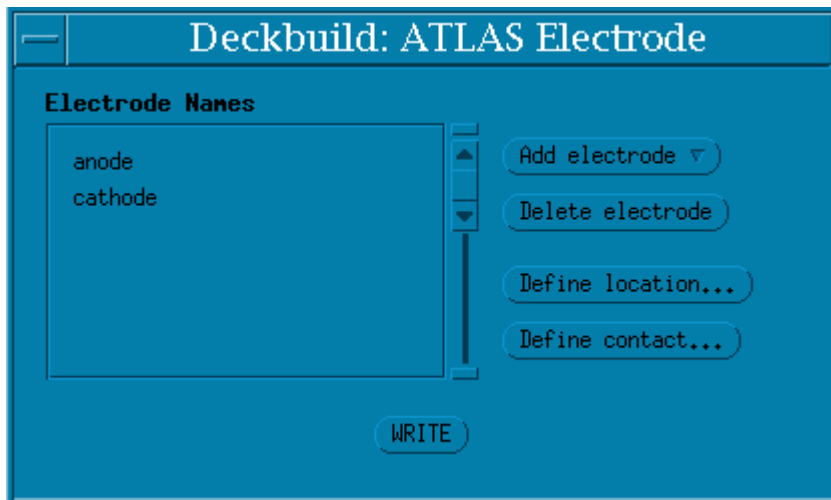
- Select the *Read from file* button and write the name of the structure you want to load in.
- Press the *Write* button and the corresponding command line will appear in the Deckbuild Text Subwindow.



Structure Specification: the ELECTRODE statement

To define the electrodes an `ELECTRODE` statement has to be generated:

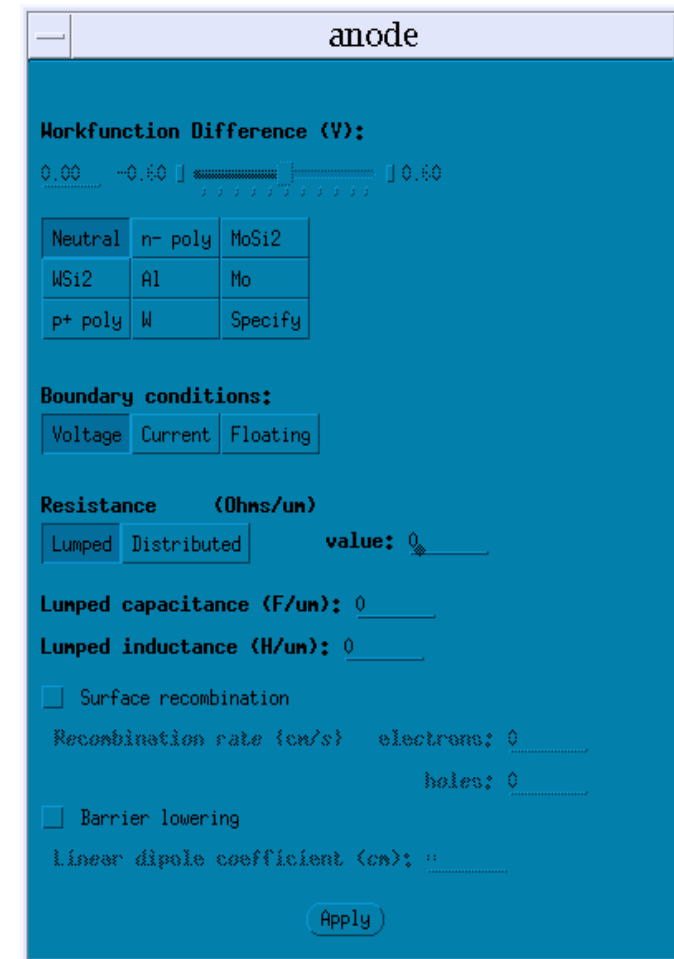
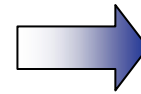
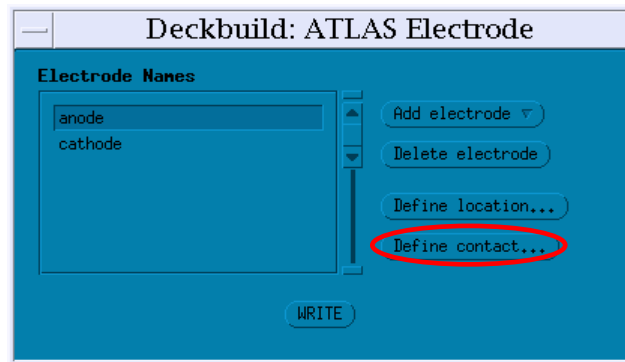
Select *Structure* → *Electrode...* from the *Commands* menu



- Electrodes must be specified in the same sequential order of Devedit or Athena.
- To add an electrode press the *Add electrode* button and select a name. The name will appear in the scrolling list.
- Repeat this procedure once per electrode in the device.
- Before writing the electrode information into the input file, assign boundary conditions to the electrode.

Structure Specification: the CONTACT statement (1)

To assign boundary conditions to the electrode a CONTACT statement must be generated. To do this, select the electrode name and click on *Define contact...*

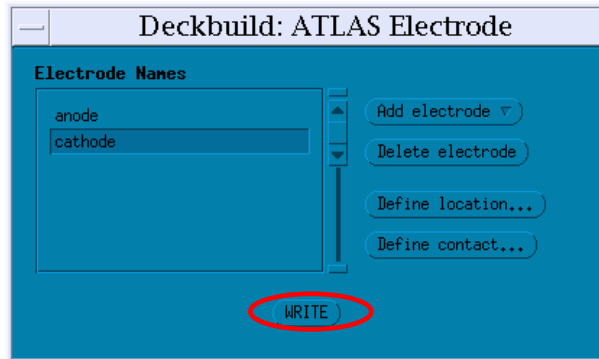


In the popup window that will appear, you can:

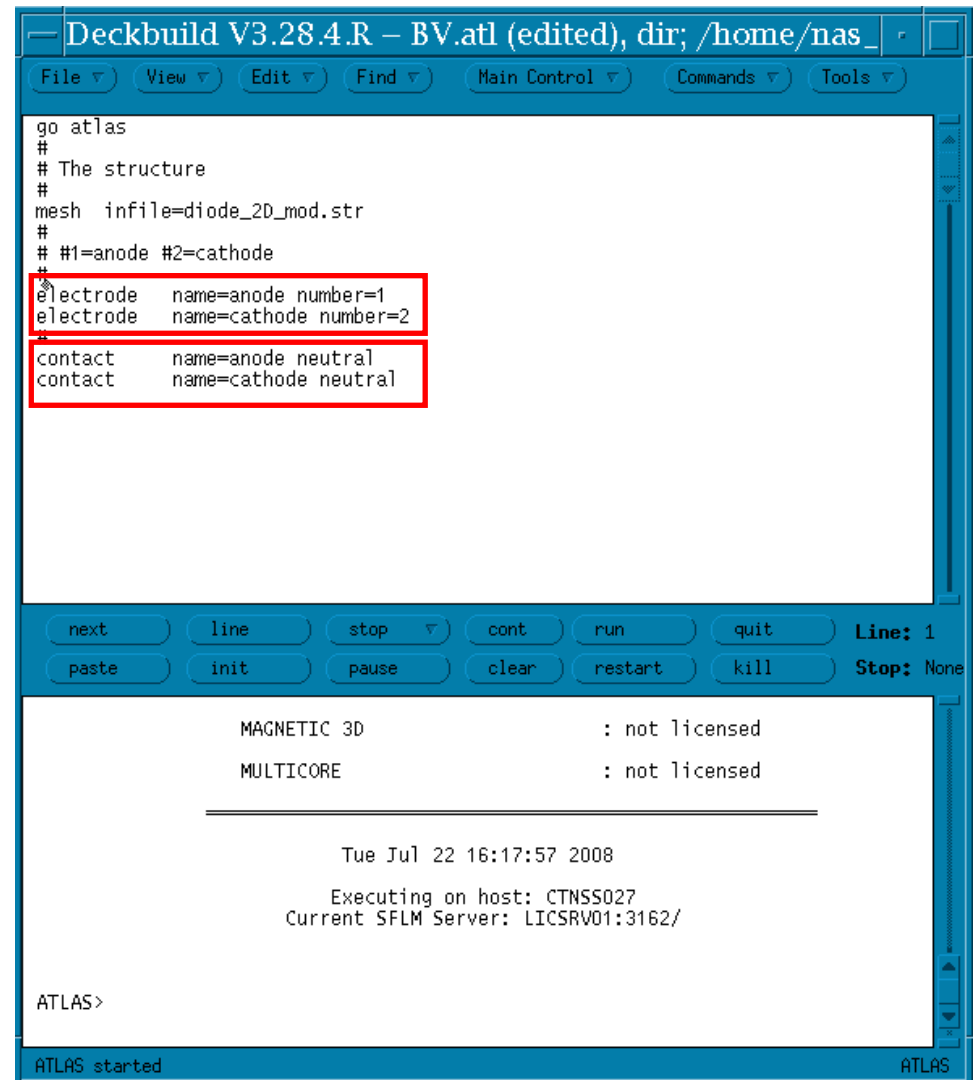
- Define the electrode *workfunction*
 - by default an electrode is ohmic (Neutral)
 - the workfunctions of commonly used materials can be specified using the name of the material.
- Change an electrode from voltage to *current control*
- Specify external *resistance, capacitance, conductance*

Structure Specification: the CONTACT statement (2)

- Select the cathode electrode name and set the boundary conditions in the same way.
- Finally, press the *Write* button.



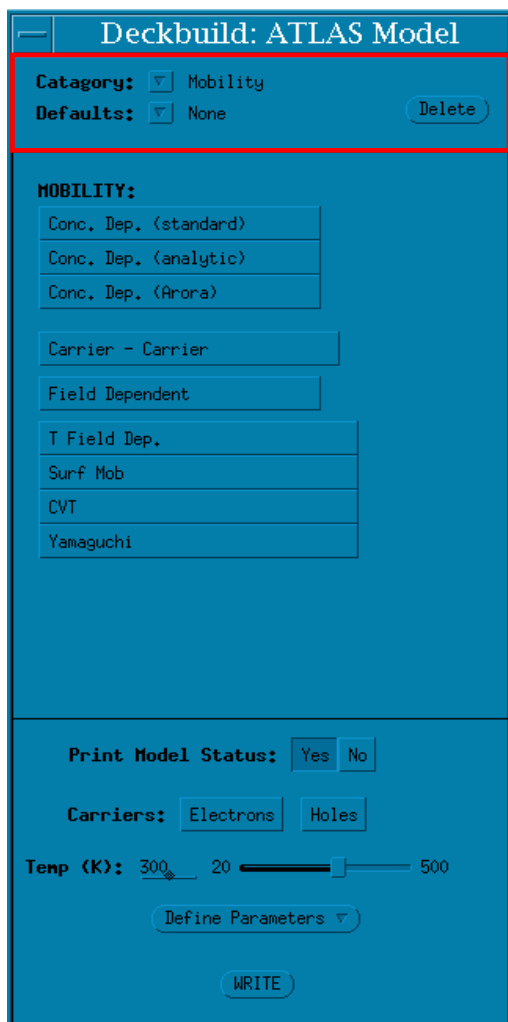
- The command lines corresponding to **ELECTRODE** and **CONTACT** statement will appear on the Deckbuild Text window.



```
go atlas
#
# The structure
#
mesh infile=diode_2D_mod.str
#
# #1=anode #2=cathode
#
electrode name=anode number=1
electrode name=cathode number=2
#
contact name=anode neutral
contact name=cathode neutral
```

Models Specification

All models with exception of impact ionization are specified on the `MODELS` statement. Impact ionization is specified in the `IMPACT` statement. To generate these statements:



Select *Models* → *Models...* from the *Commands* menu

Deckbuild provides an easy method for selecting the correct models for the different technologies. Deckbuild window for setting Atlas models shows two fields:

- *Category*, which allows to select the class of models.
- *Defaults*, which allows to configure a basic set of models for Mosfet and Bipolar devices.
 - If *MOS* is chosen in the *Defaults* field, the models suitable for Mosfet devices will be selected in each Category.
 - If *Bipolar* is chosen in the *Defaults* field, the models suitable for Bipolar devices will be selected in each Category.

Models for Bipolar devices (1)

Choosing Bipolar for simulating diode behavior, the corresponding models are selected.

Deckbuild: ATLAS Model

Category:

Defaults:

MOBILITY:

- Conc. Dep. (standard)
- Conc. Dep. (analytic)
- Conc. Dep. (Arora)
- Carrier - Carrier
- Field Dependent
- T Field Dep.
- Surf Mob
- CVT
- Yamaguchi

Print Model Status: Yes No

Carriers: Electrons Holes

Temp (K): 300 20 500

Mobility

Category:

Defaults:

MOBILITY:

- Conc. Dep. (standard)
- Conc. Dep. (analytic)
- Conc. Dep. (Arora)
- Carrier - Carrier
- Field Dependent

Statistics

Category:

Defaults:

STATISTICS:

- Boltzman
- Fermi-Dirac
- Incomplete Ionisation
- Band gap narrowing

Recombination

Category:

Defaults:

RECOMBINATION:

- Auger
- SRH (fixed lifetimes)
- SRH (conc,dep. lifetimes)

Models for Bipolar devices (2)

Pressing the *Write* button, the `MODELS` statement with the appropriate bipolar models is written in the Deckbuild window.

```
go atlas
#
# The structure
#
mesh infile=diode_2D_mod.str
#
# #1=anode #2=cathode
#
electrode name=anode number=1
electrode name=cathode number=2
#
contact name=anode neutral
contact name=cathode neutral
#
models auger consrh conmob fldmob boltzman bgn temperature=300 print
#
```

Recombination

- **auger** : Auger recombination
- **consrh** : Shockley-Read-Hall recombination with concentration dependent lifetimes

Mobility

- **conmob** : concentration dependent mobility
- **fldmob** : field dependent mobility

Statistics

- **boltzman** : Boltzmann carrier statistics
- **bgn** : band gap narrowing

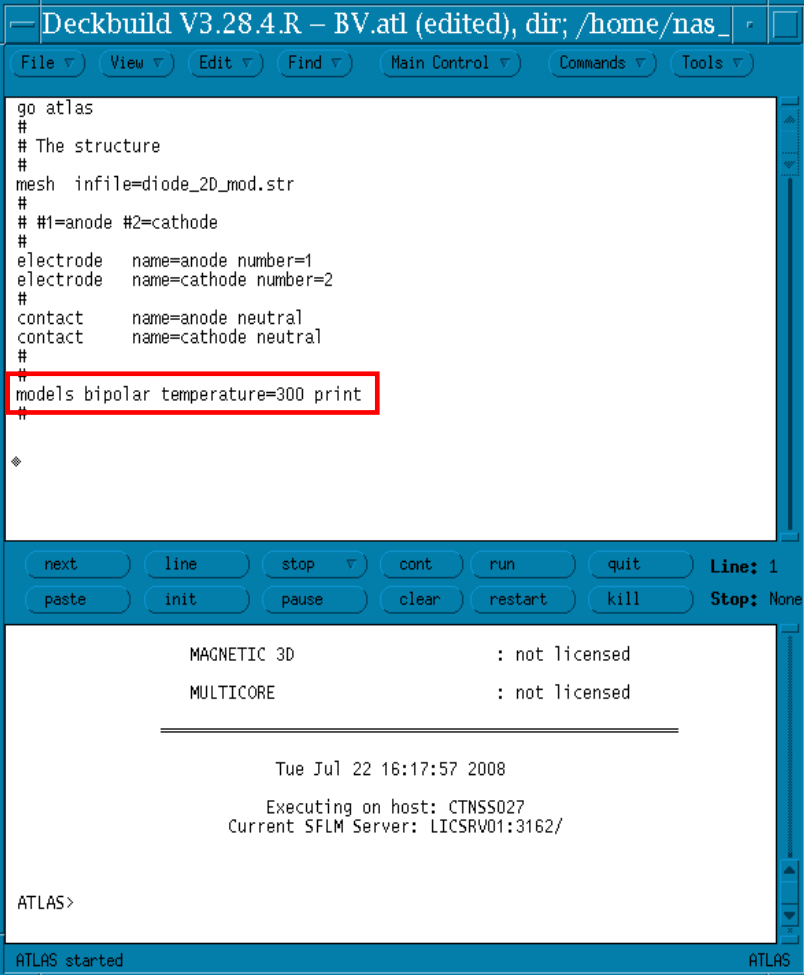
Models for Bipolar devices (3)

The same models can be selected writing the `bipolar` parameter in the MODELS statement.

■ **bipolar**: enables the *conmob*, *fldmob*, *consrh*, *auger* and *bgn* models.

■ **temperature**: specifies the lattice temperature in Kelvin

■ **print**: displays the details of material parameters and mobility models at the start of the run-time output.



```
Deckbuild V3.28.4.R – BV.atl (edited), dir: /home/nas_
File View Edit Find Main Control Commands Tools
go atlas
#
# The structure
#
mesh infile=diode_2d_mod.str
#
# #1=anode #2=cathode
#
electrode name=anode number=1
electrode name=cathode number=2
#
contact name=anode neutral
contact name=cathode neutral
#
#
models bipolar temperature=300 print
#
◆
next line stop cont run quit Line: 1
paste init pause clear restart kill Stop: None
MAGNETIC 3D : not licensed
MULTICORE : not licensed
-----
Tue Jul 22 16:17:57 2008
Executing on host: CTNSS027
Current SFLM Server: LICSRV01:3162/
ATLAS>
ATLAS started ATLAS
```


Question 8

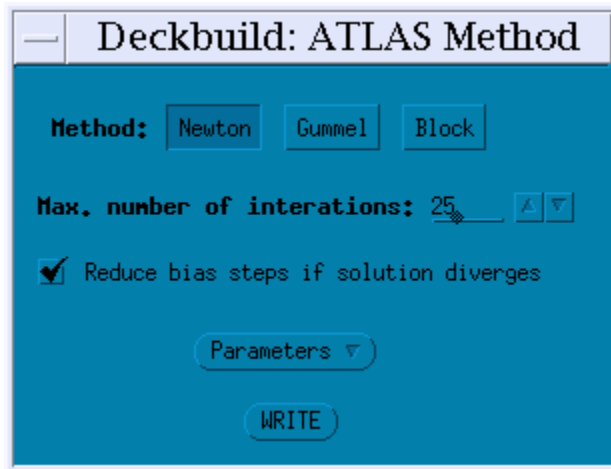
In order to perform a breakdown simulation it is crucial to set:

- a) the cvt mobility model
- b) the impact ionization model
- c) current boundary conditions

Numerical Method Selection (1)

Different numerical methods can be used to calculate the solutions of semiconductor device problems. Numerical methods are given in the `METHOD` statement:

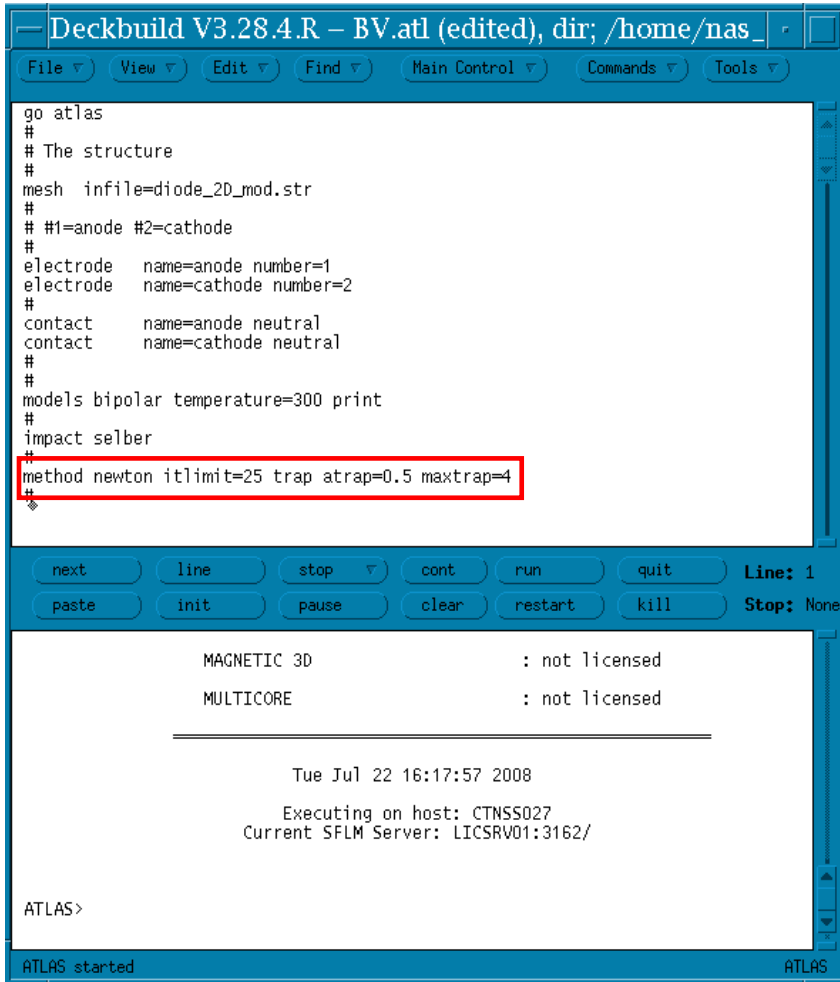
Select *Solutions* → *Method...* from the *Commands* menu



- Select one of the three available methods:
 - Newton
 - Gummel
 - Block
- Set the maximum number of iterations (default=25).
- Allow reducing bias steps if solution diverges.
- Press the *Write* button to write the method command line in the input file.

Numerical Method Selection (2)

Pressing the *Write* button the `METHOD` command line is written in the input file



```
go atlas
#
# The structure
#
mesh infile=diode_2D_mod.str
#
# #1=anode #2=cathode
#
electrode name=anode number=1
electrode name=cathode number=2
#
contact name=anode neutral
contact name=cathode neutral
#
#
models bipolar temperature=300 print
#
impact selber
#
method newton itlimit=25 trap atrap=0.5 maxtrap=4
#
#
```

■ **itlimit**: specifies the maximum number of allowed iteration (default=25).

■ **trap**: specifies that the electrode bias steps are reduced by the multiplication factor *atrap*, if a solution starts to diverge.

■ **atrap**: specifies the multiplication factor that reduces the electrode bias steps when the solution diverges (default=0.5).

■ **maxtrap**: specifies the number of times the trap procedure will be repeated in case of divergence (default=4). A value of `maxtrap=10` is recommended for breakdown simulation.

Numerical Method Selection (3)

■ Deckbuild does not support all possible Atlas syntax. Therefore not all the available parameters can be inserted in the input file by using Deckbuild interface.

■ The command lines generated in the Deckbuild Text window can be easily modified by hand. Parameters can be added and their values modified just typing on the window.

■ For all breakdown simulation it is recommended:

■ to increase the `maxtrap` value to 10

■ to add the `climit` parameter to the method statement and to reduce its value to `1e-4` (default=`1e4`)

* Note that it is not necessary to write the parameters with the default values. Therefore `itlimit=25` and `atrap=0.5` can be omitted. You need to introduce them if you want to modify their default values.

```
Deckbuild V3.28.4.R – BV.atl (edited), dir: /home/nas_
File View Edit Find Main Control Commands Tools
go atlas
#
# The structure
#
mesh infile=diode_2D_mod.str
#
# #1=anode #2=cathode
#
electrode name=anode number=1
electrode name=cathode number=2
#
contact name=anode neutral
contact name=cathode neutral
#
models bipolar temperature=300 print
#
impact selber
#
method newton trap maxtrap=10 climit=1e-4
#
next line stop cont run quit Line: 1
paste init pause clear restart kill Stop: None
MAGNETIC 3D : not licensed
MULTICORE : not licensed
-----
Tue Jul 22 16:17:57 2008
Executing on host: CTNSS027
Current SFLM Server: LICSRV01:3162/
ATLAS>
ATLAS started ATLAS
```

Question 9

The parameter `trap` in the `METHOD` statement:

- a) places donor traps at oxide/silicon interface
- b) reduces the bias step to improve convergence
- c) activates the trap numerical method

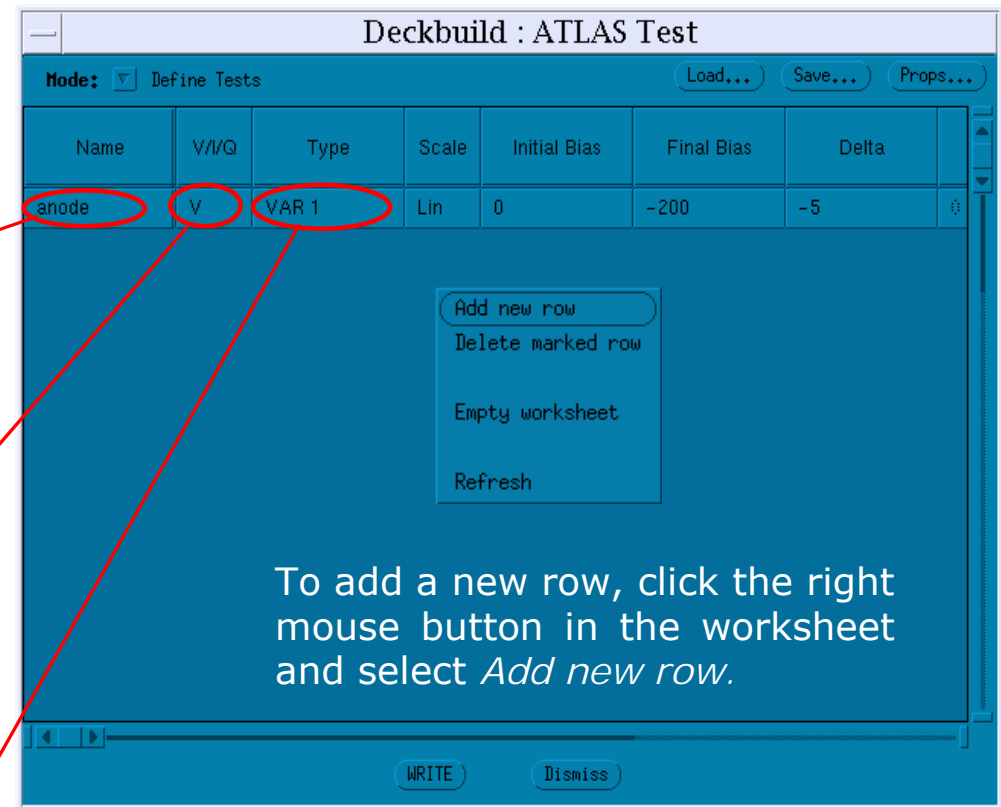
Solutions specification: the SOLVE statement (1)

To generate a SOLVE statement select *Solutions* → *Solve...* in the *Commands* menu.

■ In the first cell, to edit the electrode name press the right mouse button and select the desired name.

■ The second cell specifies if the electrode is voltage (V), current (I) or charge (Q) controlled.

■ The third cell specifies whether the SOLVE statement is to be a single DC solve (CONST), a swept DC variable (VAR1), a stepped DC variable (VAR2), or a transient solution (PULSE).



Solutions specification: the SOLVE statement (2)

The remaining cells specify the parameter required for the type of solution desired. These cells can be edited to entry the numerical values.

- To obtain the diode reverse characteristic, ramp up the anode electrode setting:

Initial Bias=0

Final Bias=-200

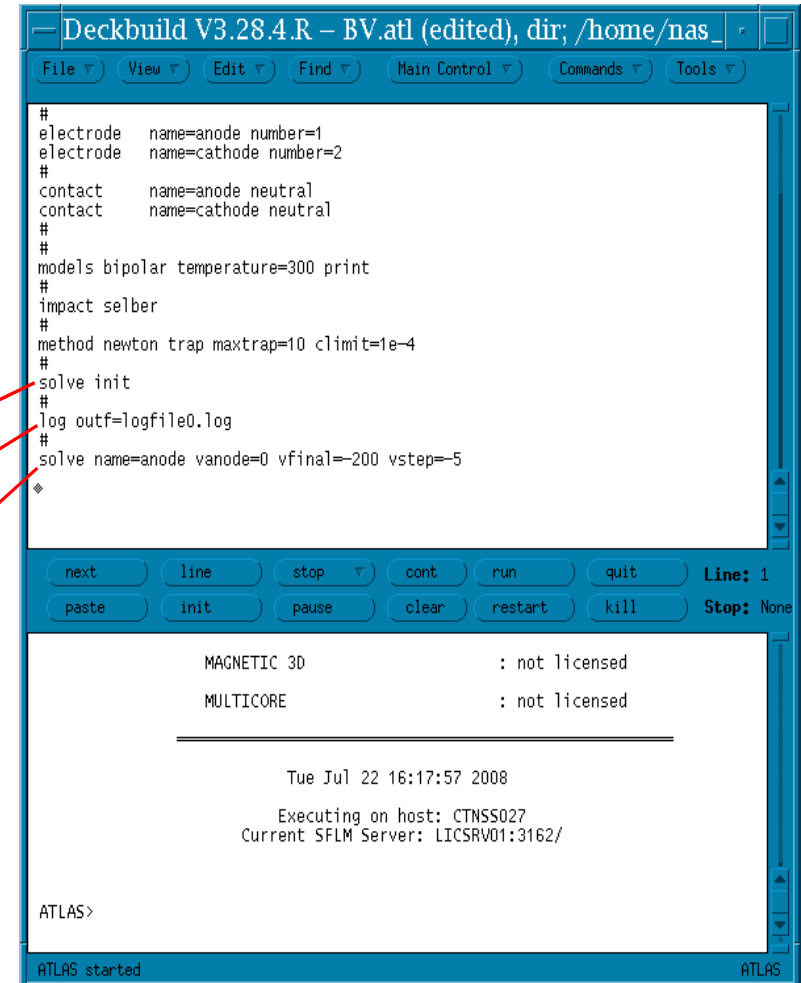
Delta=-5

- Press the *Write* button to write the command lines into the input file.

To solve the Poisson's equation

To write the log file

To ramp the anode from the initial voltage `vanode=0` to the final voltage `vfinal=-200` with a voltage increment `vstep=-5`



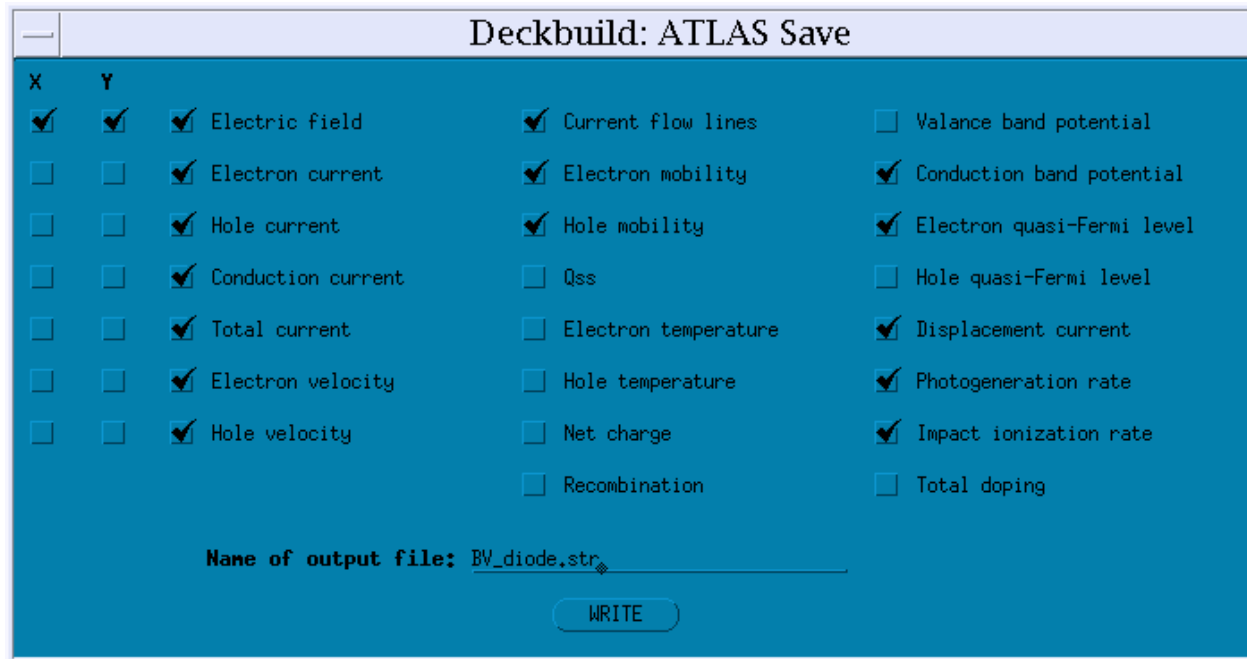
The screenshot shows the Deckbuild V3.28.4.R software interface. The main window displays the following text:

```
#  
electrode name=anode number=1  
electrode name=cathode number=2  
#  
contact name=anode neutral  
contact name=cathode neutral  
#  
#  
models bipolar temperature=300 print  
#  
impact selber  
#  
method newton trap maxtrap=10 climit=1e-4  
#  
solve init  
#  
log outf=logfile0.log  
#  
solve name=anode vanode=0 vfinal=-200 vstep=-5  
◆
```

Below the text is a control panel with buttons: next, line, stop, cont, run, quit, Line: 1, paste, init, pause, clear, restart, kill, Stop: None. At the bottom, there is a status bar with the text: MAGNETIC 3D : not licensed, MULTICORE : not licensed, Tue Jul 22 16:17:57 2008, Executing on host: CTNSS027, Current SFLM Server: LICSRV01:3162/, ATLAS>, ATLAS started, ATLAS.

Solutions specification: the OUTPUT statement

To save a structure file select *Solutions* → *Save...* in the *Commands* menu.



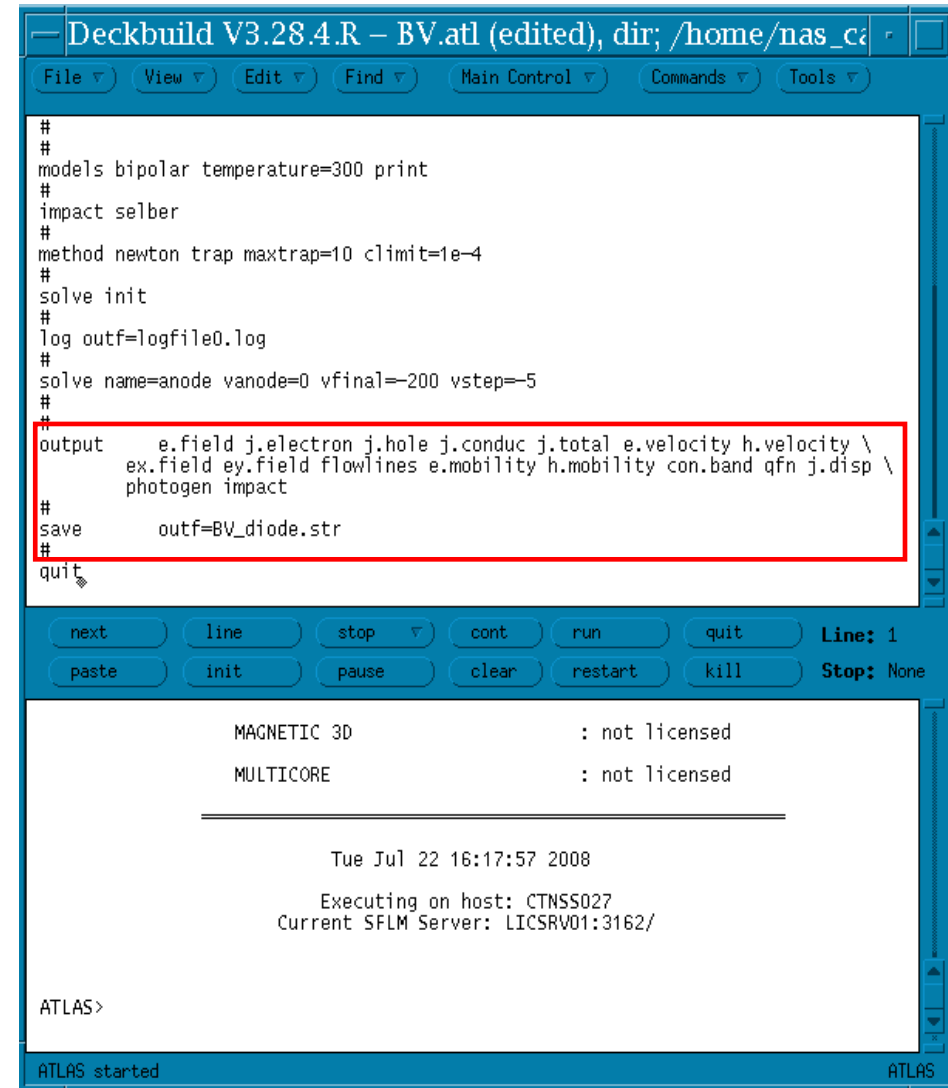
- In the popup window select the electrical information you want to be stored in the standard structure file format.
- Specify a file name (the file extension *.str* is recommended) and click on the *Write* button.

Solutions specification: the SAVE statement

Pressing the *Write* button, two statements appear in the input file:

- **OUTPUT** allows to specify electrical quantities to be stored in the structure file and subsequently displayed using Tonyplot.

- **SAVE OUTF** saves in a structure file all electrical data specified in the **OUTPUT** statement. If a solve statement has preceded a save statement the data from the last solution is stored.



```
Deckbuild V3.28.4.R – BV.atl (edited), dir: /home/nas_ca
File View Edit Find Main Control Commands Tools
#
#
models bipolar temperature=300 print
#
impact selber
#
method newton trap maxtrap=10 climit=1e-4
#
solve init
#
log outf=logfile0.log
#
solve name=anode vanode=0 vfinal=-200 vstep=-5
#
#
output e.field j.electron j.hole j.conduc j.total e.velocity h.velocity \
ex.field ey.field flowlines e.mobility h.mobility con.band qfn j.disp \
photogen impact
#
save outf=BV_diode.str
#
quit
next line stop cont run quit Line: 1
paste init pause clear restart kill Stop: None
MAGNETIC 3D : not licensed
MULTICORE : not licensed
Tue Jul 22 16:17:57 2008
Executing on host: CTNSS027
Current SFLM Server: LICSRV01:3162/
ATLAS>
ATLAS started ATLAS
```

Question 10

The **OUTPUT** statement:

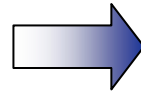
- a) saves an output structure file
- b) loads a previously saved structure file
- c) allows to specify the electrical information to be stored in the structure file

Obtaining Solutions around the breakdown voltage

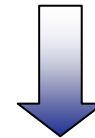
Obtaining solutions around the breakdown voltage requires special care. The breakdown curve is flat up to a voltage very close to breakdown and then almost vertical. The *current change* by orders of magnitude for very small bias increments produces some *convergence problems*. Consider the following statement:

```
SOLVE NAME=ANODE VANODE=0 VFINAL=-200 VSTEP=-5
```

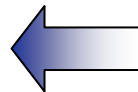
If the breakdown occurs at 78V, there are no solutions for voltages greater than 78V.



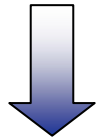
Atlas is trying to ramp to 200V, so it is inevitable it will fail to converge at some point.



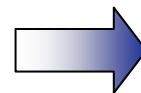
Atlas will continually try to increase the drain voltage until it reaches the limit set by the `maxtrap` parameter.



Bias step reduction will take place due to the `trap` parameter.



Typically, to see the breakdown point the current should increase by two orders of magnitude in a small voltage increment.



If the current does not reach a sufficiently high level, instead of reducing the voltage step, increase the `maxtrap` value.

Run-time output (1)

Run-time output is provided at the bottom of the Deckbuild Window. Errors occurring during the simulation run will be displayed in this output.

```
#
# ramp the anode
#
solve init
#
solve varnode=0.0 vstep=-5.0 vfinal=-200.0 name=anode
#
output  e.field j.electron j.hole j.conduc j.total e.velocity h.velocity \
        ex.field jx.electron jx.hole ex.velocity hx.velocity ey.field \
        jy.electron jy.hole ey.velocity hy.velocity flowlines e.mobility \
        h.mobility e.temp h.temp con.band qfn j.disp photogen impact

save  outf=BV_diode.str
#
quit
◆
```

next line stop cont run quit Line: 40
paste init pause clear restart kill Stop: None

```
V( anode ) = -10

proj      psi      n      p      psi      n      p
direct   x      x      x      rhs      rhs      rhs
i      j      m
-----
1      N      0.677  1.090  1.031 -16.99 -12.09 -5.669
2      N      0.080  0.145  1.514 -17.64 -12.99 -6.044
3      N      -0.838 -0.000  0.802 -28.7* -15.36 -7.672
4      N      -2.318 -0.901 -0.589 -29.8* -18.4* -10.93
5      N      -5.62* -3.304 -4.209 -29.6* -23.7* -17.4*

Electrode  Va(V)  Jn(A/um)  Jp(A/um)  Jc(A/um)  Jt(A/um)
-----
anode      -1.000e+01 -3.224e-18 -1.506e-13 -1.506e-13 -1.506e-13
cathode    0.000e+00  1.210e-13  2.951e-14  1.506e-13  1.506e-13
Total                                2.224e-19

Time for bias point:  0.00 sec.
Total time:          6.07 sec.
```

ATLAS started ATLAS

- Not all errors are fatal because Deckbuild tries to interpret the file and continue. This may cause a statement to be ignored, leading to unexpected results.

- During the running simulation it is recommended to check the run-time output to intercept any errors or warnings.

- During SOLVE statements, the error numbers of each equation at each iteration are displayed. It can provide important insights in the case of convergence problems.

Run-time output (2)

The output can be interpreted as follows:

XNORM and RHSNORM errors

proj direct		psi x	n x	p x	psi rhs	n rhs	p rhs
i	j	-5.00*	-5.00*	-5.00*	-26.0*	-17.3*	-17.3*
1	N	0.677	1.090	1.031	-16.99	-12.09	-5.669
2	N	0.080	0.145	1.514	-17.64	-12.99	-6.044
3	N	-0.838	-0.000	0.802	-28.7*	-15.36	-7.672
4	N	-2.318	-0.901	-0.589	-29.8*	-18.4*	-10.93
5	N	-5.62*	-3.304	-4.209	-29.8*	-23.8*	-17.4*
Electrode		Va(V)	Jn(A/um)	Jp(A/um)	Jc(A/um)	Jt(A/um)	
anode		-1.000e+01	-3.224e-18	-1.506e-13	-1.506e-13	-1.506e-13	
cathode		0.000e+00	1.210e-13	2.951e-14	1.506e-13	1.506e-13	
Total						2.220e-19	

iteration numbers (points to i, j)

solution method (points to N):
N = Newton
G = Gummel
B = Block

tolerance values (points to -5.00*, -5.00*, -5.00*, -26.0*, -17.3*, -17.3*)

error values (points to -17.4*)

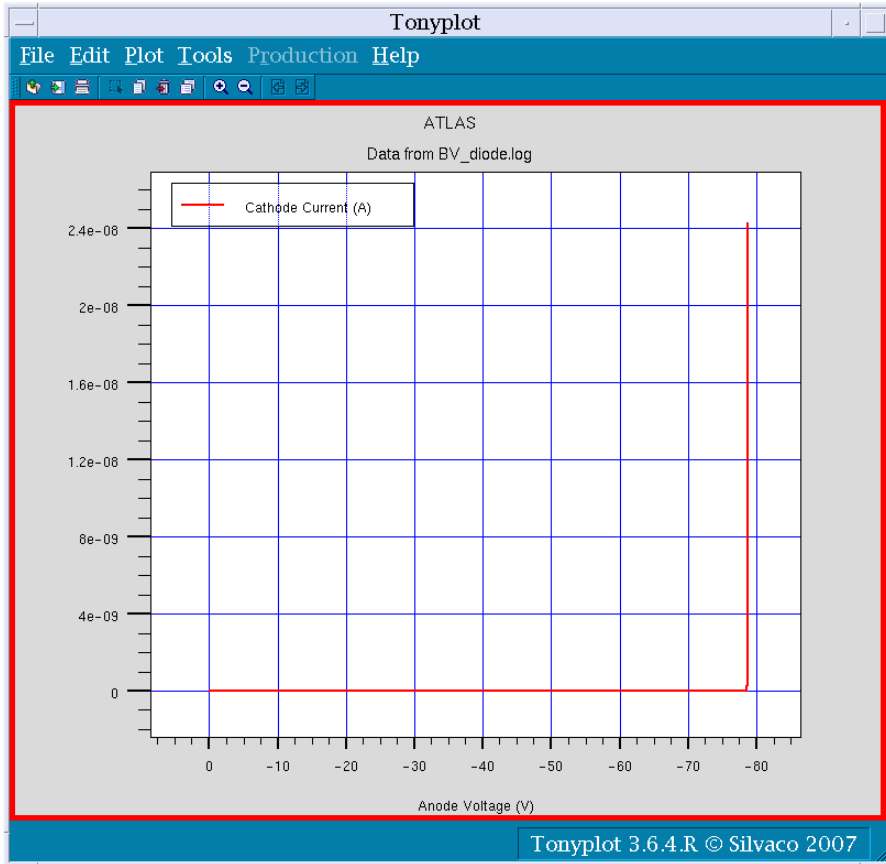
This error has met its tolerance (points to -17.4*)

voltage at the contact surface (points to Va(V))

electron, hole, conduction, and total currents (points to Jn, Jp, Jc, Jt)

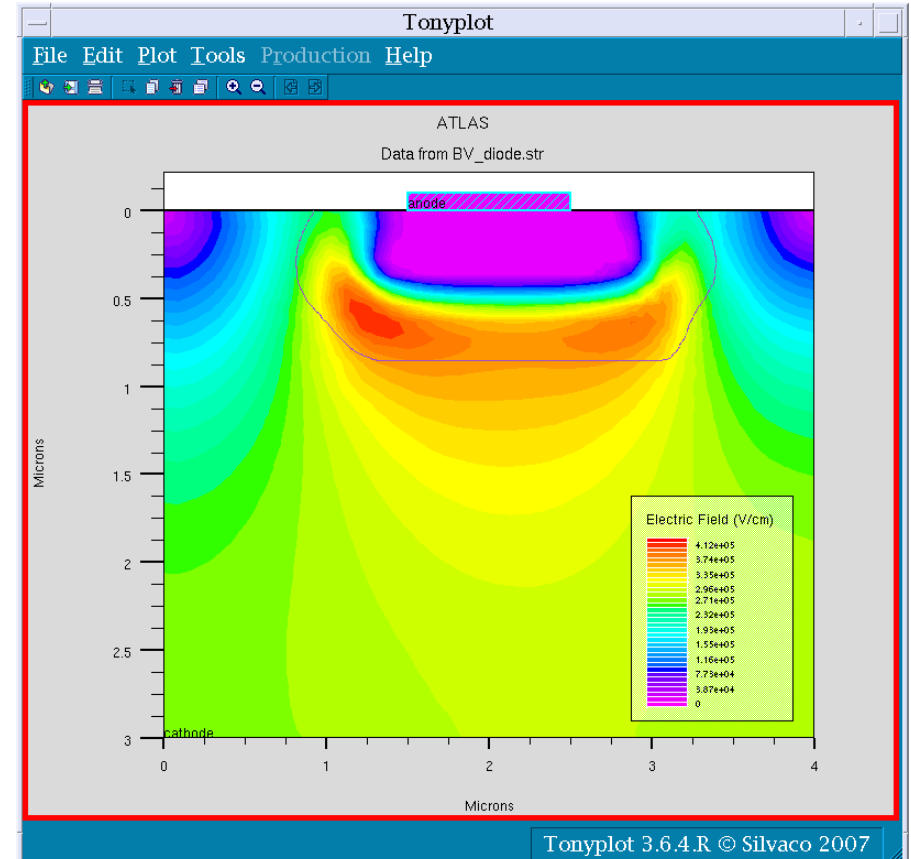
Displaying the results

LOG FILE



A typical *breakdown curve* is showed (BV=78V). The cathode current is displayed as function of the anode voltage.

STRUCTURE FILE



The *electric field* at breakdown is displayed. The higher electric field regions (in red) show where the breakdown occurs.