

# Semiconductor Device Modeling and Simulation

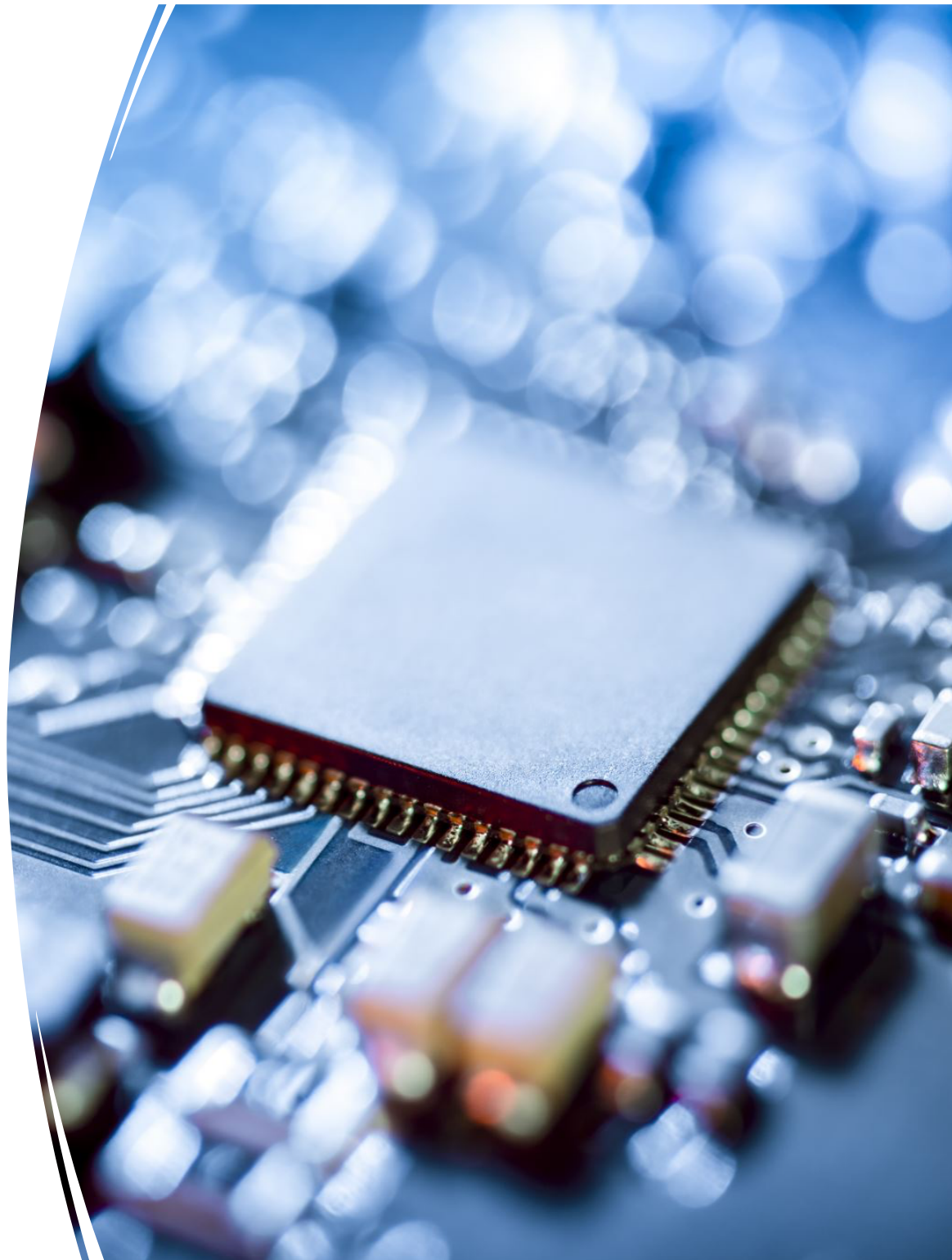
L4.01 Silvaco Atlas –  
Silvaco Syntax, Part 1

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National Nanotechnology  
Coordinated Infrastructure



# Introduction to Silvaco ATLAS Tool

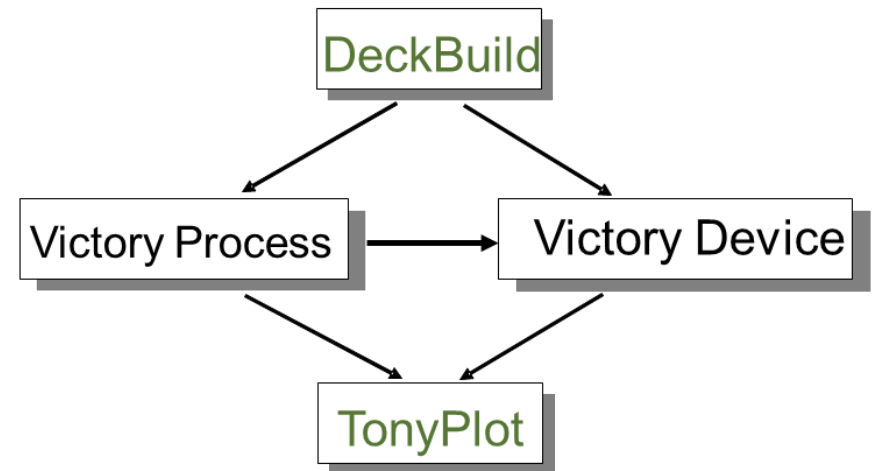
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1. Some general comments
2. Deckbuild overview
3. ATLAS syntax
  - a) Structure specification
  - b) Materials models specification
  - c) Numerical method selection
  - d) Solution specification
  - e) Results analysis
4. ATLAS Extract description

# Some General Comments

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- **VICTORY PROCESS** – process simulation tool:
  - Predicts the physical structure that results from the processing steps
  - Treats process simulation as a serial flow of events
- **VICTORY DEVICE (ATLAS)** – device simulation tool:
  - Performs physically-based 2D/3D device simulations
  - Predicts the electrical behavior of specified semiconductor structures and provides insight into the internal physical mechanisms associated with the device operation
  - Various tools that comprise ATLAS include: S-PISCES, BLAZE, GIGA3D, TFT, LUMINOUS, LASER, MIXEMODE, DEVICE3D, INTERCONNECT3D, THERMAL3D

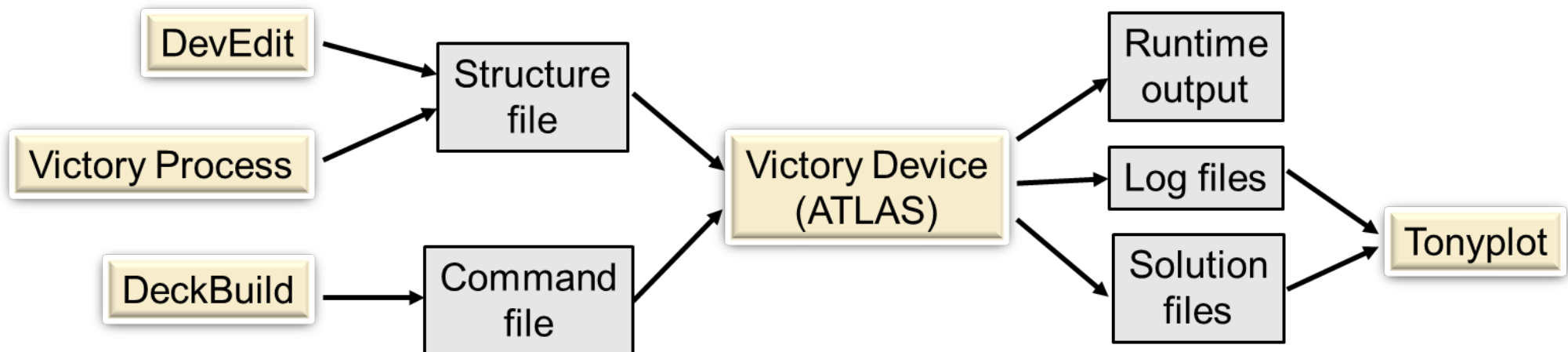


# Some General Comments

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- **ATLAS (Victory Device) Inputs and Outputs:**

- Most ATLAS simulations use two types of inputs: **text files** and **structure files**
- There are three types of outputs produced by ATLAS:
  - 1) **Runtime output** – guide to the progress of simulation that is running
  - 2) **Log files** – summaries of the electrical output information
  - 3) **Solution files** – store 2D and 3D data relating to the values of the solution variables



# DeckBuild Window

```
DeckBuild - C:/Users/Dragica Vasileska/Desktop/Abdul Silvaco/test_CdTe_stack_1.in
File Edit View Run Tools Commands Help
Deck
#####
### Solar cell simulation
#####
go atlas
set vFinal=1.5
set vStep=$vFinal/15

mesh space.mult = 1

x.m loc = 0 spacing = 1
x.m loc = 10 spacing = 5

y.m loc = 0 spacing = 0.001
y.m loc = 0.2 spacing = 0.001
y.m loc = 4 spacing = 0.001

region number = 1 material=CdTe y.min = 0. y.max = 0.5
region number = 2 material=CdTe y.min = 0.5 y.max = 3.5
region number = 3 material=CdTe y.min = 3.5 y.max = 3.54
region number = 4 material=CdTe y.min = 3.54 y.max = 4

electrode name = anode y.min = 0 y.max = 0
electrode name = cathode y.min = 4 y.max = 4

doping uniform conc = 2.8e18 p.type y.min = 0 y.max = 0.5
doping uniform conc = 7e16 p.type y.min = 0.5 y.max = 3.5
doping uniform conc = 1e16 n.type y.min = 3.5 y.max = 3.54
doping uniform conc = 3.397e17 n.type y.min = 3.54 y.max = 4

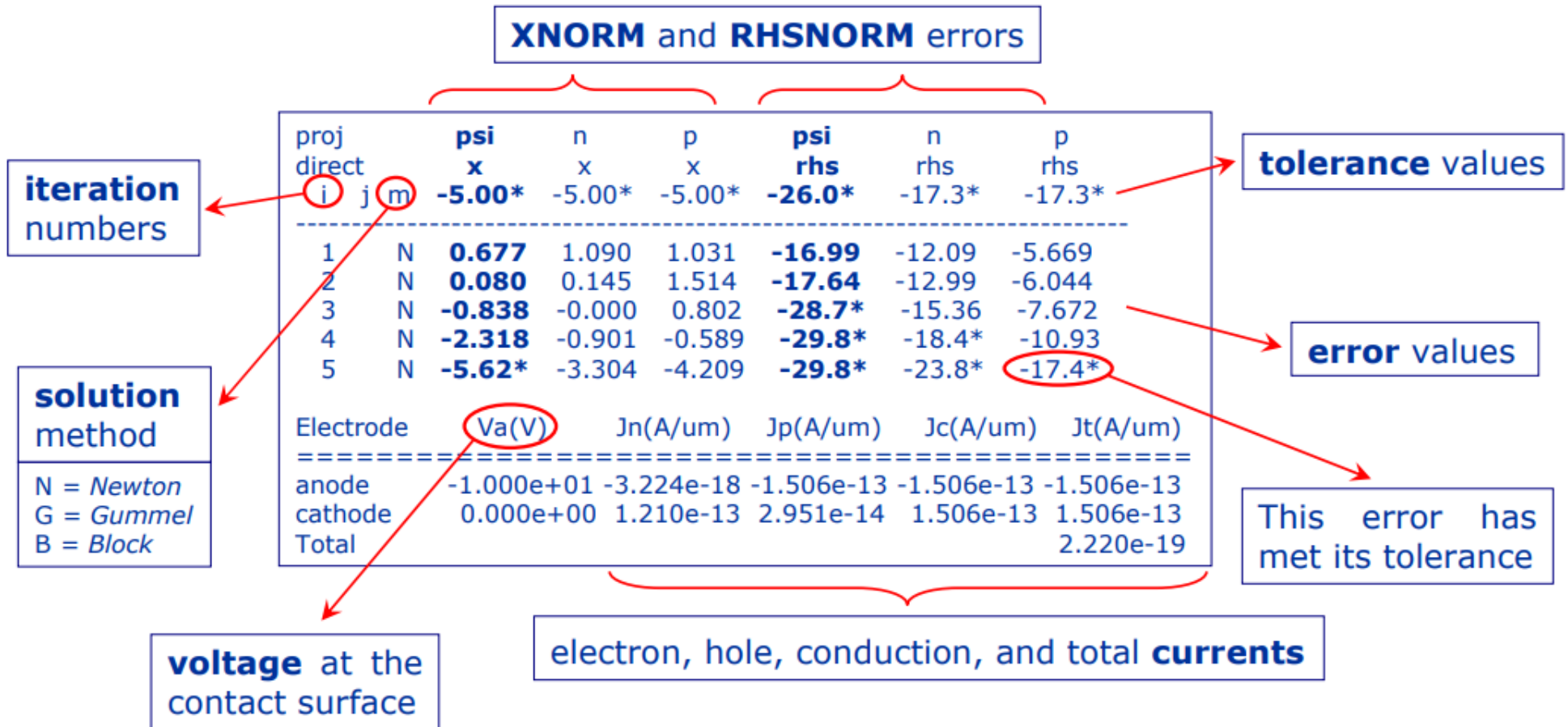
material num=1 EG300=2.28 PERMITTIVITY=11 AFFINITY=3.53 MUN=400 MUP=200 NC300=7.8e17 NV300=
1.8e19 index.file=abs_ZnTe_test COPT=1e-11 taun0=1.e-11
material num=2 EG300=1.51 PERMITTIVITY=11 AFFINITY=4.4 MUN=400 MUP=200 NC300=7.8e17 NV300=
1.8e19 index.file=abs_CdTe_test COPT=1e-11 taun0=8.3e-11 taup0=1.82e-13
material num=3 EG300=2.468 PERMITTIVITY=11 AFFINITY=4.4 MUN=400 MUP=200 NC300=7.8e17 NV300=
1.8e19 index.file=abs_CdS_test COPT=1e-11 taup0=2.27e-11
material num=4 EG300=3.6 PERMITTIVITY=11 AFFINITY=4.4 MUN=400 MUP=200 NC300=7.8e17 NV300=
1.8e19 index.file=abs_TCO_test COPT=1e-11 taup0=8.7e-11

contact name=anode
contact name=cathode

Runtime output

Output  Scroll to bottom Clear
```

# Run-Time Output (From Silvaco)



# ATLAS Syntax

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- The form of the input file statements is:  
**<STATEMENT> <PARAMETER> = <VALUE>**  
The parameter can be **real, integer, character** and **logical**
- The order in which the ATLAS commands occur is the following:
  - a) Structure specification:** MESH, REGION, ELECTRODE, DOPING
  - b) Material models specification:** MATERIAL, MODELS, CONTACT, INTERFACE
  - c) Numerical method selection:** METHOD
  - d) Solution specification:** LOG, SOLVE, LOAD, SAVE
  - e) Results analysis:** EXTRACT, TONYPLOT
- The input file can be created using the DeckBuild Command Menu:

**Commands/Command Menu**

# STRUCTURE Specification

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- **MESH** statement specification

**INFILE, OUTFILE** → file with previously saved mesh, new file

**SPACE.MULT** → scale factor applied to all specified grid spacing

**CYLINDRICAL, RECTANGULAR** → describes mesh symmetry

**NX, NY** → number of nodes along the x- and y-direction

**mesh nx=36 ny=30**

- **X.MESH, Y.MESH** statements - Specify the location of grid lines along the x- and y-axes

**NODE** → specifies mesh line index

**LOCATION** → specifies the location of the grid line

**RATIO** → ratio to be used when interpolating grid lines between given locations

**SPACING** → specifies mesh spacing at a given location

**x.mesh loc = 0.0 spacing = 0.2**

**x.mesh loc = 0.85 spacing = 0.01**

**x.mesh loc = 2 spacing = 0.3**



# STRUCTURE Specification (cont'd)

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- **ELIMINATE** statement  
Eliminates every second mesh point in a rectangular grid specified by **X.MIN**, **X.MAX**, **Y.MIN** and **Y.MAX**  
**COLUMNS, ROWS** → columns, rows elimination  
**eliminate x.min=0 x.max=4 y.min=0 y.max=3**
- **REGION** statement - Specifies regions and materials  
**NUMBER** → denotes region number  
**material** → can be SILICON, OXIDE  
**position** → defines the location of the region in terms of (1) actual position and (2) grid nodes  
**region num=1 ix.lo=1 ix.hi=25 iy.lo=1 iy.hi=20 silicon**  
**region num=1 y.max=0 oxide**  
**region num=2 y.min=0 silicon**
- **ELECTRODE** statement - must specify at least one electrode within the simulation domain  
**NAME** - defines the name of the electrode: **SOURCE, DRAIN, GATE**  
**position parameter** - **BOTTOM, LEFT, RIGHT, TOP, SUBSTRATE, IX.LOW, IX.HIGH, X.MIN, X.MAX, LENGTH**

# STRUCTURE Specification (cont'd)

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- **DOPING** statement

Can be used to set the doping profile analytically. Analytical doping profiles can be defined with the following parameters:

**distribution type** → UNIFORM, GAUSSIAN

**doping type** → N.TYPE, P.TYPE

**CONCENTRATION** → peak concentration specification for Gaussian profiles

**CHARACTERISTIC** → principal characteristic length of the implant (standard deviation). One can specify junction depth instead.

**PEAK** → specifies the location of a peak of a Gaussian profile

**position** → X.LEFT, X.RIGHT, REGION

**doping uniform concentration=1E16 n.type region=1**

**doping gaussian concentration=1E18 characteristic=0.05 \**

**p.type x.left=0 x.right=1.0 peak=0.1**

The doping profile can also be imported from SSUPREM. One must use the **MASTER** parameter in the doping statement combined with the **INFILE** parameter to be able to properly import the doping profile.

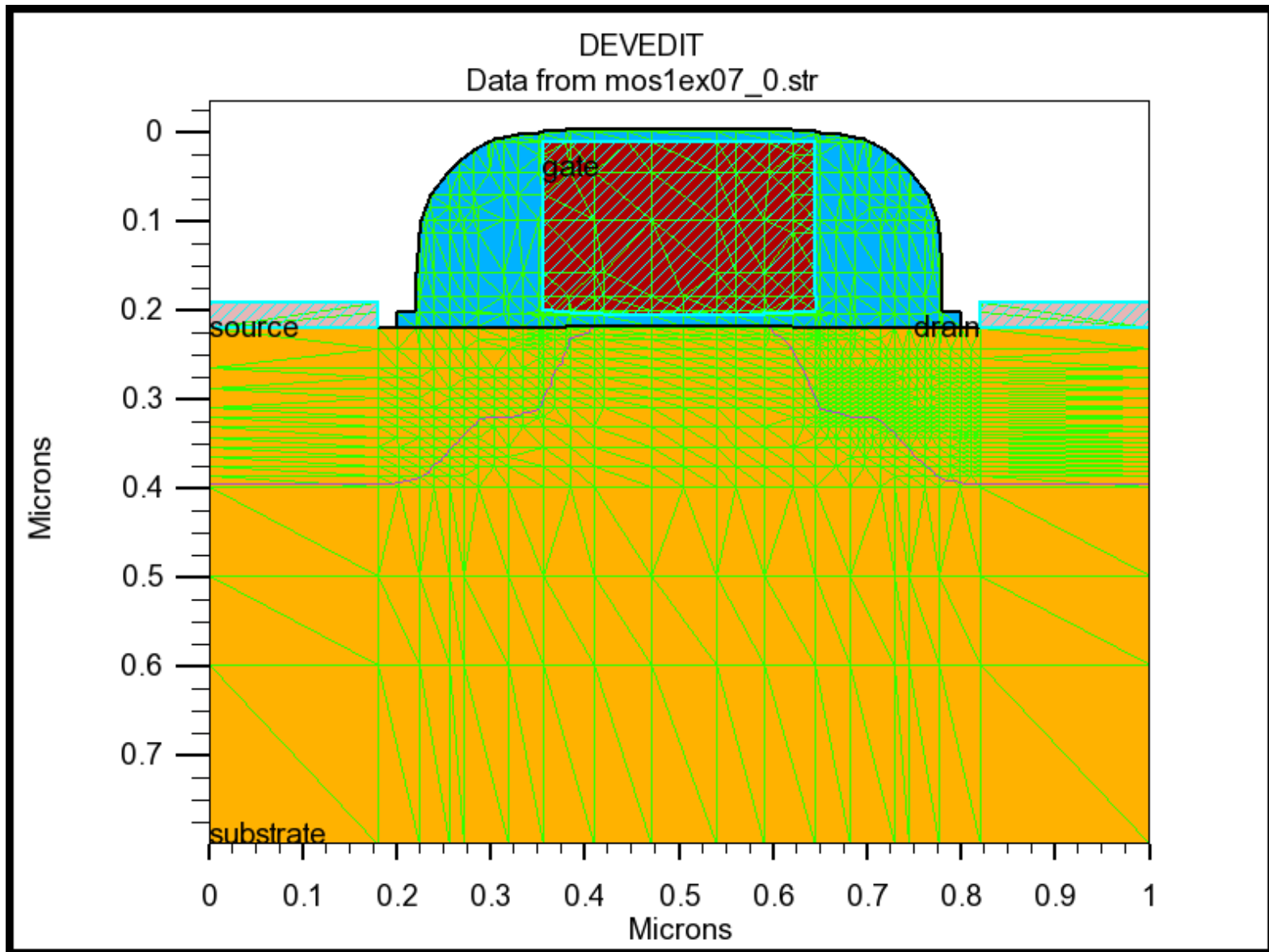
# STRUCTURE Specification (cont'd)

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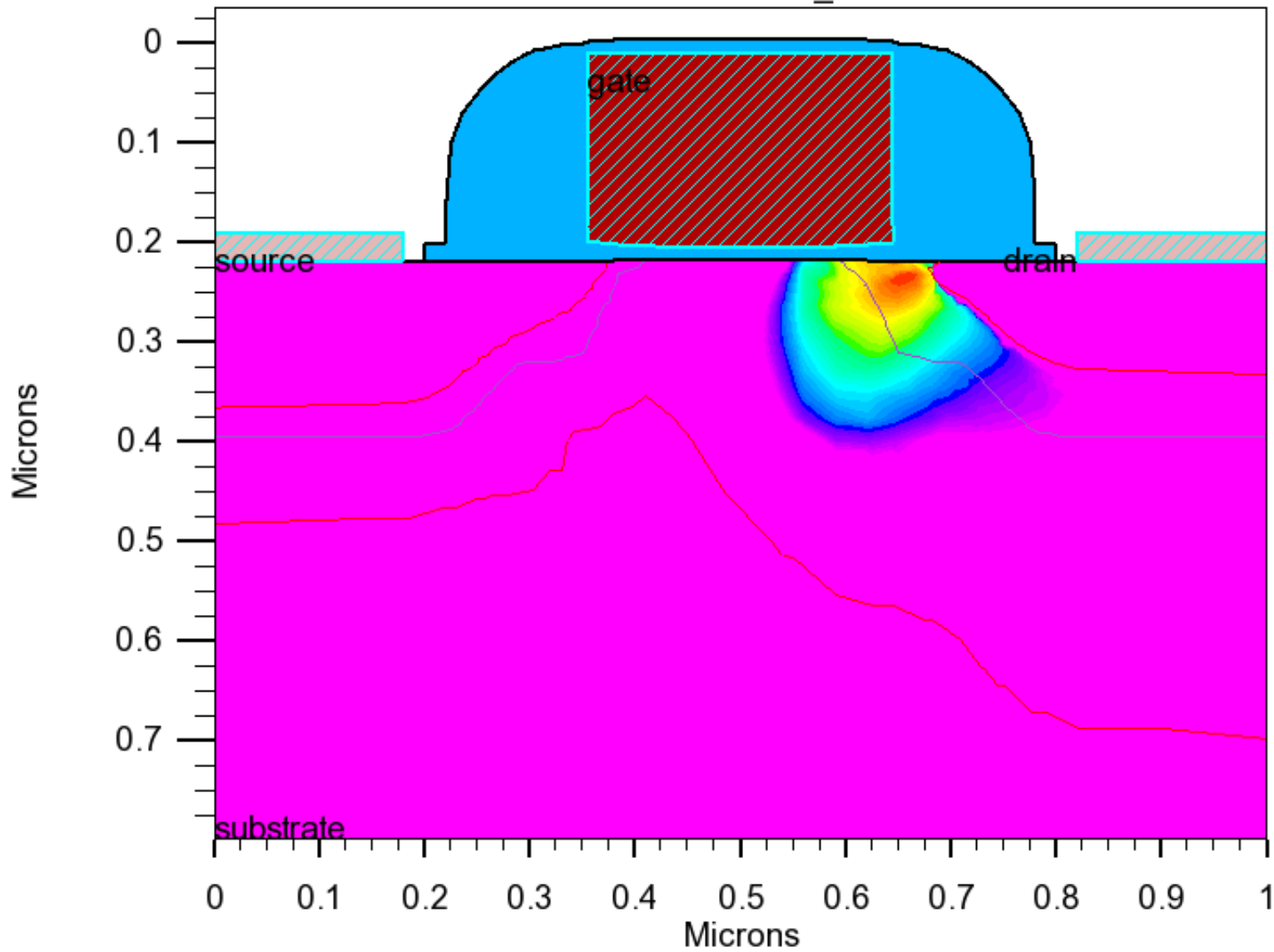
## COMMENTS ON THE MESH SET-UP

- 1) Defining a good mesh is a crucial issue in device simulations. There are several factors that need to be considered when setting the mesh:
  - ACCURACY** - fine mesh is needed to properly resolve the structure
  - EFFICIENCY** - for the simulation to finish in a reasonable time, fewer grid points must be used
- 2) Critical areas where fine mesh is needed include
  - depletion regions:** high-field regions
  - Si/SiO<sub>2</sub> interface:** high transverse electric field region
  - emitter/base junction of a BJT:** recombination is important
  - impact ionization areas**
- **REGRID** statement allows fine mesh generation in critical device areas. This statement is used after the MESH, REGION, MATERIAL, ELECTRODE, and DOPING statements. There are two ways in which regriding can be done:
  - regrid on **DOPING**
  - regrid using **SOLUTION VARIABLES**

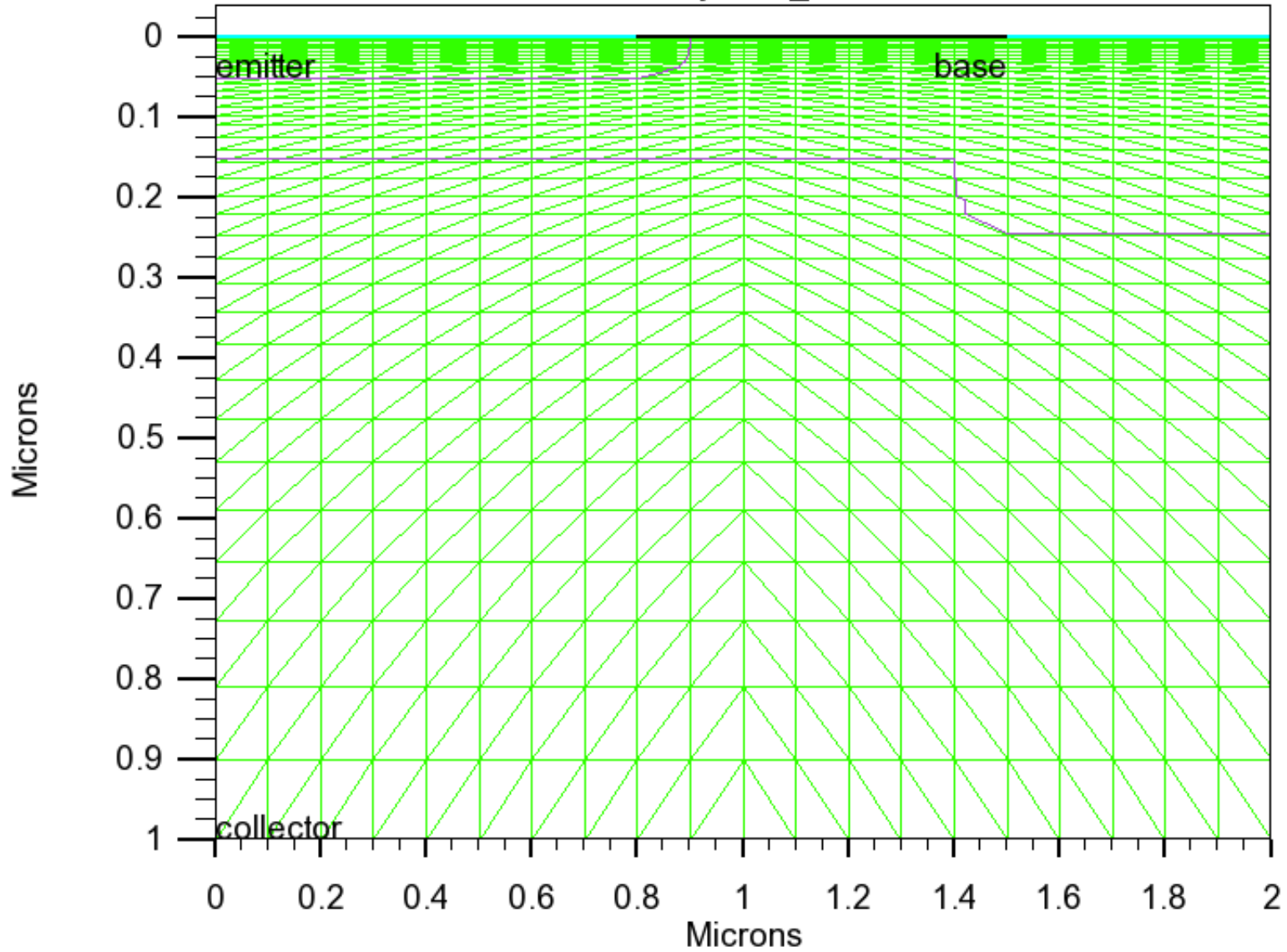
# STRUCTURE Specification (cont'd)



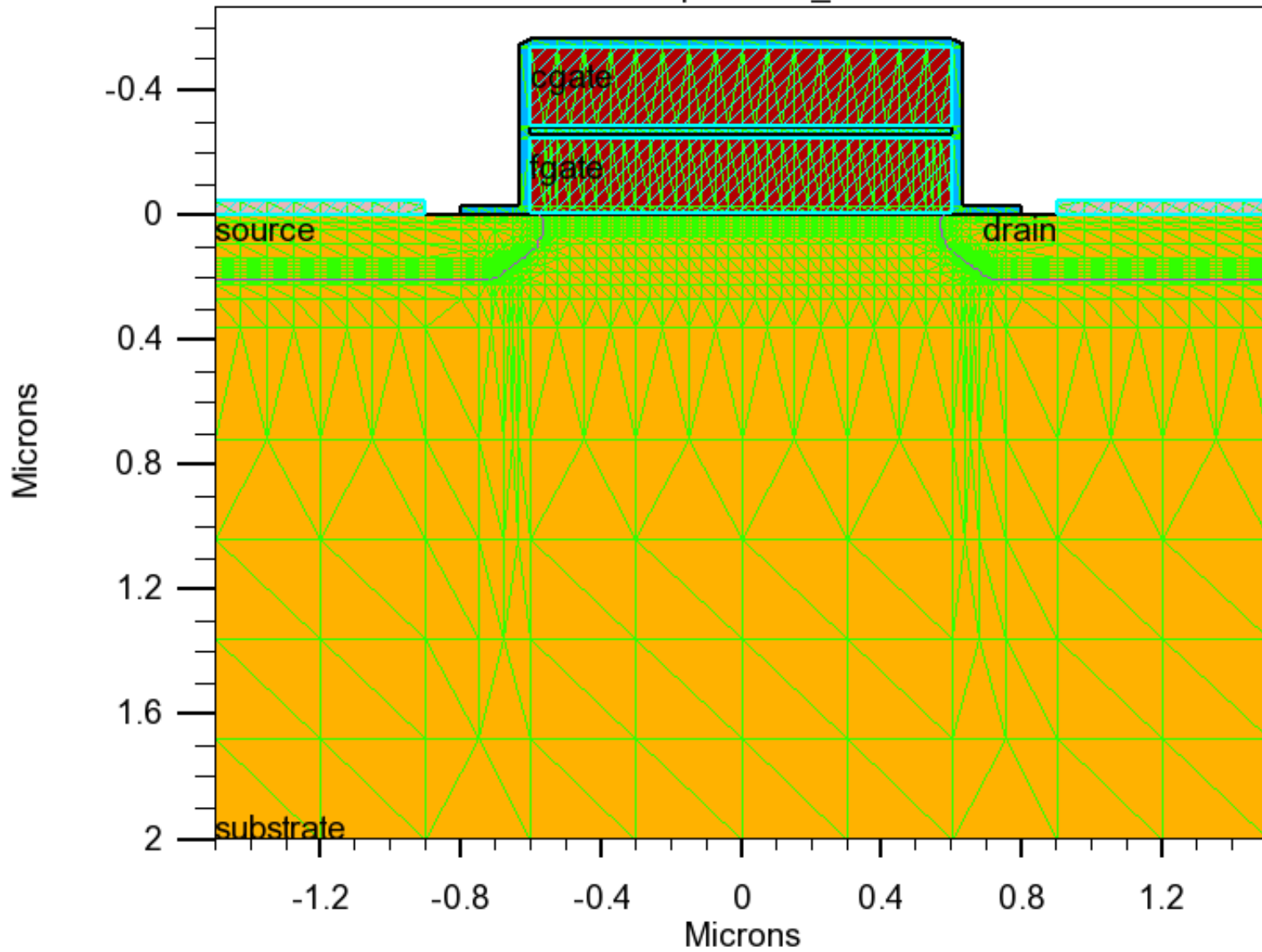
ATLAS  
Data from mos1ex07\_1.str



ATLAS  
Data from bjtex05\_0.str



DEVEDIT  
Data from eprmex01\_1.str



# Material Models Specification

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- **CONTACT** statement

**NAME** → specifies the name of the contact: GATE, DRAIN, ANODE

**WORKFUNCTION** → specifies workfunction of a metal, or if specifies N.POLYSILICON, then it implicitly assumes one

**type** → specifies the type of a contact: CURRENT, VOLTAGE, FLOATING

**CONTACT IMPEDANCE** → uses RESISTANCE, CAPACITANCE, INDUCTANCE, CON.RESISTANCE (used for distributed contact resistance specification)

**Schottky barrier** → BARRIER (turns on barrier lowering mechanism), ALPHA (specification of the barrier lowering)

**contact name=gate workfunction=4.8**

**contact name=gate n.polysilicon**

**contact name=drain current**

**contact name=drain resistance=40.0 \  
capacitance=20.E-12 inductance=1.E-6**



# Material Models Specification

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- **MATERIAL** statement

Atlas also supplies a default list of parameters for the properties of the material used in the simulation. The parameters specified in the MATERIAL statement include, for example: *electron affinity, energy bandgap, density of states function, saturation velocities, minority carrier lifetimes, Auger and impact ionization coefficients, etc.*

**REGION** → specifies the region number to which the above-described parameters apply

**parameters** → Some of the most commonly used parameters include: AFFINITY, EG300, MUN, MUP, NC300, NV300, PERMITTIVITY, TAUN0, TAUP0, VSATN, VSATP

```
material taun0=5.0E-6 taup0=5.0E-6 mun=3000 \  
mup=500 region=2
```

```
material material=silicon eg300=1.2 mun=1100
```

# Material Models Specification

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- **INTERFACE** statement – Specifies interface charge density and surface recombination velocity.

**QF, S.N, S.P** → amount of interface charge density,  
surface recombination velocity for electrons  
and holes

**interface qf=3E10 x.min=1. x.max=2. y.min=0. y.max=0.5**

**interface y.min=0 s.n=1E4 s.p=1E4**

# Material Models Specification (cont'd)

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- **MODELS** and **IMPACT** statements

The physical models that are specified with the MODELS and IMPACT statements include:

**mobility model** → CONMOB, ANALYTIC, ARORA, FLDMOB, TASCH, etc.

**recombination models** → SRH, CONSRH, AUGER, OPTR

**carrier statistics** → BOLTZMANN, FERMI, INCOMPLETE, IONIZ, BGN

**impact ionization** → CROWELL, SELB

**tunneling model** → FNORD, BBT.STD (band to band - direct transitions), BBT.KL (direct and indirect transitions), HEI and HHI (hot electron and hot hole injection)

**models conmob fldmob srh fermidirac**

**impact selb**

# Material Models Specification (cont'd)

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Additional important parameters that can be specified within the MODELS statement include:

**NUMCARR** → specifies number of carriers,  
and is followed by a carrier type  
specification (ELECTRONS or  
HOLES or both)

**MOS, BIPOLAR** → standard models used for  
MOSFET and BIPOLARs

**models MOS numcarr=1 holes**

**models BIP print**

# Summary

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- We have introduced the main components of the Silvaco simulation package:
  - Victory Process and Victory Device.
- We have also introduced the **structure** and the **material models** specification.
- Meshing is very important part of device analysis. Proper meshing is crucial for device phenomena description.
- Next: **numerical method** and **solution** specification.