ATLAS

2D and 3D Device Simulator: Detailed Overview

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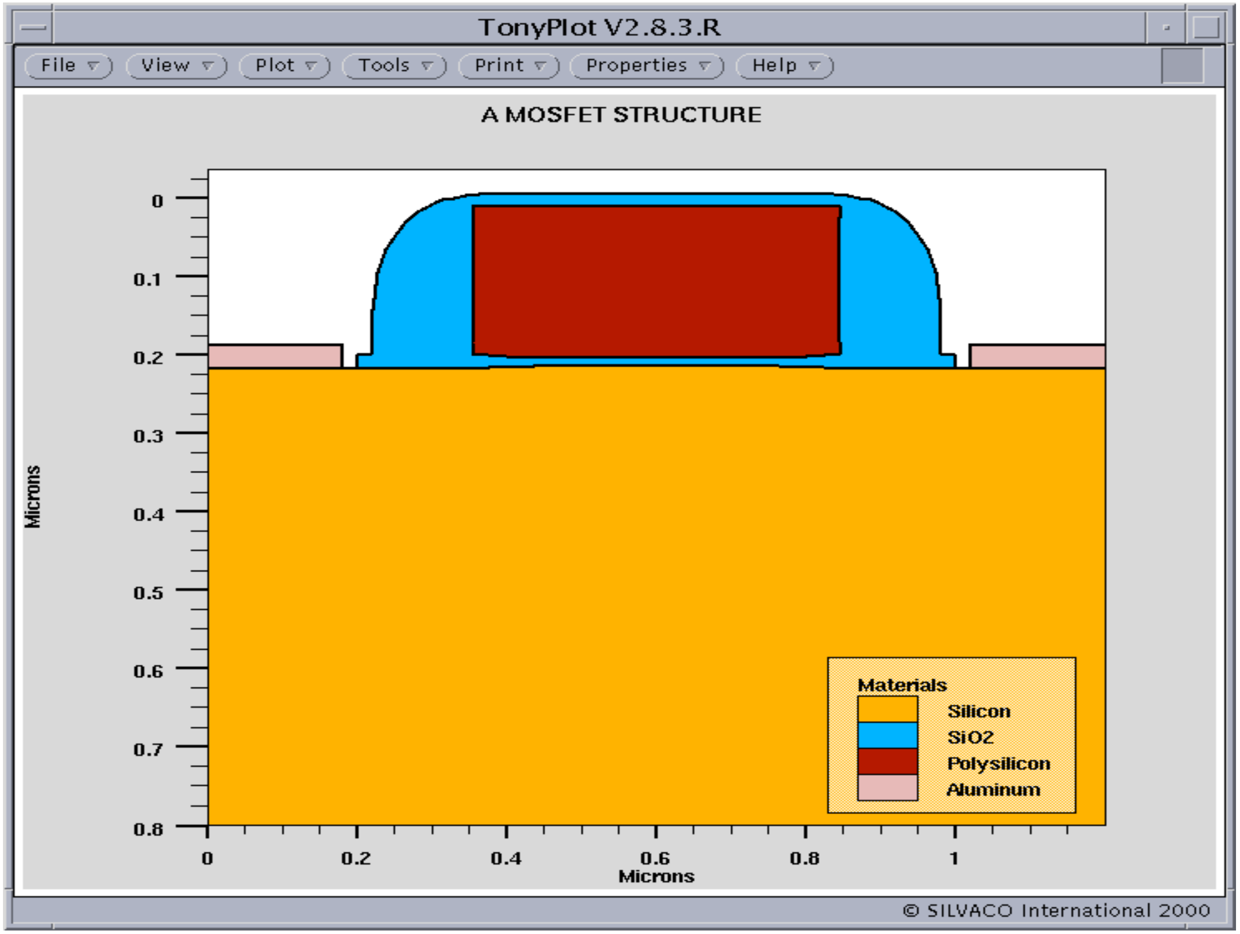
Overview

- Basic principles of device simulation
- ATLAS Framework and Modules
- Input/Output and Core processing
- ATLAS input deck structure
- Mesh design
- Pisces Physical Models
- Numerics
- Tuning device simulators
- 3D simulations

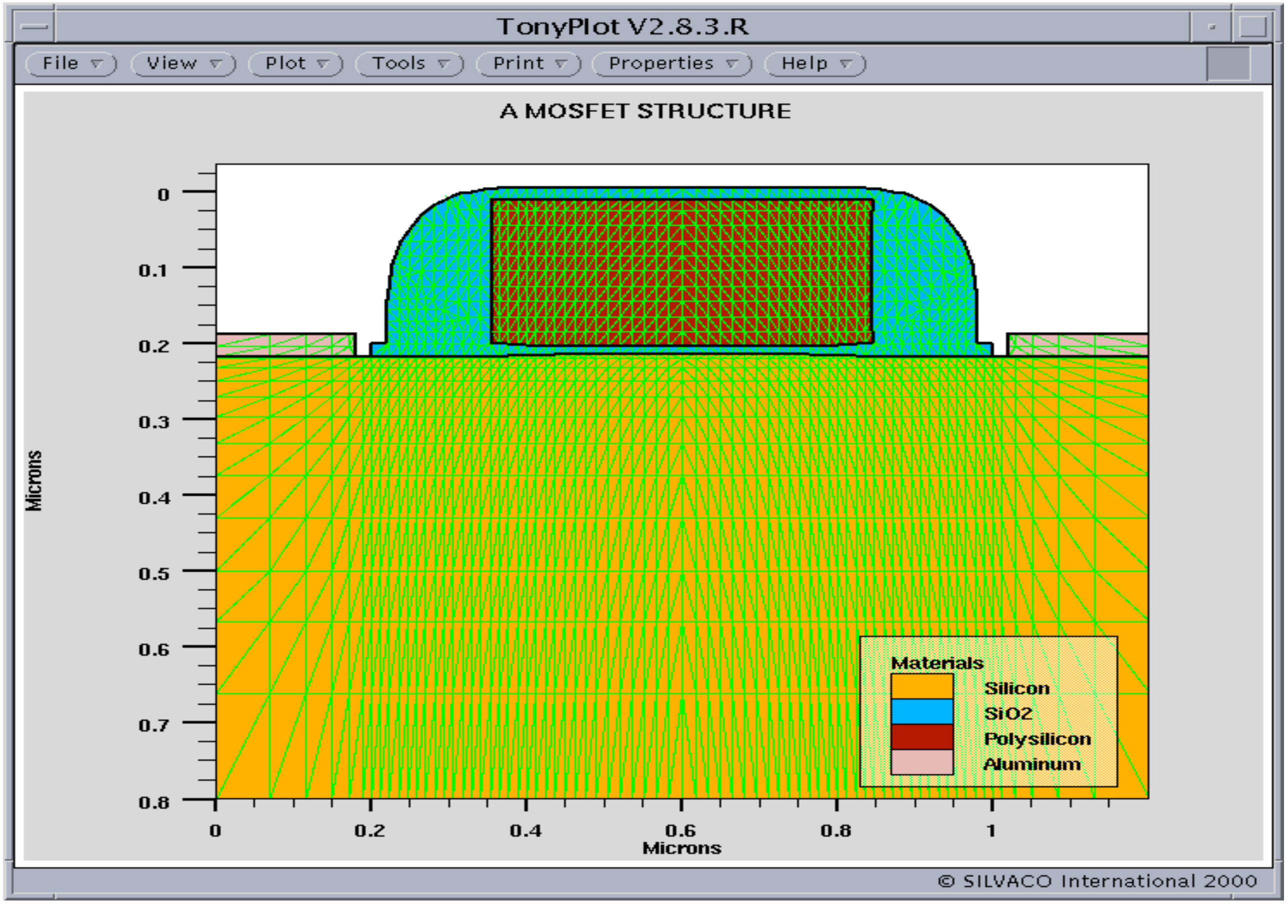
Basic Principles: What is ATLAS?

- ATLAS is a 2D and 3D Device Simulation Framework
- ATLAS solves the fundamental physical equations describing the dynamics of carriers in semiconductor devices for arbitrary device structures
- ATLAS predicts terminal characteristics of semiconductor devices for steady state, transient, and small signal AC stimuli
- ATLAS gives insight into the internal characteristics of semiconductor devices (e.g. carrier densities, fields, ionization/ recombination rates, current densities etc.)

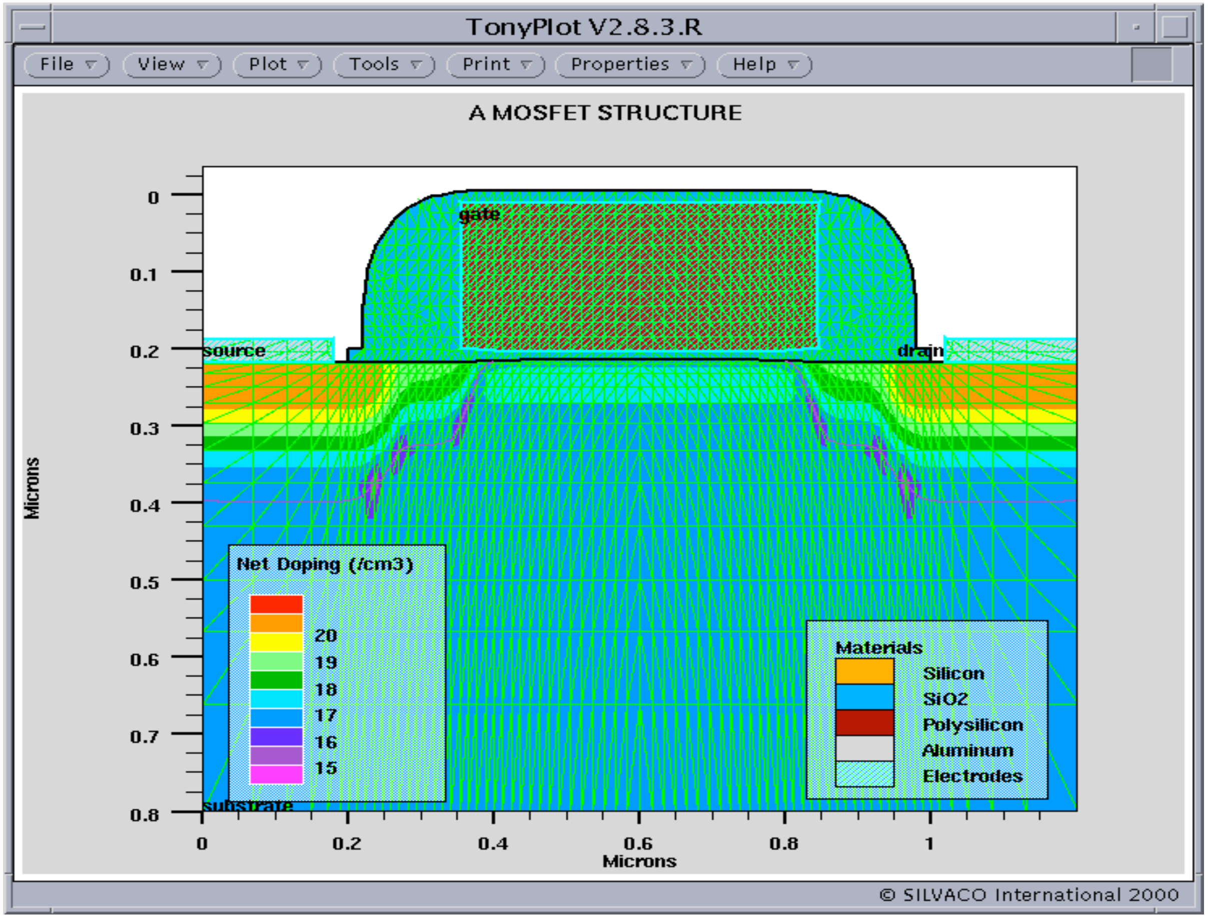
Basic Principles: Create a Structure for Simulation



Basic Principles: Create the Mesh



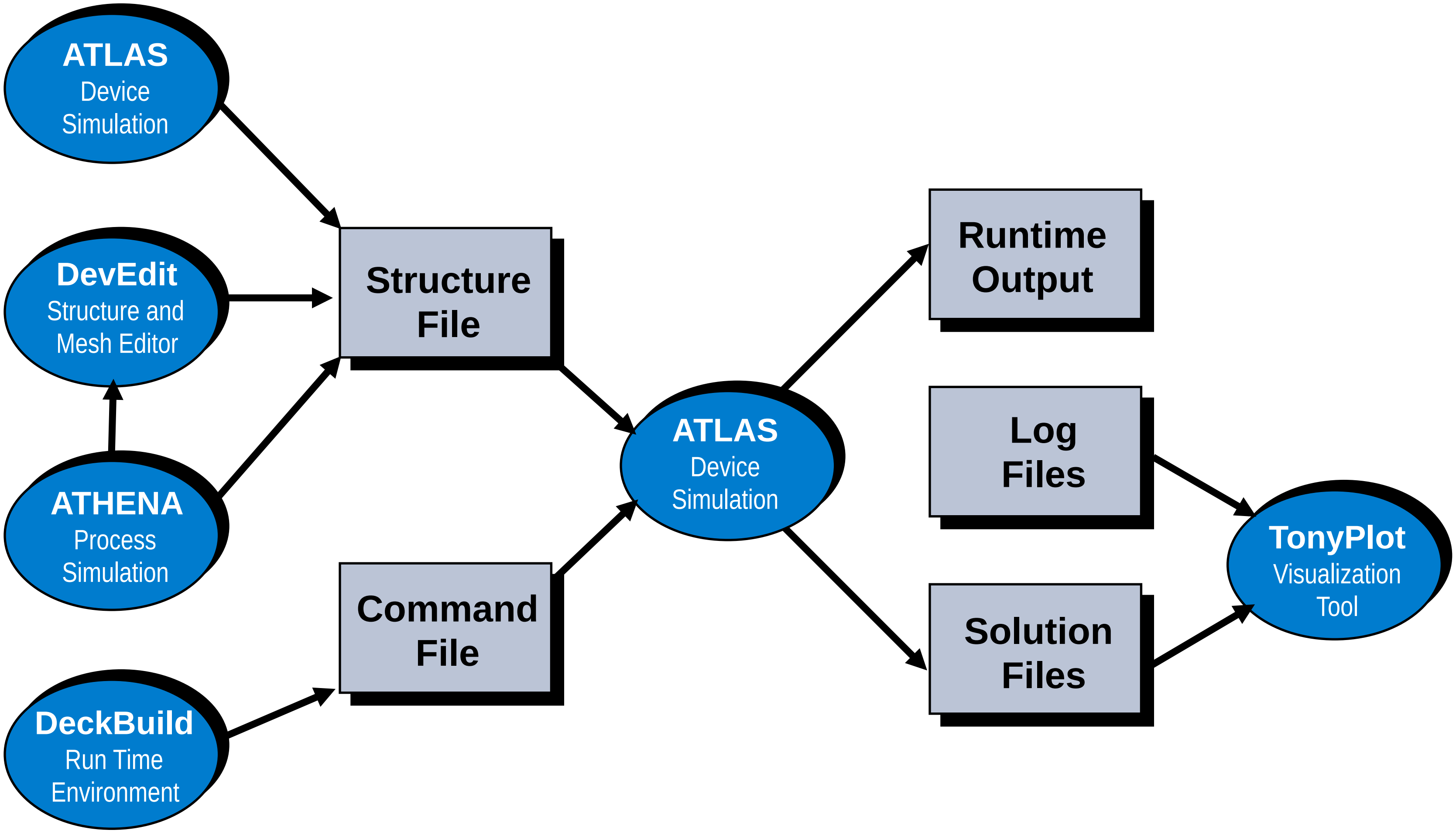
Basic Principles: Define the Doping Profiles



Elements of ATLAS Input Deck

Group	*Statements*
1. Structure Specification	MESH REGION ELECTRODE DOPING
2. Material Models Specification	MATERIAL MODELS CONTACT INTERFACE
3. Numerical Models Specification	METHOD
4. Solution Specification	LOG SOLVE LOAD SAVE
5. Results Analysis	EXTRACT TONYPLOT

ATLAS Inputs and Outputs



ATLAS Device Simulation

DevEdit Structure and Mesh Editor

ATHENA Process Simulation

DeckBuild Run Time Environment

Structure File

Command File

ATLAS Device Simulation

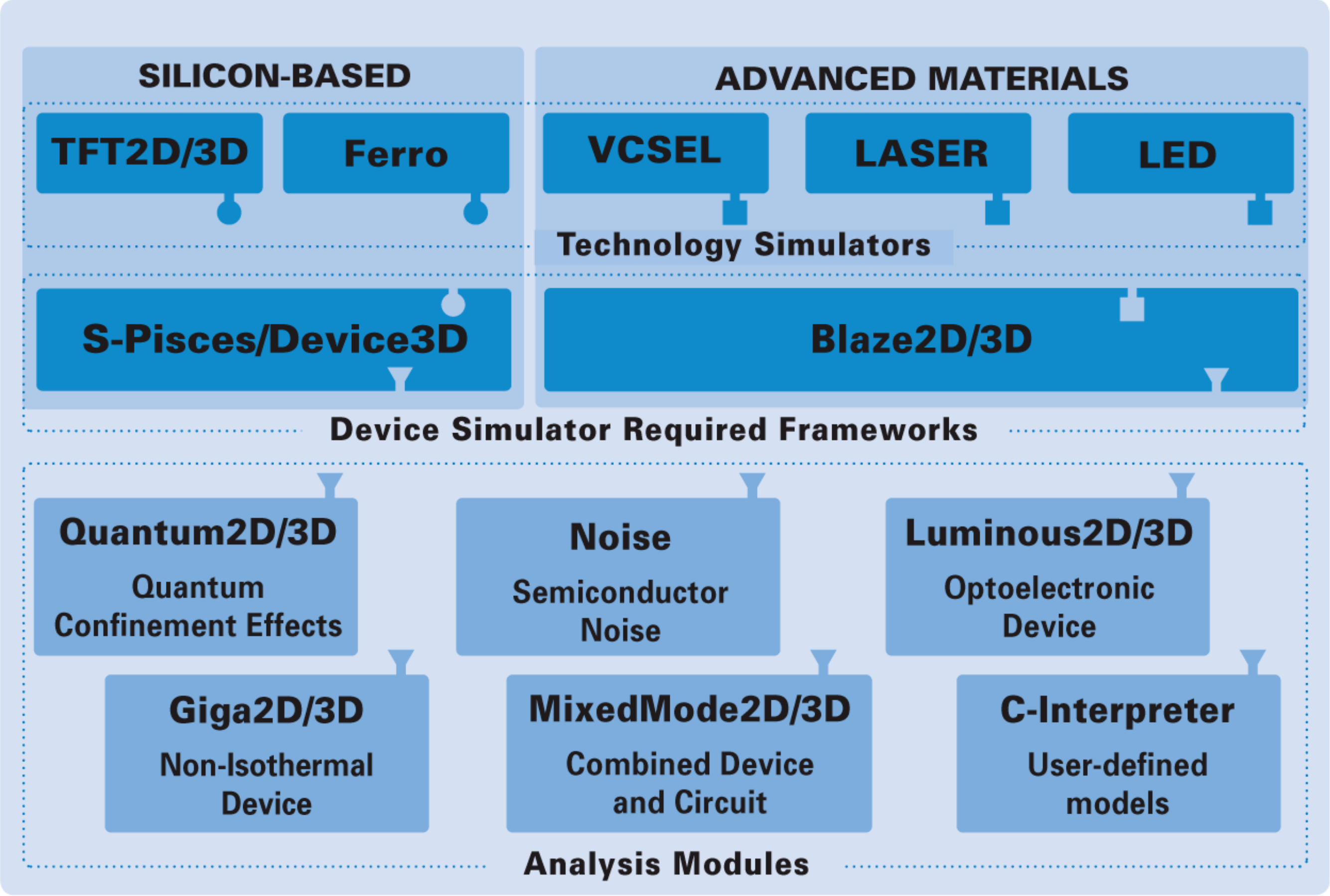
Runtime Output

Log Files

Solution Files

TonyPlot Visualization Tool

ATLAS Framework Architecture



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ADVANCED MATERIALS

TFT2D/3D

Ferro

VCSEL

LASER

LED

Technology Simulators

S-Pisces/Device3D

Blaze2D/3D

Device Simulator Required Frameworks

Quantum2D/3D
Quantum Confinement Effects

Noise
Semiconductor Noise

Luminous2D/3D
Optoelectronic Device

Giga2D/3D
Non-Isothermal Device

MixedMode2D/3D
Combined Device and Circuit

C-Interpreter
User-defined models

Analysis Modules

ATLAS Framework and Modules: S-Pisces

- Drift-diffusion equation set
- Full energy balance / hydrodynamic equations
- Cartesian and cylindrical coordinate systems
- DC, AC and Transient simulation domains
- Extensive database of physical models
- Impact ionization for device breakdown effects
- Acceptor-like and Donor-like Trap dynamics

Able to accurately simulate the basic operation of MOS, bipolar, diode and power devices which contain silicon, silicon dioxide, polysilicon or metal regions.

ATLAS Framework and Modules: Giga

- Significant local heating can occur which affects terminal characteristics for example:
  - High current devices
  - Breakdown characteristics
  - SOI device simulation (Oxide is a good thermal insulator)
  - III-V devices (substrates are poor conductors)

- Fully Coupled into Energy Balance Model
  - 6 equation solver
  - Important to treat Energy balance and lattice heating effects together

ATLAS Framework and Modules: Quantum

- 1D Schrodinger solver
- Van Dort Correction Model
- Hansch Correction Model
- Quantum moments model

ATLAS Framework and Modules: MixedMode

- Embeds up to 10 ATLAS devices within a standard spice netlist and solves the complete system
  - ESD simulation of human body model and machine model specifications
  - SEU simulation of memory cells where the logical mode switches after an alpha particle strike
  - circuit analysis of devices with no accurate compact model for example certain power devices
  - verification of newly developed compact models

ATLAS Framework and Modules: Luminous

- General purpose 2D ray trace and photogeneration. Enables simulation of optoelectronic devices:
  - Photodectors, photoconductors, solar cells, CCDs, LEDs, etc.
  - Si-pased optoelectronic devices in conjunction with S-Pisces
  - Optoelectronic devices based on advanced material systems including heterostructures in conjunction with Blaze
  - Optical and self-heating effects (with Giga)
  - Optoelectronic device-circuit simulation (with MixedMode ray tracing algorithms
  - Allows simulation of anti-reflective coatings

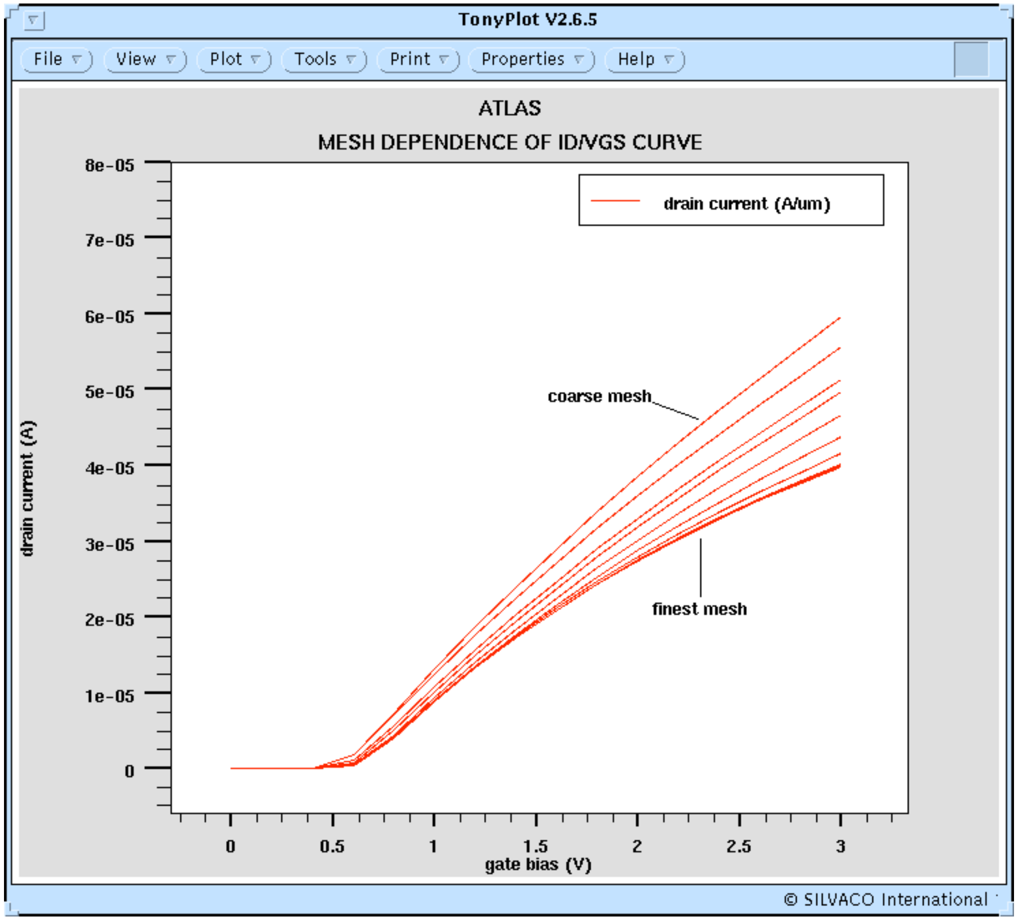
Mesh Design: Basic Guidelines

- A good mesh is crucial to accurate simulation results.
- Creating a good mesh is learned mainly from experience.
- Some basic guidelines are to refine in key areas:
  - Around junctions and depletion regions
  - Inversion regions
  - Areas of high electric field
  - Areas of current flow
  - Base region of BJTs
  - E-B junction is very critical
- DevEdit is an ideal tool for creating and modifying the mesh only where the user wishes it

Mesh Design: Basic Guidelines (con’t)

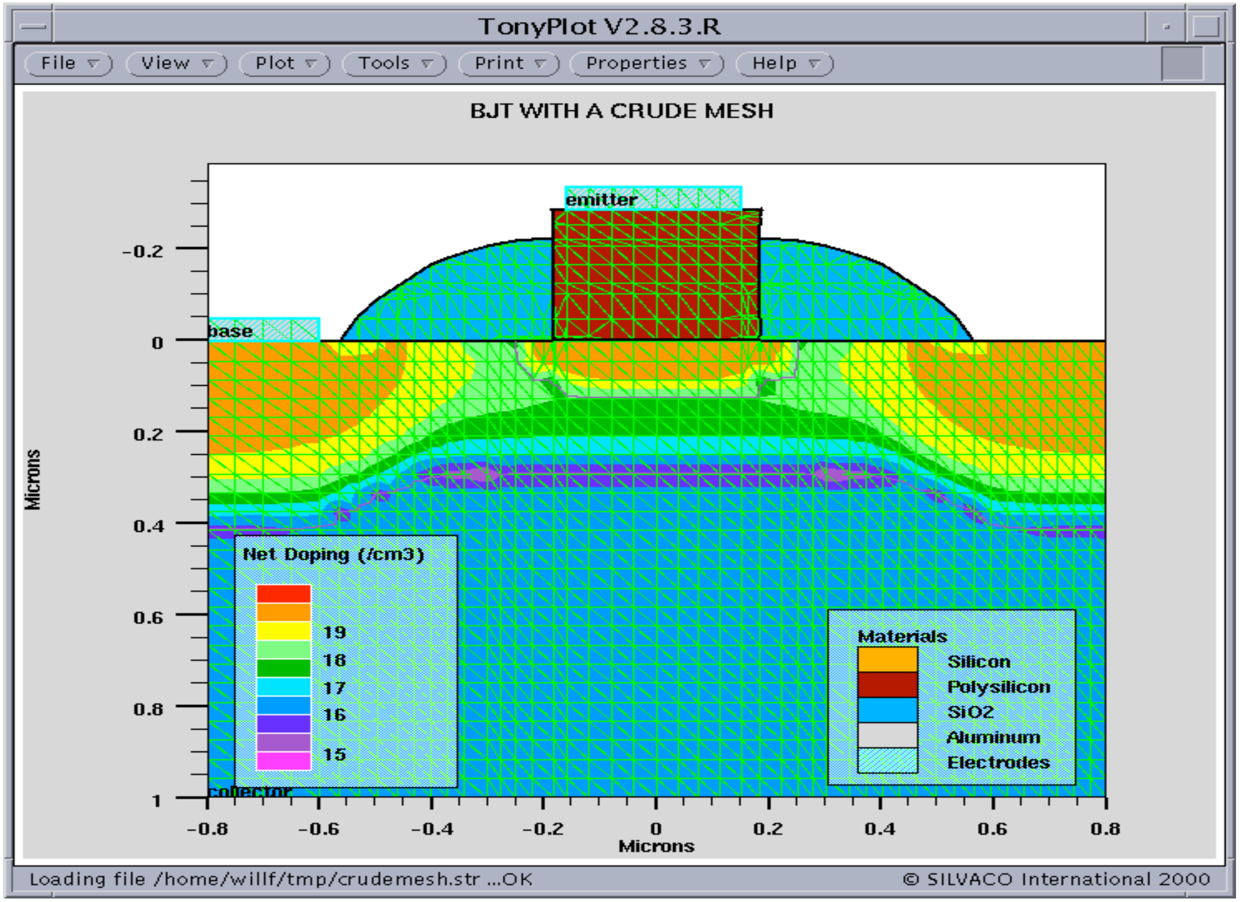
- A suitable grid for process simulation may not be suitable for device simulation
- In general, minimize the number of mesh points
    - Solution time »k*(mesh points)1.5 –> 2.5
- BUT... too few mesh points can take LONGER since each solution takes longer to converge. You cannot beat experience here
- Use DevEdit to remove unnecessary mesh points and to concentrate the mesh where it’s needed
- 10Å mesh in inversion regions. Concentrate mesh at junctions

Mesh Design: Effect on MOSFET Drain Current

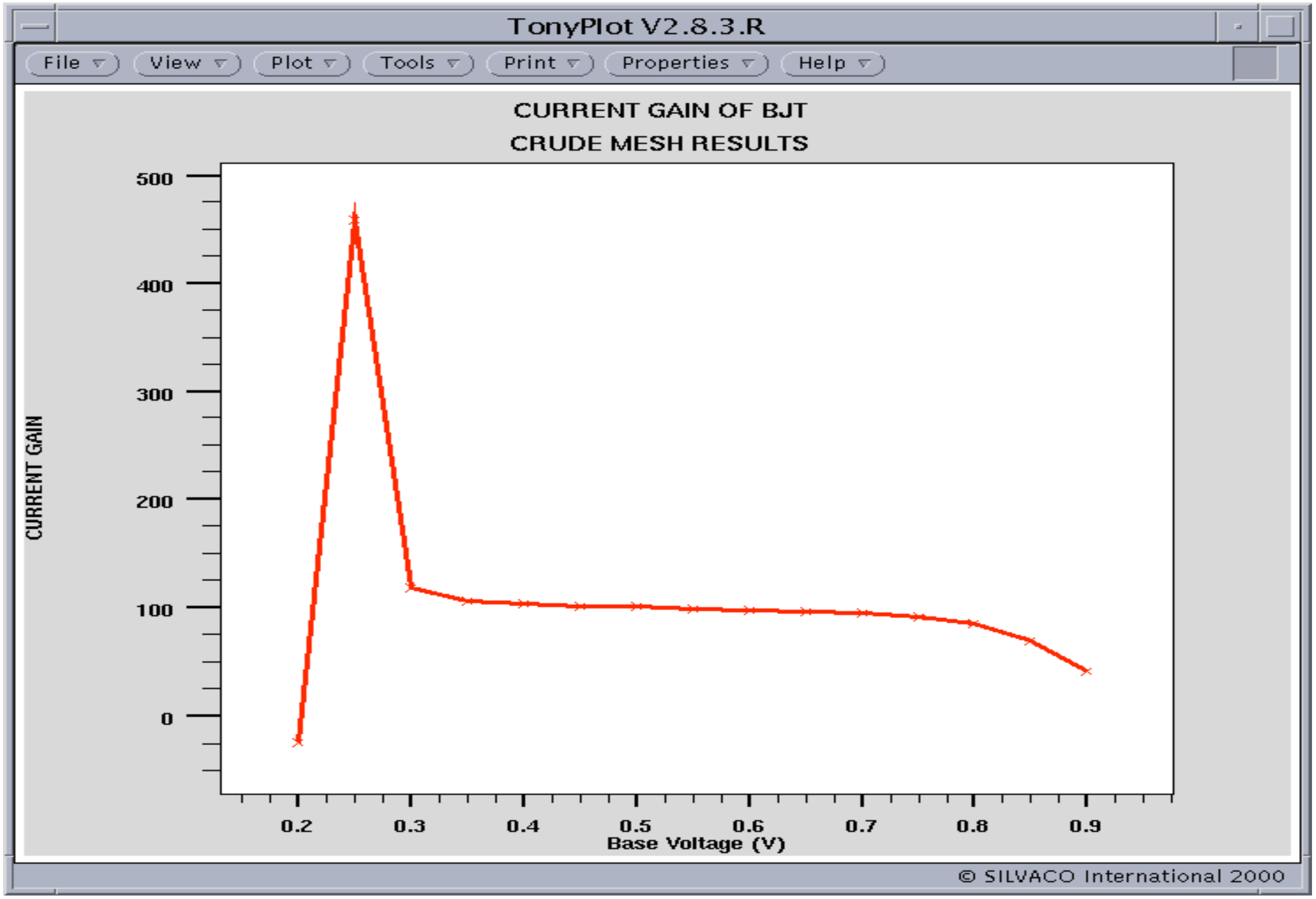


- Graph showing effect of increasing drain current with grid spacing
- This shows the requirement for a grid density for the inversion region of 10Å typically

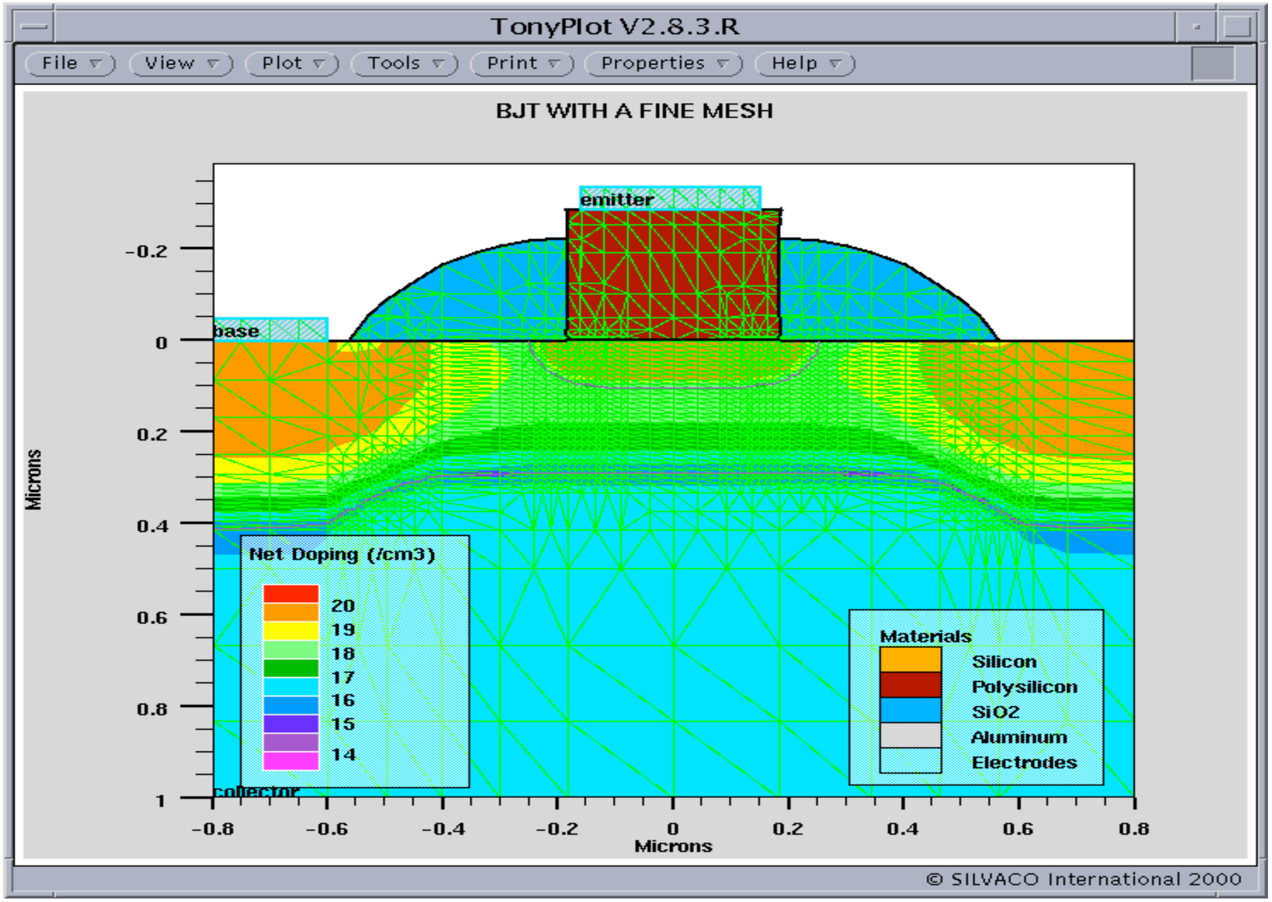
Mesh Design: Effect on Current Gain of a BJT



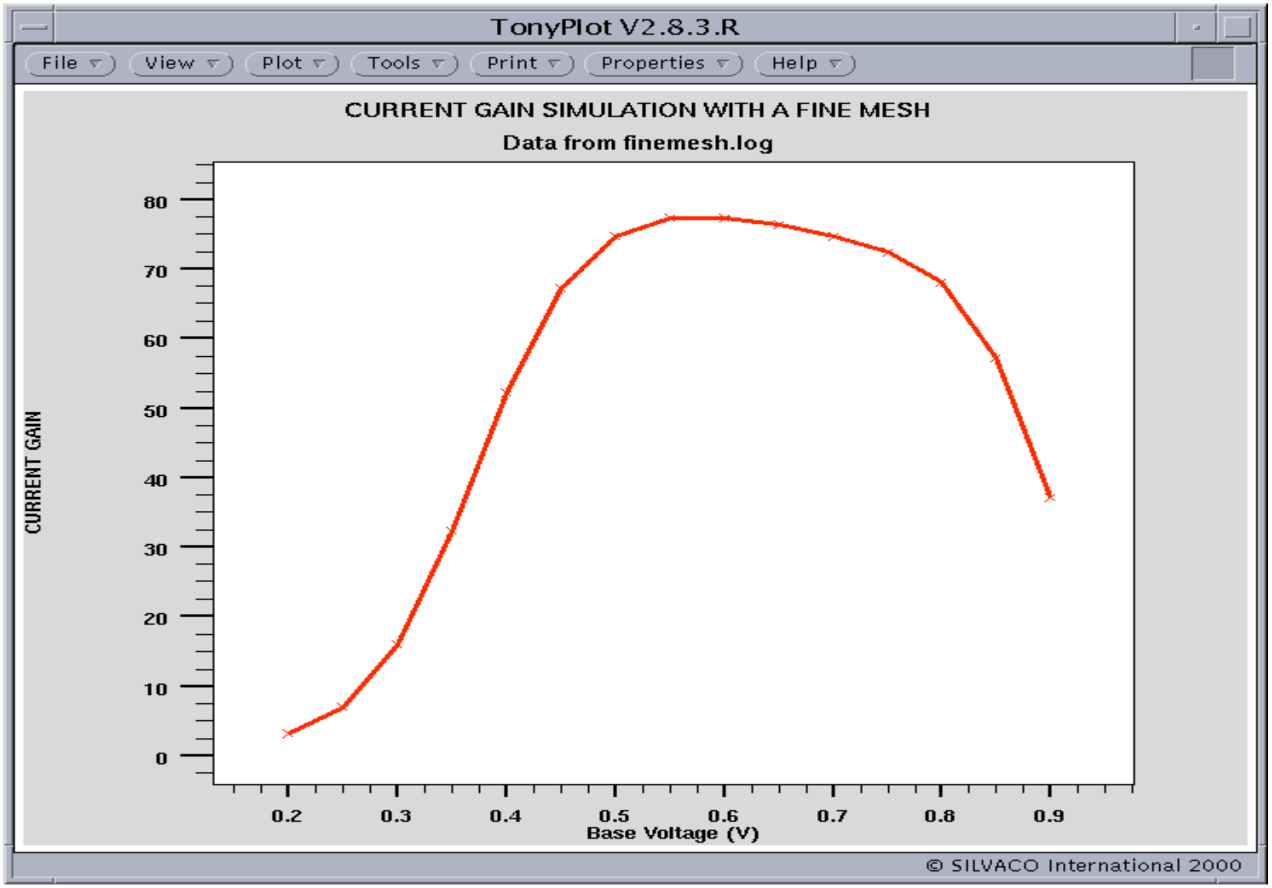
Mesh Design: Effect on Current Gain of a BJT



Mesh Design: Effect on Current Gain of a BJT



Mesh Design: Effect on Current Gain of a BJT



Contact Definition

- CONTACT statement is used to:
  - set workfunctions for example N+/P+ POLY gate (MOSFETs)
  - Surface recombination velocity (BJT emitter)
  - contact slaving and voltage control (BJT dual base contacts)
  - Schottky contacts (MESFETs, pHEMTs, Diodes, etc)
  - floating contacts (EEPROMs)
  - switch to current boundary conditions (latchup)
  - lumped contact R, L and C
  - distributed contact resistance

S-Pisces Physical Models: Which Model?

- All simulation programs use a hierarchy of models from simple to complex models. These are key to accurate simulations
- More complex models are generally:
  - More complete description of the actual physics
  - Have physically based parameters
  - More predictive

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S-Pisces Physical Models: Which Model?

- Why not just choose the most complex model each time?
  - CPU time vs. accuracy gain whilst considering the goal of the simulation
  - Simpler model gives the same answer in many cases
  - More tuning parameters

Device Simulation Models

- Mobility Models
- Recombination Models
- Generation Models
- Carrier Statistics
- Energy Balance
- Lattice Heating

Model choice tends to be technology specific as well as application specific. Recommendations will be given.

Mobility Models: Which one?

- Models describing separate physical effects can be combined together
  - Concentration dependence (CONMOB)
  - Concentration and temperature dependence (ANALYTIC, ARORA)
    - uses local temperature in Giga
  - Carrier concentration dependence (CCSMOB)
  - Parallel electric field dependence (FLDMOB)
    - velocity saturation
    - separate negative differential mobility model for GaAs (EVSATMOD=1)
  - Transverse electric field dependence (TASCH, WATT, SHIRAHATA)
    - surface mobility
  - Integrated models (CVT, YAMAGUCHI, KLA.x)

Recombination Model Hierarchy

- Shockley-Read-Hall two carrier recombination
  - used in almost all simulations
  - based on fixed lifetimes (SRH)
  - concentration dependent lifetimes (CONSRH and KLASRH)
  - trap assisted tunneling (TRAP.TUNNEL)
- Auger three carrier recombination (AUGER and KLAAUG)
  - significant when carrier concentrations high
- Optical recombination (OPTR)
  - for direct band-gap materials
  - dominant recombination in GaAs
- Surface Recombination
  - at semiconductor/insulator interfaces (S.N, S.P)
  - at metal/semiconductor interfaces (SURF.REC)
- Traps
  - discrete bulk traps (TRAP statement)
  - interface traps (INTTRAP statement)
  - continuous trap density for non-crystalline materials (DEFECT statement)

Generation Model Hierarchy

- Impact Ionization
  - required for any sort of breakdown voltage simulation
  - Selberrherr’s Model (IMPACT SELB)
  - Grant’s Model (IMPACT)
  - Crowell-Sze Model (IMPACT CROWELL)
  - Concannon (IMPACT N.CONCAN P.CONCAN)
  - Valdinoci Model (IMPACT VALDINOCI)
  - Toyabe Model (IMPACT TOYABE)
- Band to Band Tunneling
  - standard model with E (BBT.STD)
  - Klaassen’s model with E (BBT.KL)
  - narrow bandgap model (KAGUN KAGUP)

Generation Model Hierarchy (con’t)

- Fowler-Nordheim Tunneling (FNORD)
  - tunneling through insulators
  - used in EEPROM erasing
- Hot Carrier Injection (HEI, HHI)
  - energetic carrier transport through thin insulators
  - used in EEPROM programming
- Thermionic Emission (EMISS.xx)
  - used to model transport across potential barriers at heterojunctions

Carrier Statistics Models

- Boltzmann statistics
  - default
- Fermi-Dirac statistics (FERMI)
  - high concentration effects
- Incomplete Ionization (INCOMP)
  - for dopant freezeout
  - required for low temperature simulations
  - extra model for heavy dopants in silicon (IONIZ)
- Band Gap Narrowing (BGN)
  - important in heavily doped regions
  - critical for bipolar simulations

Lattice Heating and Energy Balance Simulations

- Lattice Heating activated by MODELS LAT.TEMP
- Energy Balance activated by MODELS HCTE.EL HCTE.HO
- Additional numerical techniques available
- See Six Equation Solver Training for more details

Recommended Physical Model Selections

- Recommended physical models for MOS type FETs:
  - MODELS SRH CVT BGN
- Recommended physical models for BJTs, thyristors, etc:
  - MODELS KLASRH KLAAUG KLA BGN
- Also include impact ionization to model breakdown:
  - IMPACT SELB
- In general do not switch on a model unless it is really needed

Numerical Methods for Isothermal Drift Diffusion

- All numerics settings chosen on METHOD statement
  - All structure/parameter specification must be before this statement
  - All solution specification must be after it
- Fully Coupled Method solves for potential and carriers coupled (METHOD NEWTON)
  - recommended for all cases even including SOI simulations
- De-Coupled method solves potential and carriers sequentially (METHOD GUMMEL)
  - faster for low current cases
- Combined method (METHOD GUMMEL NEWTON)
  - runs initial decoupled iterations and switches to coupled
  - GUM.INIT parameter controls the number of initial decoupled iterations
  - most robust (but slowest) method

ATLAS Syntax Guide

- Recommended numerical settings
  - METHOD NEWTON MAXTRAP=10 CLIMIT=1E-4

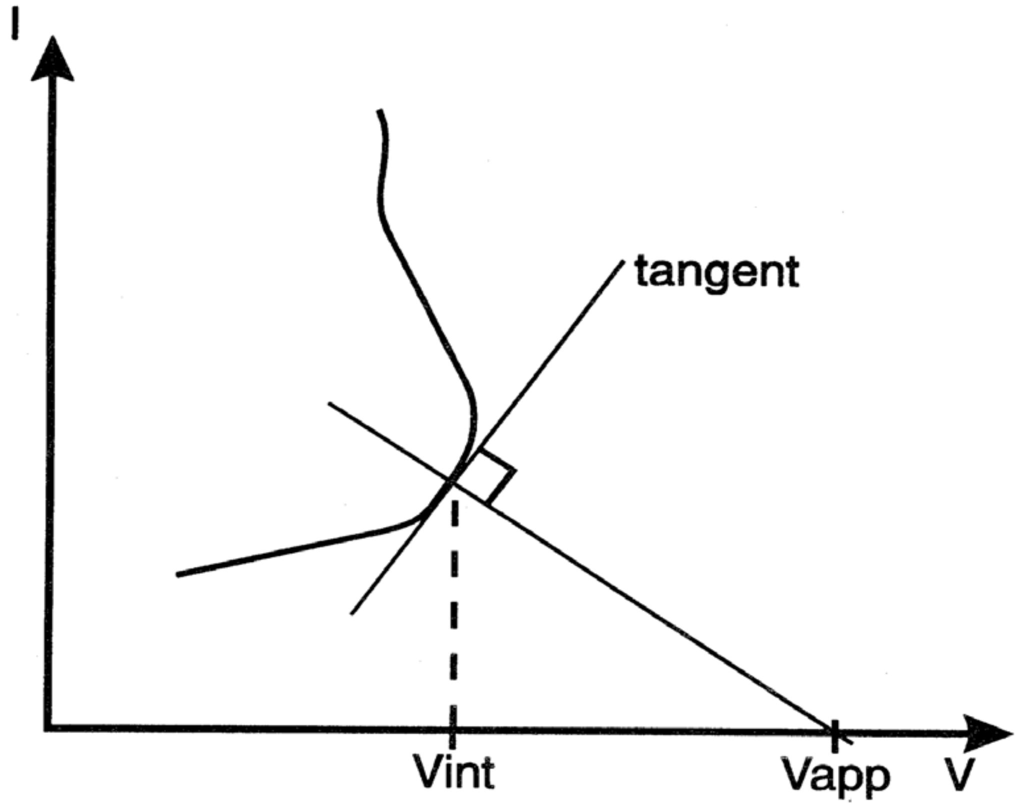
The Curvetracer: An Overview

- Algorithm to enable ATLAS to trace out complex IV curves
- Avoids user intervention in switching from voltage to current boundary conditions
- Ideal method for simulating snapback
- Improves simulation of breakdown

The Curvetracer: Features

- Dynamic Load Line Approach from “An Automatic Biasing Scheme for Tracing Arbitrarily Shaped IV Curves”, Goosens et al., IEEE Trans CAD 1994, Vol 13, pp. 310-317
- Automatic boundary condition selection
- Automatic selection of voltage/current step size
- A single SOLVE statement can be used to trace entire curves
- Only in DC mode. Transient and MixedMode already have similar capability

The Curvetracer: A Load Line Approach



The Curvetracer: Typical Applications

- CMOS Latch-up
- Snapback Effects
- Breakdown Voltages
- Second Breakdown

The Curvetracer: Syntax Guide

- A single command is used to trace an IV curve SOLVE CURVETRACE
- The TRACE statement sets up the parameters for the curve trace
- When viewing results in TonyPlot the INT.BIAS rather BIAS should be used as the voltage axis of the IV curve

The Curvetracer: TRACE Parameters

CONTR.NAME	is the name of the electrode to be ramped
STEP.INIT	defines the initial voltage step on the ramped electrode
NEXT.RATIO	specifies the factor used to increase the voltage step in areas on the IV curve away from turning points
MINCUR	may be used to set a small current value above which the dynamic load line algorithm is used. Below this STEP.INT and NEXT.RATIO are used. Highly recommended
END.VAL	is used to stop tracing if the voltage or current of ramped electrode equals or exceeds END.VAL
VOLT_CONT	denotes that END.VAL is a voltage
CURR_CONT	denotes that END.VAL is a current

ATLAS Syntax Guide: Data Output

- Two dimensional structure files use the syntax:
  - OUTPUT EFIELD
  - SAVE OUTF=2D.STR
  - SOLVE OUTF=<filename>.str

- All terminal characteristics are saved in logfiles:
  - LOG OUTF=<filename>.str
- To stop sending data to a logfile either QUIT or insert another LOG statement or use LOG OFF statement

ATLAS Syntax Guide

- Numerics:
  - METHOD NEWTON CARRIERS=2 Use syntax for most cases
  - Use CARRIERS=0 for initial guesses
  - Use METHOD GUMMEL NEWTON for devices with floating regions (e.g. SOI) This uses Gummel iterations to supply initial guess for Newton solver. It is more robust, but slower than regular Newton.
  - Contents of method statement statement vary with solution type
    - GUMMEL DAMPED
    - Newton AUTONR
    - Always TRAP

Sources of Error in Device Simulation

- Inaccurate doping profiles
- Insufficient physics
- Unknown or inaccurate material parameters
- Inaccurate model parameters
- Reliance on empirically fitted models
- Mesh induced errors
- External effects

Solving Doping Profile Errors

- This is the largest source of error for ‘small geometry devices’
    - Apply correction to doping if using SRP results
    - Use a process simulator
    - Account for CD biasing in mask edge locations
    - For further information see “Calibrating Process Simulators”

Solving Material Parameter Errors

- Silicon parameters generally well-tuned already
- For non-silicon materials, all parameters are subject to tuning
- Some parameters are substrate dependent and MUST be tuned
  - e.g. minority carrier lifetime
- Some parameters are process dependent
  - e.g. Qss

Solving Model Parameter Errors

- Remember that most models are empirically fitted to a particular set of data
- Should be used only after other errors are handled
- Most common parameters used are VSAT for saturation region tuning and Impact Ionization parameters for breakdown

Solving Mesh Errors

- Avoid obtuse triangles in the current path or high field areas
- Avoid discontinuities in mesh density
- Ensure adequate mesh density in high field areas

External Effects

- You are trying to compare measured data so you must understand your measurement system. The simulation is of a ‘perfect intrinsic device structure.”
    - External resistances
        - Long tracks in street structures, substrate contacts
    - Temperature. Simulator uses 300K. Do you?
    - Test systems use transients. Can be important for some device effects
    - Variations in measured data. Best to tune to a curve of data rather that a single point.
    - Ensure extraction technique is the same
        - e.g at least 4 ways to get MOS Vt

How to Tune Device Simulators

- Problem
  - too many parameters to change
- Run many simulations
  - slow and tedious
- Use Optimizer
  - easier, but may not converge in difficult cases
- User VWF
  - using parameterized input decks

How to Tune Device Simulators (con't.)

- Tactic
  - Eliminate or account for external effects
  - Measure what you can first to eliminate variables in the tuning
  - Thoroughly check all process related information
  - Use ‘unknown’ material parameters first
  - Use ‘major’ model parameters such as VSAT

Lattice Heating Simulations

- Wachutka’s model of lattice heating accounts for
  - Joule heating
  - Heating/cooling from generation and recombination
  - Peltier and Thomson heating
- Lattice heating is required for many reasons
  - High power devices
  - ESD protection devices
  - SOI device operation
  - III-V material systems
  - Bipolar carrier injection processes
  - Accurate impact ionization
  - External heat sources

Tuning Lattice Heating Simulations

- There are four additional calibration requirements when simulating lattice heat flow
  - 1. Temperature dependent physical models
  - 2. Temperature dependent thermal conductivities
  - 3. Temperature dependent heat capacities
  - 4. Thermal boundary conditions
  - Tactic
    - choose correct models 1
    - control material heating by 2
    - transient heat flow control with 3
    - apply external heat sources/sinks 4

Energy Balance Simulations

- Energy balance simulations are required for today’s technologies:
    - Deep sub-micron CMOS transistors
    - Advanced high mobility materials
    - Accurate substrate current modeling
    - Velocity overshoot effects
    - Gate leakage currents
    - Transconductance modeling
    - Nonlocal transport phenomena

Reference: Simulation Standard article, Volume 6, Number 4, April 1995.

Tuning Energy Balance Equations

- The relaxation times of the energy balance equations are the critical parameter but are difficult to measure.
  - 1. Energy relaxation times
  - 2. Energy dependent mobilites
  - 3. temperature dependence of relaxation times
  - 4. Energy dependent impact ionization
  - Tactic
    - apply previous drift-diffusion calibration strategies
    - modify 1 to control velocity overshoot
    - 2 is then coupled to 1
    - 3 is uncharacterized but implemented for research purposes
    - specify energy relaxation length for 4

Examples of Calibration Parameters

- Threshold Voltage

Gate workfunction (WORKF)	CONTACT
Surface states (QF)	INTERFACE

- Subthreshold Slopes

Surface states (QF)	INTERFACE
Interface defect traps	INTTRAP
Discrete Bulk defect traps	TRAP
Distributed bandgap defect traps	DEFECTS

- Theta

Physical models (MOS)	MODELS
Mobility equations coefficients (DELTAN.CVT)	MOBILITY

- Bipolar Gain

Physical models (BIPOLAR)	MODELS
Mobility equations coefficients (MUN, MUP)	MOBILITY
Recombination coefficients (TAUN0)	MATERIAL
Extrinsic resistances (RESISTANCE)	CONTACT
Surface recombination (SURF.REC)	CONTACT

Examples of Calibration Parameters (con't.)

- I - V Curves

Physical models (MOBILITY, BGN)	MODELS
Mobility equations coefficients (VSAT)	MOBILITY

- Leakage Currents

Physical models (TUNNELING)	MODELS
Recombination coefficients (TAUN0)	MATERIAL
Trap density (see subthreshold slope)	

- Breakdown

Current level (Vt, Theta, Gain, etc)	
Impact ionization coefficients (SELB, AN1, BN1)	IMPACT

- EPROM Write/ Erase

Floating contacts (FLOATING)	CONTACT
Physical models (PROGRAM, ERASE)	MODELS
Tunneling equation coefficients (IG. ELINR)	MODELS
Coupling capacitances	CONTACT

Examples of Calibration Parameters (con’t)

- Lattice Heating

Physical models (LAT.TEMP)	MODELS
Thermal conductivities (TC.A, TC.B, TC.C)	MATERIAL
Heat capacities coefficients (HC.A, HC.B, HC.C)	MATERIAL
Thermal boundary conditions	THERMCONTACT

- Energy Balance

Physical model (HCTE)	MODELS
Relaxation times (TAUREL.EL)	MATERIAL
Impact ionization coefficients (LREL.EL)	IMPACT

3D Device Simulation with ATLAS

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3D Device Simulation Modules in ATLAS

- Device3D - Drift diffusion simulator with standard 2D models available
- Blaze3D - III-V and II-VI simulator
- Giga3D - Self-consistent lattice heat flow solution
- MixedMode3D - Missed Spice and Device 3D simulation
- Quantum3D - Quantum correction theory in 3D
- TFT3D - Amorphous Poly Device simulation
- Thermal3D - Heat dissipation only simulator

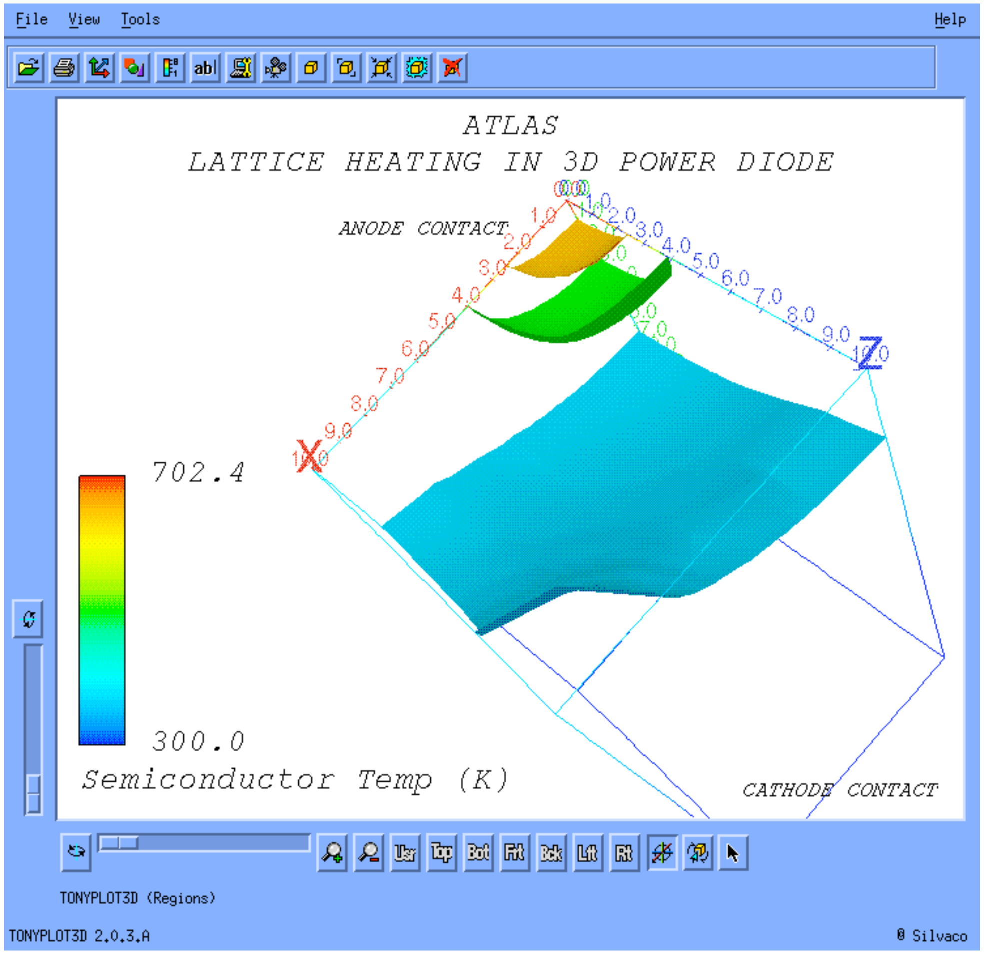
Device 3D - 3D Silicon Device Simulator

- Solves Poisson’s and electron/hole continuity equations
- Prismatic based mesh structures
- dc, ac and transient analysis modes
- Choice of numerical solvers
- Comprehensive physical models
  - mobility
  - recombination
  - generation
  - carrier statistics
- R, L and C lumped elements
- C-interpreter functionality

3D Device Simulation

- Giga 3D
  - Giga 3D contains most the functionality of the 2D Giga but works with the 3D products
  - This allows modeling of heatflow and self heating effects in 3D devices
  - The only functionality not supported in this version of Giga 3D that is supported in 2D is the BLOCK method

Lattice Heating in 3D Using Giga3D

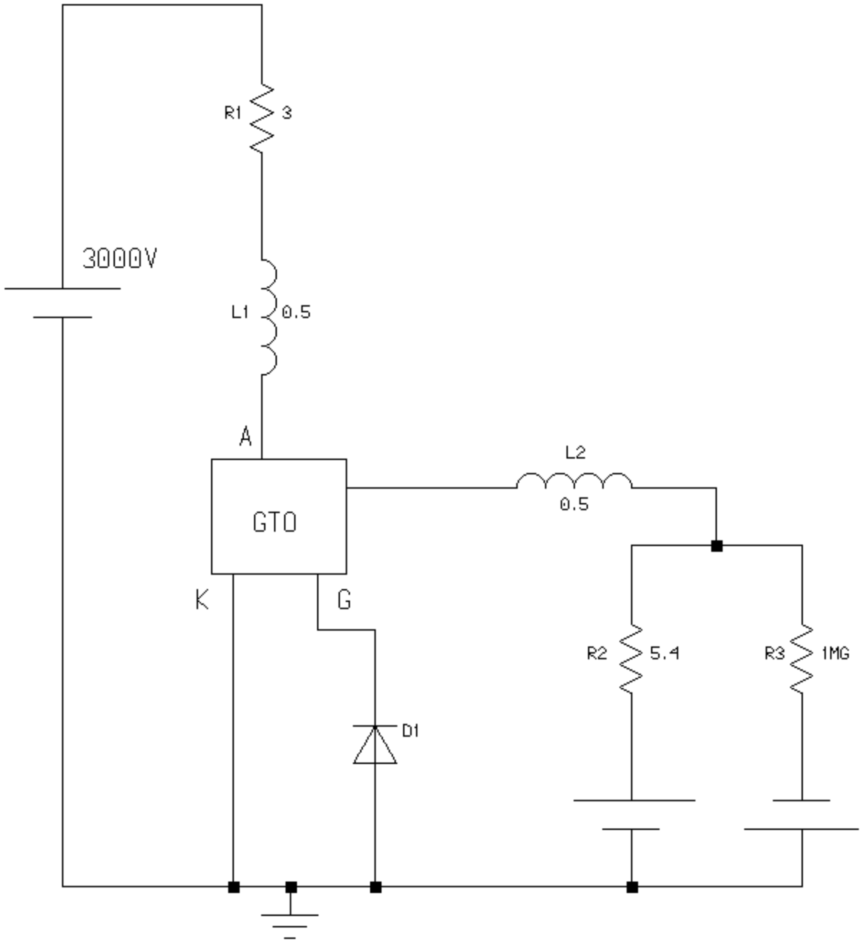


- Isosurfaces of temperature in a power diode with current crowding into the anode

3D Device Simulation

- MixedMode3D
  - This improvement allows simulation of 3D devices embedded in lumped element circuits
  - MixedMode3D contains all the functionality of 2D MixedMode simulator

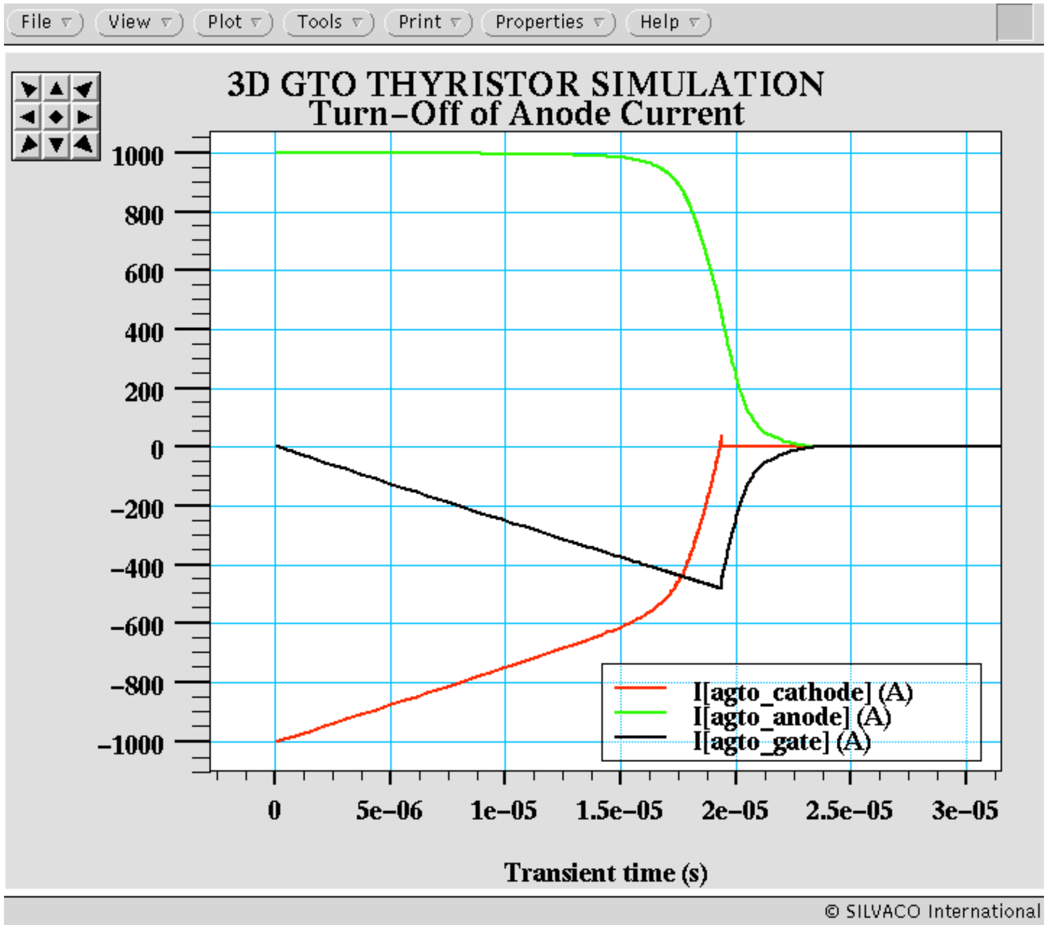
MixedMode3D



Circuit schematic for a GTO thyristor

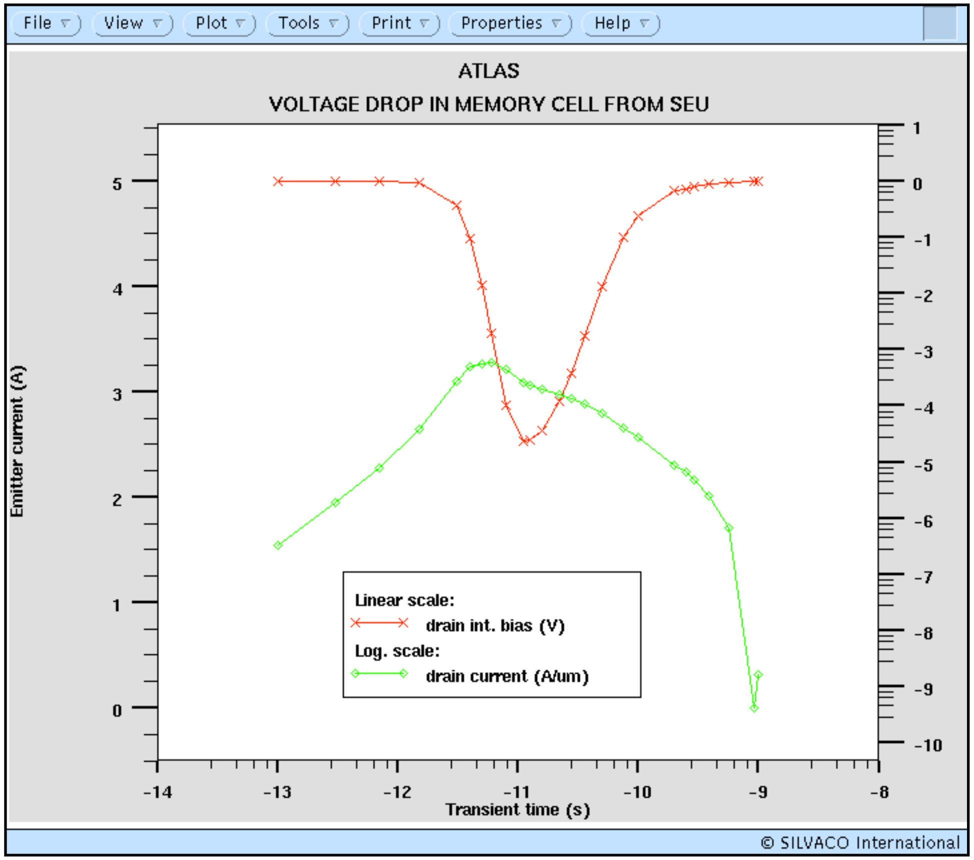
The GTO element is simulated using 3D device simulation

MixedMode3D



- Currents in the GTO thyristor during turn-off through external circuit

SEU in Memory Cell Using MixedMode3D

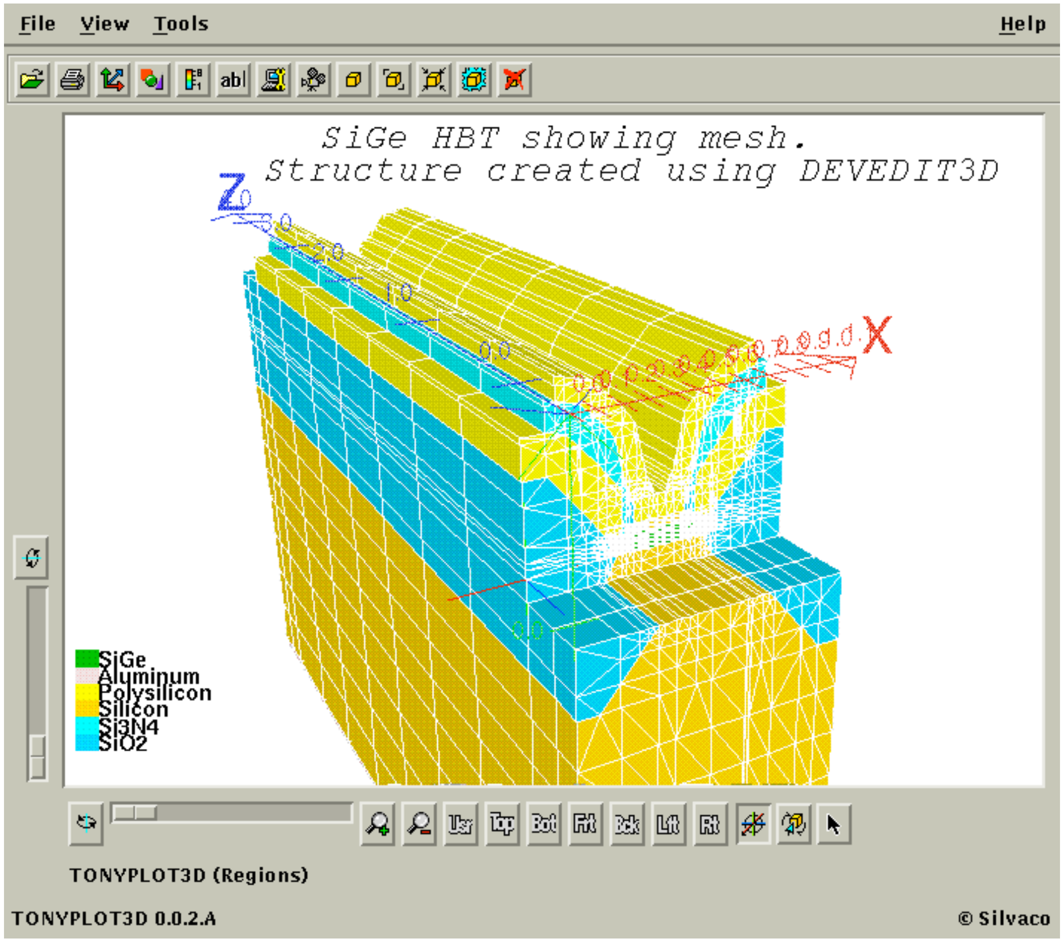


- Voltage drop on mode of SRAM cell during single event upset
- Circuit boundary conditions are required to model the cell behavior
- 3D device simulation is required to model the SEU

3D Device Simulation

- Blaze 3D
  - This version accounts for spatial variations in bandgap due to variations in material composition in 3D This version supports all the same models as are supported in 2D Blaze with the exception of thermionic emission at heterojunctions and energy transport
  - This version also does not support compositional variation in the z direction

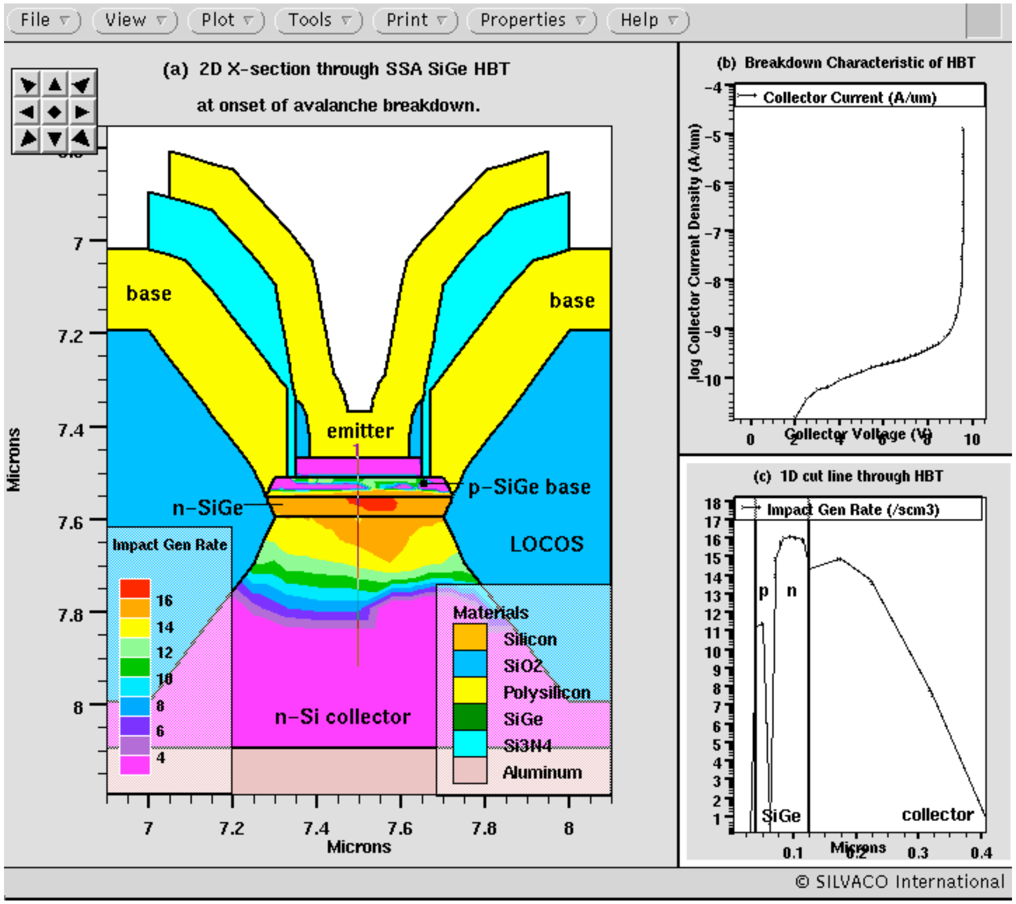
HBT in Blaze3D



SiGe HBT showing mesh.
Structure created using DEVEDIT3D

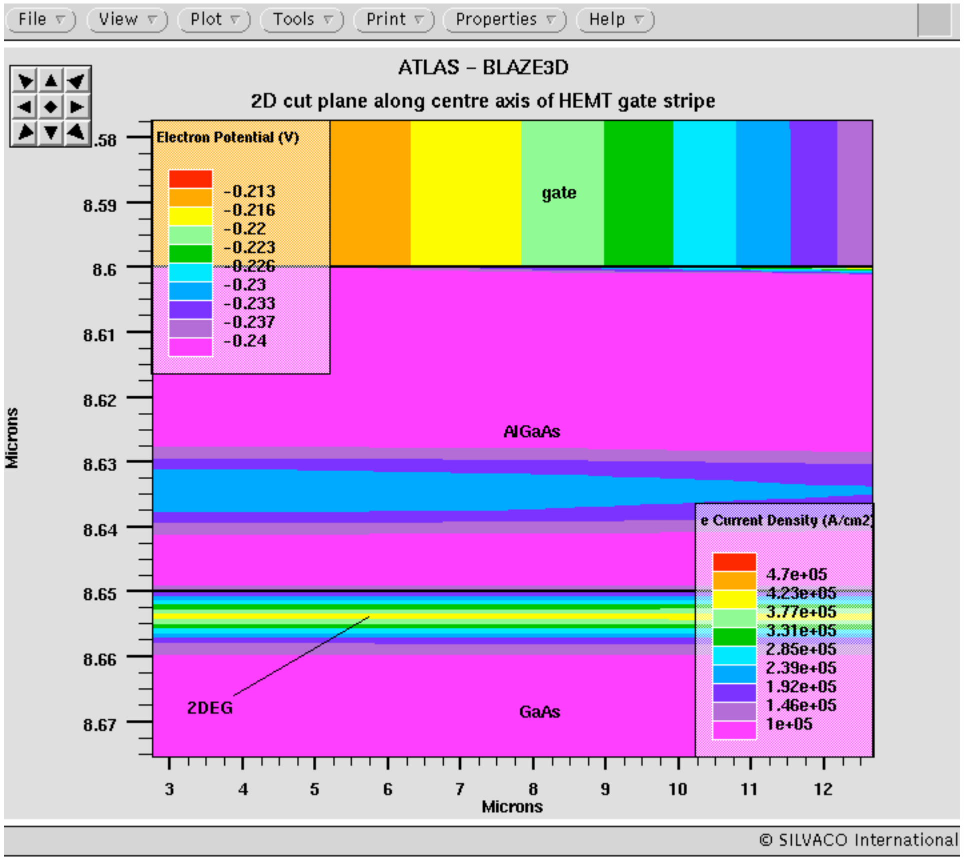
- 3D super self aligned SiGe HBT structure created and meshed using DevEdit3D
- Emitter and base contacts are polysilicon
- A section of oxide isolation is removed from the view to reveal the confined SiGe base region with denser mesh

HBT in Blaze3D



- (a) cut plane through 3D HBT structure at onset of avalanche breakdown. Note the concentration of impact ionization in the center of the n-SiGe collector extension region.
- (b) HBT collector breakdown characteristic. (c) cut line through
  2D section showing graph of impact ionization rate with depth under poly emitter stripe.

HEMT in Blaze3D

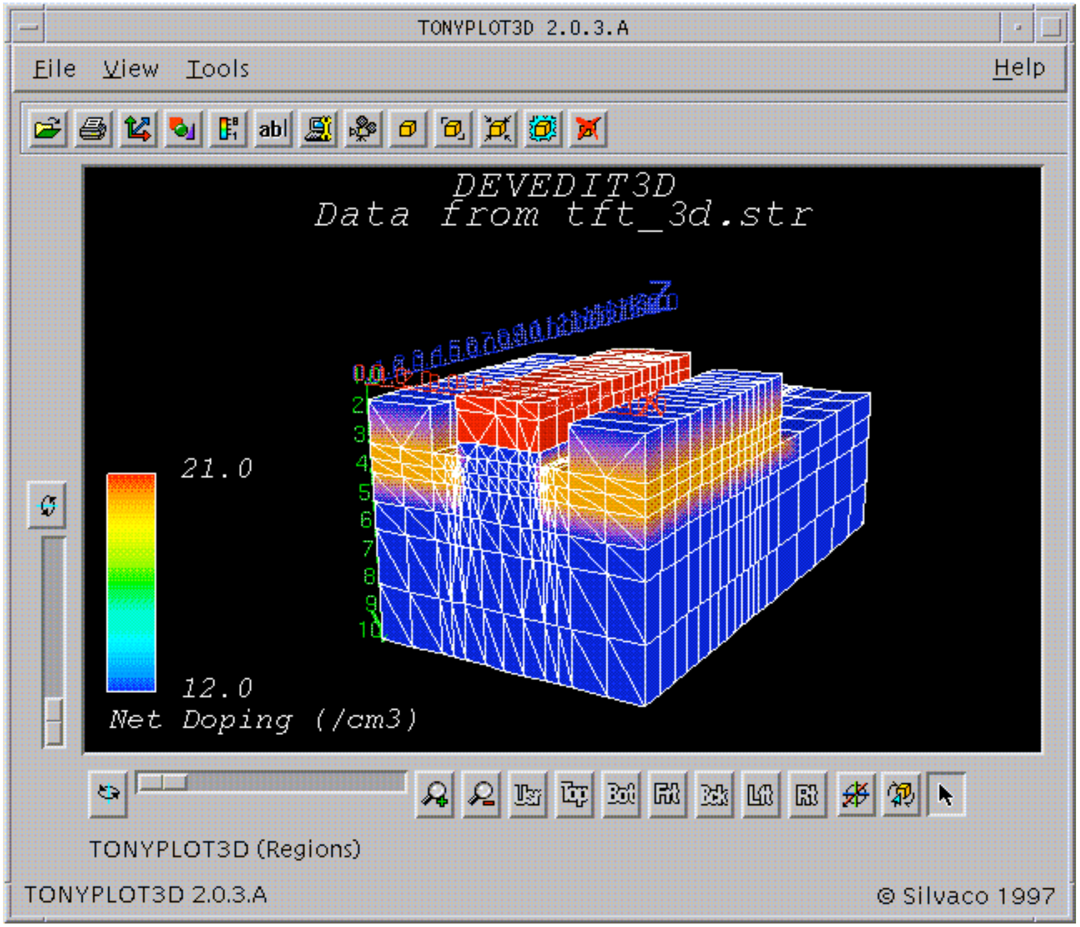


- 2D cut plane taken from a Blaze3D solution for the 3D HEMT during a negative gate bias transient
- The section is along the major axis of the resistive T-gate and shows the potential gradient along its length
- The channel conduction (particularly the parasitic conduction in the AlGaAs) is consistent with the gate potential profile

3D Device Simulation

- TFT 3D
  - This model allows modeling of poly and amorphous semiconductor devices such as TFTs in 3D
  - This model has all the functionality of the 2D TFT simulator

TFT 3D

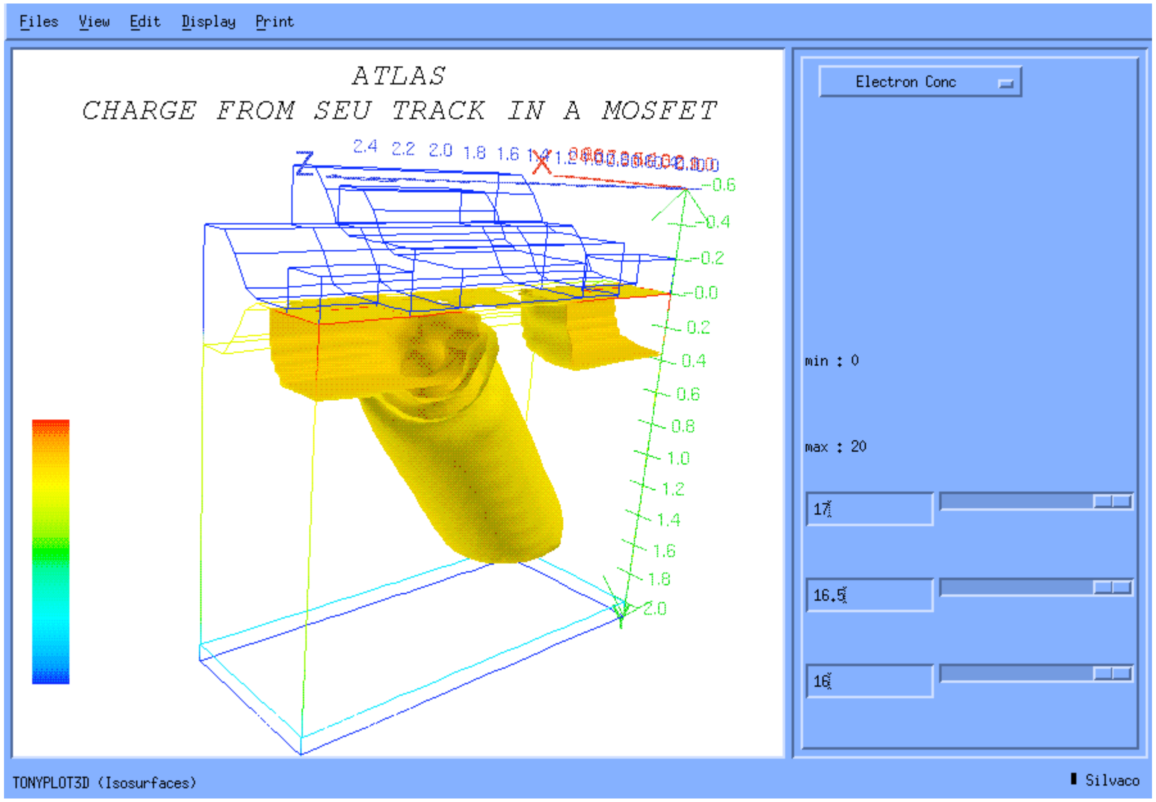


- 3D device simulation of high performance TFT device

3D Device Simulation

- Quantum3D
  - This allows modeling of the effects of quantum confinement using the quantum moment approach
  - This model has all the functionality of the 2D Quantum model

SEU in Device 3D



ATLAS
CHARGE FROM SEU TRACK IN A MOSFET

Electron Conc

min : 0

max : 20

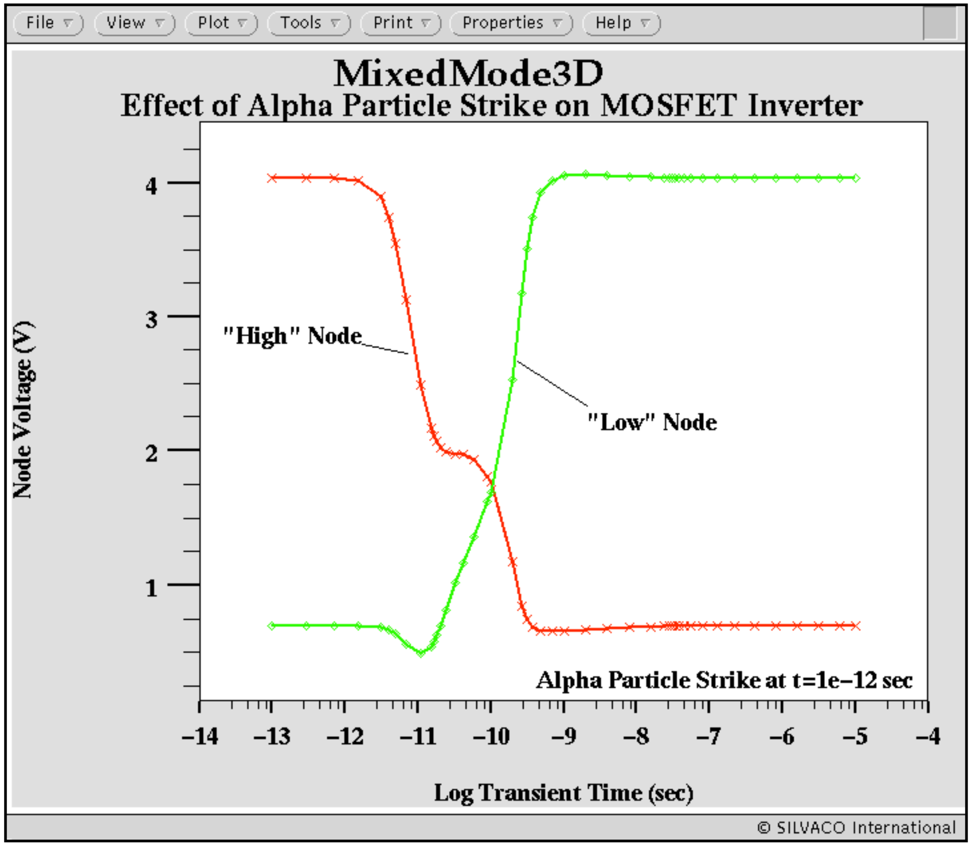
17

16.5

16

- More control parameters for radial distribution and transient intensity of SEU pulses have been added

SEU in MixedMode3D



- Effect of an alpha particle strike on an inverter circuit simulated with MixedMode 3D
- The memory bits are seen to switch during the event
- Data corruption such as this could cause critical failure of the circuit