Introduction to Process and Device Simulations with ATHENA and ATLAS

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General Tips on Using TCAD Tools

- **A simulator is only as good as the physics put into it**
  - Only what is well understood can be modeled
  - Always with clear objectives for a simulation
  - Rely on your own judgement, not simulation nor experimental results
- **Be fully aware of the model assumptions and the default parameters**
  - Make sure the model is used in its region of validity
  - Justify if defaults are to be used
- **The result of a simulation is grid dependent**
  - Trade-off between accuracy and speed
  - Use coarse grids initially, refine the grids as you proceed
- **Look for trends, not for “accurate” values**
  - Never try to “perfectly fit” a single set of parameters to an experimental curve
  - Overall 10–20% accuracy would be a reasonably good fit

Role of Process and Device Simulation

- **Process simulation**
  - **Stand-alone**: simulate processing steps for evaluating process alternatives,sensitivity, and yield improvement
  - **Front-end to device simulator**: provide realistic structure and impurity profile for meaningful device simulation
- **Device simulation**
  - **Stand-alone**: simulate single-device electrical characteristics for understanding physical effects, advanced device design, and reliability study
  - **Front-end to circuit simulator**: provide accurate parameters for transistorlevel models to predict circuit performance

Trends in VLSI Technology Development and Simulation

- **Device scaling and scale of integration** — How far can we go?
- **Device physics and modeling** — Will the device physics at 0.1 µm still work?
- **Processing technology**
  - More complex/expensive processes and equipment, multiplayer interconnect
- **Lithography**
  - Electron, X-ray, and ion based techniques (0.1 µm resolution)

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- **Packaging and interconnection technology**
  - Larger I/O numbers, surface mount, MCM's, printed wiring boards
- **Design process**
  - Higher levels of abstraction to cope with complexity, self-test capability
- **CAD tools** (major gap)
  - 3D process/device simulation, on-chip signal integrity, full-cell characterization, full-chip verification

ATHENA: Simulation Capabilities

- **Arbitrary 2D structures composed of different semiconductor materials**
- **Profiles of different impurities, diffused, implanted, or incorporated into deposited layers**
- **Semiconductor processing steps**
  - Diffusion of impurities in all layers
  - Oxidation of silicon and polysilicon
  - Ion implantation of impurities
  - Expitaxial growth of doped and undoped silicon layers
  - Deposition and etching of all materials
  - Exposure and development of photoresist
- **Calculation of stress due to oxidation, thermal expansion and material Deposition**
- **Generation, diffusion and recombination of point defects in silicon**

SSUPREM4: Physical Models

- **Diffusion**
  - Oxidation enhancement/retardation; high-concentration and coupled-impurity effects; transient enhancement effects; diffusion and saturation of dopant/defect pairs; generation, diffusion and recombination of point defects; …
- **Oxidation**
  - 2D viscous flow with stress dependence; high-concentration effects; thinoxide enhancement; gas partial pressure; effect of HCl on oxidation rates; user-defined ambients; different rates for polysilicon and single crystal; …
- **Implantation**
  - Gaussian, Pearson and dual-Pearson analytic models; energy, dose, tilt and rotation effects; shadowing effects; implant damage model; Monte Carlo model including channeling, amorphization, temperature, substrate tilt, etc.;

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- **Deposition, masking, and etching**
  - Conformal deposition; epitaxial growth with impurity diffusion; dry etching with masked undercutting and angled sidewalls; etching of arbitrary regions; exposure and development of positive and negative photoresist
- **Optolith**: 2D Lithography simulator with Maskviews Interface through GDS
  - Arial image, resis profile, OPC(Optical Proximity Correction)
- **Elite :** more complex non-isotropic step coverage and etch model (PECVD)

ATHENA: Input/Output

- **Input** — A series of statements
  - Grid generation
  - Mask definition
  - Structure initialization
  - Process step specification
  - Output control
- **Output** — Ascii, binary, graphical data
  - Structure and mesh
  - Profiles: minima or maxima, or arbitrary points
  - 2D contour and vector plots
  - Extraction of concentrations, depths, junction locations, …
- **Interface — *Deckbuild/Tonyplot/Maskviews/DevEdit***

ATLAS(S-PICES): Simulation Capabilities

- **Electrical characteristics of arbitrary 2D structures under users-pecified operating conditions**
- **Self-consistent solution of Poisson's equation, current continuity equations, energy balance equations and the lattice heat equation**
- **Steady-state, transient, small-signal AC analysis**
- **Arbitrary doping from analytic functions, tables, or process simulation**
- **Voltage, current, or charge boundary conditions; lumped element or distributed contact resistance**
- **Multiple materials (Si, Ge, SiGe, GaAs, AlGaAs, SiC, GaN, InP) as well as arbitrary use-defined materials**
- **Automatic regridding and I–V curve tracing**
- **Parameter extraction (V_T, I_{dsat}, b , f_t, *RSH*, …)**
- **Optimization for tuning device performance and model calibration**

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ATLAS(S-PICES): Physical Models

- **Recombination and generation**
  - SRH, Auger, band-to-band, recombination including tunneling
- **Mobility models**
  - Dependencies on lattice temperature, impurity concentration, carrier concentration, carrier energy, parallel and perpendicular electric fields
- **Fermi–Dirac and Boltzmann statistics**
- **Bandgap narrowing and band-to-band tunneling**
- **Field-, carrier energy- and lattice temperature-dependent impact ionization**
- **Gate-current analysis**
- **Advanced application modules (Blaze, Giga, ESD, Lase, Luminous, TFT, Quantum, Fram)**

ATLAS(S-PICES): Input/Output

- **Input** — A series of statements
  - Mesh generation
  - Physical model/coefficient selection
  - Solution and boundary specification
  - Electrical analysis, parameter extraction and optimization
  - Output control
- **Output** — Ascii, binary, graphical data
  - Structure, mesh, boundary, junction location, depletion regions
  - Solutions and various physical quantities extracted from the solution
  - 1D, 2D, 3D, surface, contour, and vector plots of physical quantities
- **Interface** — *Deckbuild, SSUPREM4, Tonyplot, DevEdit ,Maskviews, MixedMode, Utmost*

Utmost: Device Characterization

- **Applications**
  - Measure and analyze device electrical characteristics through direct control of parametric testers, network analyzers, wafer probers, …
  - Extract physically meaningful parameters for SPICE or proprietary models
  - Develop new device models and custom extraction/optimization strategies
  - Obtain skew models from simulated/measured data for best/worst case Design
  - Create macromodels for complex devices

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- **Models**
  - MOS2, MOS3, BSIM2, BSIM3, BSIM4, Gummel–Poon, junction capacitance model, JFET model, diode model, TFT, HBT, Fram, VBIC, High voltage CMOS, Maxtram, user-defined model, etc
- **Circuit simulator interface**
  - SmartSpice – Silvaco's Analog Circuit Simulator, HSPICE,..

VWF(Virtual Wafer Fab): Virtual IC Factory

- **Integrated graphical environment for physical simulation**
- **Comprehensive data management**
- **Post-simulation graphical and statistical data analysis**
- **Design of experiment capabilities**
  - **DOE** — efficient design of simulated experiments based on the number of input variables
  - **RSM** — rapid approximation and responses in a design space, which can be further explored via graphical acceptable design window or optimization
  - **Split run** — design comparison and tradeoff
- **Easy-to-use GUI**

Other Silvaco TCAD Tools

- **Decbuild – Input file parsing and analysis**
- **Optimizer – Process and Device parameters optimization in Deckbuild**
- **DevEdit/DevEdit3D — Graphical Device Generation and Mesh Optimization**
- **Maskviews — Layout interface**
- **Tonyplot /Tonyplot3D— Graphical Analysis**
- **Device3D — 3D device simulation**
- **Elite — 2D deposition and etch simulation**
  - **Use physically-based deposition/etch models for arbitrarily shaped structures**
- **Optolith — 2D photolithography (imaging, exposure and development)**
  - **Simulate photolithographic processes and aerial images affecting topography**
- **Interconnect3D — 3D interconnect analysis**
  - **Simulate parasitics of interconnnect and 3D cell using field solver and RC**

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Simulator Calibration

- **Paramount importance**
  - Obtain meaningful simulation results related to your real process
  - Provide reliable predictions from process alterations and extensions
- **Basic ideas**
  - Compare with experimental data from SIMS, SEM, TEM, SRP, I–V, C–V,
  - Choose a process model and a set of parameters associated with that model, then, numerically fit the result of the model to that of the experimental data using optimization
  - Fit major physical parameters independently first

Process Simulation with SSUPREM4

- **Overview of process simulation**
- **Structure specification**
- **Major process steps and models**
  - Diffusion, oxidation, implantation, epitaxy, deposition, masking, etching, exposure and development
- **Models and coefficients**
- **Electrical calculation and parameter extraction**
- **Data post-processing**
- **A tutorial example**

Structure Specification

MESH	Sets grid spacing scale factor and defaults for automatic grid generation
LINE	Specifies a grid line in a rectangular mesh
ELIMINATE	Specifies grid lines to be removed from the mesh
BOUNDARY	Sets boundary conditions for a rectangular mesh
REGION	Sets material types for a rectangular mesh
INITIALIZE	Initializes a rectangular mesh or reads mesh and solution information from a file
LOADFILE	Reads mesh and solution information from a file
SAVEFILE	Writes mesh and solution information to a file
STRUCTURE	Reflects or truncates a structure
MASK	Reads mask information from a file
PROFILE	Reads a one-dimensional doping profile from a file
ELECTRODE	Specifies the name and position of electrodes

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Grid in SSUPREM4

- **The simulation structure**
  - 2D cross-section of a portion of a semiconductor wafer
  - X-coordinate: distance parallel to the wafer surface
  - Y-coordinate: depth into the wafer
  - Top surface: exposed where deposition, etching, impurity predeposition, oxidation, silicidation, reflow, out-diffusion, and ion implantation occur
  - 1 to 40 regions of arbitrary shape

- **The grid structure**
  - The continuous physical process are modeled numerically by using finite difference (for diffusion) and finite element (for oxide flow) solution techniques
  - Each region is divided into a mesh of nonoverlapping triangular elements
  - Solution values are calculated at the mesh nodes (at the corners of the triangular elements), values between the nodes are interpolated
  - Up to 40,000 triangles, up to 20,000 use-defined and temporary nodes

Other Structure-Related Statements

- **Boundary conditions**
  - `BOUNDARY {EXPOSED|REFLECT} XLO XHI YLO YHI`
- **Material type of a mesh region**
  - `REGION MATERIAL XLO XHI YLO YHI`
- **Structure truncation or reflection**
  - `STRUCTURE {TRUNC|REFLECT} {RIGHT|LEFT} {BOTTOM|TOP}`
- **Impurity profile (1D)**
  - `PROFILE IMPURITY IN.FILE`
- **Electrode definition**
  - `ELECTRODE {X Y|BOTTOM}`

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Diffusion Theory

- **Goal — develop models for predicting diffusion results based on calculation of electrical characteristics from processing parameters**
- **Two major approaches**
  - **Continuum theory**
    - Solution of Fick's diffusion equation with appropriate diffusivities
    - Suitable when impurity concentrations are low (< ni)
    - For high dopant concentrations, use concentration-dependent diffusivities
  - **Atomistic theory**
    - Interactions between point defects, vacancy and interstitial atoms, and impurity atoms
    - Atomic movement of the diffusant in the crystal lattice by vacancies or selfinterstitials

–

Diffusion of Point Defects

- **Point-defect based diffusion**
  - Impurities diffuse in semiconductor materials as dopant–defect pairs via vacancies and interstitials
  - The diffusion coefficients (D_m and D_n) are sums of the diffusivities of impurities paired with defects in various charge states
- **"Fermi" model** — the point defect concentrations depend only on the Fermi level (without OED)
- **Transient model** — the simplest model that includes a full 2D transient solution for the point defect concentrations (with OED)
- **Full model** — the most complete diffusion model, including saturation of dopant-defect pairs and dopant-assisted recombination

Oxidation Enhanced Diffusion

- **Enhancement (or retardation) of diffusion**
  - Due to nonequilibrium point defect concentrations
  - Oxidation produces point defects (interstitials) which alter dopant diffusivity
- **Models**
  - `METHOD FERMI ( no OED )`
  - `METHOD TWO`
  - `METHOD FULL.CPL`

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Choosing a Diffusion Model

METHOD {PD.FERMI|PD.TRANS|PD.FULL}

- **"Fermi" model** — use only in special cases when speed is more important than accuracy (*No OED*)
  - Use for faster simulation of diffusion in inert ambients
  - Use for oxidation under extrinsic conditions (high impurity concentration and low oxidation temperatures, e.g., S/D reoxidation) to avoid multiplication of point-defect effects
- **Transient model** — use most of the time
  - Simulate OED effects
  - Require deep substrate (~200 µm), which can have very coarse grid
- **Full model** — use for ultimate accuracy
  - High-concentration effects (e.g., kink effect)
  - Post-implant anneals (when using the implant damage model)

Numerical Oxidation Models

- **The VERTICAL model** — the simplest of the numerical oxidation models
  - The oxide/silicon interface is constrained to move in the + y direction
  - The expansion of the oxide occurs in the – y direction
- **The COMPRESS model** — simulates the compressible viscous flow of the oxide and 2D movement of the oxide/silicon interface
- **The VISCOUS model** — simulates the incompressible viscous flow of the oxide, with or without stress dependence

Choosing an Oxidation Model

METHOD {ERFC|ERFG|ERF1|ERF2|VERTICAL|COMPRESS|VISCOUS}

- **ERFC, ERFG, ERF1, ERF2 models** — do not use!
  - Useful only in special case of bare, planar, silicon surface and uniform or nonrecessed local oxidation. Requires careful calibration and parameter setup. Does not include concentration dependence
- **VERTICAL model** — use for early process steps (default)
  - Only accurate for planar or near-planar structures. Much easier to use than ERFC etc. Does not oxidize polysilicon. Somewhat faster than COMPRESS
- **COMPRESS model** — use most of the time
  - Good for general structures. Reasonably fast. Does not use too much memory. Error due to compressibility is negligible

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- **VISCOUS model (without stress dependence)** — use in special cases only
  - Negligible increase in accuracy over COMPRESS. More accurate solution of oxidant diffusion sometimes useful. Slow compared to COMPRESS
- **VISCOUS model (with stress)** — use when maximum accuracy is needed
  - Most accurate but very slow (20–200 times slower than that without stress). Requires modified viscosities and extra parameters

Silicide Models

- **Specification of silicide models and parameters**
  - The new materials must be defined (**MATERIAL NEW**)
  - Any diffusing species that participates in the growth reactions must be defined(**IMPURITY NEW**)
  - The growth reactions themselves (one at each interface) must be defined (**REACTION**)
  - The deposition of initial layers must be specified
  - The diffusion and segregations of impurities in the new materials and at interfaces must be specified
- **Impurities and point defects**
  - **Impurities in silicides are modeled in the same way as in other non semiconductor materials**
  - **Point defects can participate in reactions at interfaces with silicon (suggested model: FERMI)**

Diffusion Simulation — Basic Statements

DIFFUSION TIME TEMP PRES [IMPURITY DOSE] {Ambient}

- **Temperature ramp**

$$T_c = \begin{cases} \mathbf{TEMP} + \mathbf{T.RATE} \times \mathbf{t} \\ \mathbf{TEMP} + \dfrac{\mathbf{T.FINAL} - \mathbf{TEMP}}{\mathbf{TIME}} \mathbf{t} \end{cases}$$

- **Ambient**
  - Specify a previously defined ambient with one of the parameters **DRYO2,WETO2, INERT**
  - Define the ambient gas directly by specifying the flows of the oxidizing and nonoxidizing species with the parameters **F.O2, F.H2O, F.H2, F.N2**, and **F.HCL2 or HCL**

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Diffusion Simulation — Relevant Statements

- **METHOD** — selects models for oxidation and diffusion, and specifies numerical methods
- **AMBIENT** — specifies oxidation coefficients
- **MATERIAL** — sets the physical properties of materials
- **IMPURITY** — defines impurities or modifies their characteristics
- **REACTION** — defines the reactions that occur at material interfaces
- **INTERSTITIAL** — sets the coefficients for interstitial kinetics
- **VACANCY** — sets the coefficients for vacancy kinetics
- **ANTIMONY** — sets some of the properties of antimony
- **ARSENIC** — sets some of the properties of arsenic
- **BORON** — sets some of the properties of boron
- **PHOSPHORUS** — sets some of the properties of phosphorus

Ion Implantation

- **Goal — model the implantation of ionized impurities (specifically, dose and range) into the simulation structure for accurate subsequent thermal cycling**
- **Major models**
  - ***Analytic models***
    Gaussian distribution
    Pearson distribution
  - ***Numerical (Monte Carlo) model*** — models the nuclear collision energy loss according to classical binary scattering theory
    - Crystalline silicon or amorphous material
    - Profile dependence on tilt and rotation angles
    - Dose, energy, and temperature dependence
    - Effects of reflected ions
  - ***Implant damage model*** — models the transition from crystalline to amorphous material

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Monte Carlo Ion Implant Model

- **Basic theory**
  - Binary scattering theory — the ion interacts with only one target atom at a time
  - Monte Carlo statistical calculation — calculates the ion trajectories using random distributions
  - **Ion energy loss mechanisms**
  - Nuclear scattering — the nucleus of the ion elastically scatters off the nucleus of an atom in the target
  - Inelastic interaction of the ion with the electrons of the target atoms
- **Major models**
  - Amorphous implant model
  - Crystalline implant model
  - Implant damage model

Amorphous Implant Model

- **Major features**
  - Generates secondaries for collisions which impart energy above a threshold to lattice atoms (results in vacancy and interstitial profiles)
  - Models crystal-to-amorphous transition by treating the target as amorphous
    with a probability which is a function of the point defect concentration
  - Models self-annealing using a temperature dependent recombination distance
- **Final ion positions**
  - Initial ions are implanted into an undamaged substrate
  - The channeled component is reduced and ions are being stopped closer to the surface
- **Point defect information**
  - Produces profiles of point defects created by the implant process, which are important for post-implant diffusion and are useful for RTA model development

Crystalline Implant Model

- **Major difference**
  - *Amorphous model* — selects the collision of the implanted ion with target atoms based on the density of the target material and a random number
  - *Crystalline model* — determines an impact parameter based on the implanted ion's position relative to sites on an idealized lattice

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- **Major features**
  - Includes explicitly the crystal structure information and lattice vibrations
  - Models effects of tilt and rotation angles (“channeling”), and different crystal orientations
  - Simulates individual ion trajectories with full 3D calculation through ideal crystal structure
  - Allows explicit specification of the electronic stopping along a particular crystal axis

Implant Damage Model

- **When used with the analytic models**

• **TWO** point defect diffusion model is enabled and the interstitial and vacancy distributions created by implantation are added to those that may have existed in the structure prior to implantation

• The model approximates the damage profiles by combinations of Gaussian and exponential functions

• The model can produce point defect concentrations that are much greater than those produced by oxidation, thus, may require **FULL.CPL** diffusion model. Very small time steps are required in the initial stages of follow-up diffusion

- **When used with the Monte Carlo model**

• The transition from crystalline to amorphous is based on the degree of damage

• Calculates the trajectories of the knock-ons (secondaries) with the same detail as the implanted ions

• The interstitials and vacancies are retained as an initial condition for subsequent diffusion

• Models self-annealing of the damage produced during implantation

Choosing an Ion Implant Model

```
IMPLANT IMPURITY DOSE ENERGY TILT ROTATION +
{GAUSSIAN|PEARSON | MONTE N.ION} + CRYSTAL DAMAGE
```

- **Gaussian model** — *useful as a rough estimate only*
- **Pearson model** — *efficient and sufficiently accurate*
  - Can fit experimental profiles quite well, including channeling
- **Monte Carlo model** — *use for modeling physical effects not available in analytic models*
  - Useful for studying new approaches

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- Useful when no implant range statistics are available
- More ions (**N.ION**) give smoother profile, but increase CPU time

o **Relevant statements**

MOMENT MATERIAL RANGE SIGMA GAMMA KURTOSIS

Epitaxy

o **Model and capabilities**

- Models the epitaxial growth of silicon layers (the top layer must consist of single crystal silicon)
- Diffusion equations are solved for all the mobile species
- One or more impurities may be incorporated into the growing layer

o **Simulation statement**

```
EPITAXY TIME TEMP THICKNESS IMPURITY
```

o **EPITAXY is equivalent to DEPOSITION + DIFFUSION**

DEPOSITION

o **Model — conformal deposition**

- All points within a distance of the exposed surface are included in the new layer
- Assuming the temperature is low enough that impurity diffusion can be ignored

o **Capabilities**

- Deposited materials: **SILICON**, **OXIDE**, **OXYNITRI**, **NITRIDE**, **POLYSILI**, **ALUMINUM**, **PHOTORES**
- Deposited layer can be doped with one or more impurities

o **Simulation statement**

DEPOSITION THICKNESS MATERIAL IMPURITY

o **Notes**

- Deposition should not be attempted when the left or bottom sides of the structure are exposed, or when the top surface is not exposed
- Deposition of one material on top of another can cause a third material to be added between them (e.g., titanium on silicon — $TiSi_2$ is inserted)

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Masking, Exposure and Development of Photoresist

o Masking

• Masking information is read from a mask file created by **Maskviews**

o Exposure and development

• Idealized model — photoresist lines always have vertical sidewalls, positioned directly beneath mask edges

• The **EXPOSE** statement uses the x coordinates to determine which portions of the photoresist should be marked as exposed

• The **DEVELOP** statement removes all the positive photoresist that has been marked as exposed, or all negative photoresist that has not been marked as exposed

o Simulation statement

```
GO ATHENA cutline="fname.sec" -> EXPOSE  MASK= name -> DEVELOP
```

Etching

o Goal — provide a means to generate the required structure for diffusion and oxidation, not intended to simulate a physical etching process

Dry/Isotropic & An-isotropic etch

Rate.etch/Etch commands

```
Rate.etch machine=WET oxide a.s wet.etch isotropic=1.0
Etch machine=WET time=1 seconds
```

Removal of a region to the left or right of a line

```
ETCH {LEFT|RIGHT} P1.X P1.Y P2.X P2.Y
```

Removal of arbitrary region

```
ETCH {START|CONTINUE|DONE} X Y
```

Removal of the entire structure

```
ETCH ALL
```

Models and Coefficients

o Models vs. coefficients

• *Model* — a mathematical abstraction of a physical phenomenon (e.g., diffusion equation, Deal and Grove model for oxidation, etc.)

• *Coefficients* — parameters used in a model (e.g., SSUPREM4 parameters in the input statements)

o Choosing or executing models and setting coefficients

• Choosing/executing models

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METHOD, DIFFUSION, IMPLANT, EPITAXY, DEPOSITION, EXPOSE, DEVELOP, ETCH, …

• ***Setting coefficients***

AMBIENT, MOMENT, MATERIAL, IMPURITY, REACTION, MOBILITY, INTERSTITIAL, VACANCY, ANTIMONY, ARSENIC, BORON, PHOSPHORUS, …

o **In SSUPREM4, oxidation and diffusion models are saved with a structure, but coefficients are not**

Electrical Calculation and Parameter Extraction

o **Electrical calculation**

• Calculates a limited set of electrical characteristics for the cut-line along a vertical axis of a simulation structure

• Solves 1D Poisson's equation for a series of specified bias conditions

o **Models**

• Poisson's equation (in semiconductor and insulator regions)

• Boltzmann or Fermi–Dirac statistics

• Incomplete ionization of donor and acceptor impurities

• Field, concentration, and temperature dependent mobilities with tabular form, Arora's model or Caughey's model

o **Electrical parameters**

• Threshold voltage

• Low-/high-frequency and deep-depletion MOS capacitances

• Spreading resistance profile and sheet resistances for all diffused regions

Other Relevant Statements

o **Extract** — extracts electrical characteristics by solving the 1D Poisson's equation. See manual for more detailed information. (VWF Interactive Vol1/2)

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Data Post-Processing

Select/Extract/Print.1D/Plot.1D/Plot.2D/Contour/Label/Color
Use Tonyplot

ex)

```
SELECT Z=log10(Boron)
FOREACH X (15 TO 19 STEP 1)
CONTOUR VALUE=X
END
```

SSUPREM4: Strengths and Weaknesses

- **Strengths**
  - Adaptive gridding algorithm
  - Comprehensive diffusion and oxidation models to simulate 2D effects
  - Accurate Monte Carlo and implant damage model
- **Weaknesses**
  - Lack of good calibration and optimization facilities
  - Too simplified etching, deposition, exposure and development models

“Proper” Use of Process Simulator

- **Variable–result dependency (relative accuracy)**
  - An inaccurate simulator can provide relatively accurate result in terms of variable–result dependencies
  - Vary one process parameter at a time — the difference of the results between two variable values can give some insight into the effect of that parameter — since “presumably” the errors in the simulator are all canceled out
- **Single-process simulation**
  - Investigate a single process alternatives
  - 1D SUPREM-3 may be adequate
- **New process development/prediction (absolute accuracy)**
  - Ultimate goal and the most difficult task
  - Require accurate process models (for all the steps involved)
  - Require accurate model coefficients (must be calibrated!)

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Device Simulation with ATLAS

- **Overview of device simulation**
- **Major physical models**
- **Solution specification**
- **Parameter extraction**
- **Interfacing with SSUPREM4**
- **Structure specification**
- **Boundary conditions**
- **Models and coefficients**
- **Data post-processing**
- **A tutorial example**

Structure Specification

MESH Initiates the mesh generation
X.MESH Specifies the grid lines perpendicular to the x-axis
Y.MESH Specifies the grid lines perpendicular to the y-axis
ELIMINATE Eliminates nodes along grid lines
SPREAD Adjusts the vertical position of nodes along horizontal grid lines

REGION Specifies the location of material regions
ELECTRODE Specifies the location of electrodes in the structure
PROFILE Specifies impurity profiles for the structure
REGRID Refines the simulation mesh

Grid in ATLAS/SPICES

- **Importance**
  - The correct grid allocation in device simulation has a direct influence on the simulation accuracy and time
  - Accurate representation of small device geometries and non-planar devices
- **Capabilities**
  - Supports general irregular grid structure for arbitrarily shaped devices
  - Allows the refinement of particular regions with minimum impact on others
  - Choice of Cartesian or cylindrical coordinate system

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Initial Mesh Specification

- **Two ways to specify an initial mesh**
  - Initiate the generation of a rectangular or cylindrical mesh manually (**MESH**)
  - Read a previously generated structure from a data file (**MESH IN.FILE**)
  - Whenever a **MESH** statement is encountered, MEDICI will perform an initialization that will allow a completely new simulation to be started

- **Sequence of mesh generation statements**

Manual Generation

```
MESH
X.MESH
Y.MESH
ELIMINATE
SPREAD
REGION
ELECTRODE
PROFILE
REGRID
MESH IN.FILE
ELECTRODE
PROFILE
REGRID
```

Reading from a File

```
MESH INFILE=<>
ELECTRODE
PROFILE
REGRID
```


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Mesh Refinement

- **Goal — refine parts of the mesh which satisfy some criterion**
- **Refinement criterion** — based on physically plausible heuristics, not geometrical grounds (structure independent)
  - Refine where a variable or the change in that variable exceeds a given value
  - The value to choose depends on the size of the structure and the desired accuracy
- **Regrid algorithm**
  - Search the initial grid (level-0) for triangles satisfying the refinement criterion
  - Each triangle found is subdivided into four congruent subtriangles, and the grid quantities are interpolated onto the new nodes (level-1)
  - The same procedure is applied to level-1 triangles, and any subtriangles become level-2 triangles
  - Refinement is continued until no triangles satisfy the criterion, or until a specified maximum level is reached

Interpolation in Mesh Refinement

- **The problem**
  - If several levels of regrid are performed in immediate succession, the refinement decisions at higher levels are made using interpolated data, which may be inaccurate due to the nonlinearity of semiconductor problems
- **Recommendation**
  - • Regrid one level at a time, re-reading the doping statements and performing a new solution between levels

Other Structure-Related Statements

- **Material type of a mesh region**
  - `REGION NAME X Y X.MIN X.MAX Y.MIN Y.MAX …`
- **Impurity profiles**
  - `DOPING N.TYPE P.TYPE REGION {UNIFORM|DOSE|X.ERFC} + { ATHENA} IN.FILE …`
- **Electrode definition and modification**
  - `ELECTRODE NAME REGION {X|Y} + {TOP|BOTTOM|LEFT|RIGHT|INTERFAC|PERIMETE} …`

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Major Physical Models

- **Basic semiconductor equation**
  - Poisson's equation
  - Continuity equations
  - Drift-diffusion equations
- **Recombination models**
  - SRH, Auger, direct, and surface recombinations
  - Concentration-dependent lifetimes
- **Semiconductor statistics**
  - Boltzmann and Fermi–Dirac statistics
  - Incomplete ionization of impurities
- **Mobility models**
  - Low-field and high-field mobilities
  - Surface scattering and electron–hole scattering

Mobility Models

- **Low-field mobilities**
  - Constant mobility
  - Concentration dependent mobility(**CONMOB**)
  - Analytic mobility (**ANALYTIC**)
  - Arora mobility (**ARORA**)
  - Carrier–carrier scattering mobility(**CCSMOB**)
  - Klassen unified mobility (**KLA**)
- **High-field mobilities**
  - Parallel field-dependent mobility/Caughey and Thomas model - FLDMOB

- **Inversion layer mobility**
  - Lombardi **CVT**
  - **Yamaguchi**
  - **Tasch**
  - Surface degradation model **- SURFMOB**
  - Transverse electric field model **- SHIRIHARA**

*** Velocity saturation model – EVSATMOD=0/1/2**
*** All are lattice temperature dependent models. Default=300K,**
m=m(*T,n,p,E,N,…*)

Lattice temperature(TL): **thermcontact …models lat.temp**
Energy-Balance Eqs.(Tn, Tp): **models hcte (or hcte.el/hcte.ho)**

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Model Selection — Recommendations

- **For MOS I–V characteristics**
  - Use 1 carrier and:
  - **ANALYTIC, FLDMOB, CONSRH, CVT**
- **For bipolar I–V characteristics**
  - Use 2 carriers and:
  - **FLDMOB; CONSRH, AUGER, BGN**
- **For breakdown or SOI simulations**
  - Use 2 carriers and:
  - **FLDMOB; CONSRH, AUGER, BGN, IMPACT**

Advanced Specific Modules

- **Lattice Temperature(Giga)** — Spatial-dependent heat equation
- **Trapped Charge & Defects (TFT)**
- **Programmable Device (EEPROM)** — FN tunneling & hot-carrier injection
- **Heterojunction Device (Blaze)** — Composition-dependent band & material
- **Optical Device (Luminous)** — Photogeneration & absorption
- **Circuit Analysis (MixedMode)** — Spice-like numerical-device circuit analysis
- **Anisotropic Material (SiC)** — Tensor dielectric constant & mobility

Boundary Conditions

- **Ohmic contacts** (Dirichlet B.C.'s) — (ψ_s, n_s, p_s) fixed, $\phi_n = \phi_p = V_{applied}$
- **Schottky contacts** — finite surface recombination velocity
- **Insulator contacts** — $n_s = p_s = 0$
- **Neumann boundaries** — homogeneous (reflecting) B.C.'s
- **Current boundary conditions**
  - The terminal current of an SCR-type structure is a multi-valued function of V_A
  - Alternative: consider voltage as a single-valued function of the terminal current
  - Current boundary condition: **CONTACT CURRENT**
- **Lumped R, L, C and distributed contact resistance**
  - **CONTACT RESISTAN CAPACITA INDUCTAN**
  - **CONTACT CON.REST**

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Solution Specification

- **Numerical methods**
  - Discretization
  - Gummel's method (decoupled)
  - Newton's method (coupled) :

$$F(\psi, n, p, T_L, T_n, T_p) = 0$$

- **Electrical analyses**
  - DC analysis
  - Transient analysis/FFT
  - Small-signal analysis
  - Impact ionization analysis
  - Gate current analysis
  -

Solution Methods

- **Importance**
  - Nonlinear iteration starting from some initial guess
  - Use the "numerical engine" efficiently (convergence)
- **Choice of methods**
  - No single method is optimal in all cases
  - At zero bias, a Poisson solution alone is sufficient
  - For MOSFETs, only one carrier need be solved for
  - In bipolar devices, both carriers are needed, and depends on the operating conditions
  - Tradeoff between stability and speed of the method

Convergence Problems

- **Common convergence problems**
- Bias steps too large; poor initial guess
- Depletion layer reaches structure edge
- Currents too low (< 1 nA/μm) under current boundary conditions
- *dI/dV* changes sign; switch boundary conditions (use automatic continuation!)
- Floating region with zero carrier — can't be solved
- Two or more adjacent floating regions — can't be solved
- **SPICES control**
- If SPICES cannot converge in **ITLIMIT** = 20 iterations, the voltage or current step will be halved

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Solution Specification Statements

- **Statements**

• **MODELS** — enables the use of physical models during solutions
• **METHOD** — sets parameters associated with solution algorithm
• **SOLVE** — generates solutions for specific biases

- **Notes**

• It is unnecessary to specify models when continuing the simulation from a saved file
• A symbolic factorization (**SYMBOLIC**) should be performed before the next **SOLVE** statement whenever the solution technique is changed, or the mesh has been refined (**REGRID**)
• The Newton's method must be used when performing a transient analysis

Initial Guess

- **SOLVE {INITIAL|PREVIOUS|PROJECT|LOCAL|P.LOCAL} + {V|I|T|Q} …**
- **Using charge-neutral assumption** (**INITIAL**)

• Obtain the first (equilibrium) bias point when no solution is available (default)

- **Using the previous solution** (**PREVIOUS**)

• The previous solution is modified by setting the applied bias at the contacts

- **Using a projection of two previous solutions** (**PROJECT**)

• The default when two previous solutions are available

- **Using the local quasi-Fermi potentials** (**LOCAL**)

• Sets the majority carrier quasi-Fermi potentials to the applied bias in the contact regions
Using the local quasi-Fermi potentials in heavily-doped regions

DC Analysis

- `SOLVE name=ELECTROD {VSTEP|ISTEP} NSTEPS …`
- **Example**

```
solve vgate=0 vsource=0 vdrainv=0
$ Bias up the gate
solve name=gate vgate=0 VSTEP=0.1 vfinal=3 outfile=sol_0
$ Drain curves
load infile="sol_0”
solve name=drain VSTEP=0.5 vfinal=5
load infile="sol_1”
solve name=drain VSTEP=0.5 vfinal=5
…
```


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Transient Analysis

ø **SOLVE {TSTEP TSTOP|NSTEPS} {RAMPTIME|ENDRAMP}** …

q **Numerical schemes**

• Time-dependent discretization of the Poisson and continuity equations

• Variable-order method (1st and 2nd order backward Euler) based on the local truncation error (LTE)

q **Time step control**

• Automatic time step selection — selects time steps so that the LTE matches the user-specified criteria (**METHOD TOL.TIME**)

• The time step size is allowed to increase at most by a factor of two

• If the new time step is less than one half of the previous step, the previous time step is re-calculated

• If a time point fails to converge, the time step is halved and the point is recalculated

Small-Signal Analysis

ø **SOLVE AC.ANALYSIS FREQUENCY FSTEP NFSTEP VSS TERMINAL +** …

q **Numerical method** — sinusoidal steady-state analysis

• Starting from a DC bias condition, a sinusoidal input of given amplitude (VSS) and frequency (**FREQ**) is applied to the device from which sinusoidal terminal currents and voltages are calculated

• The frequency-dependent admittance matrix is then calculated using

q **Capabilities**

• Cutoff frequency f_T

• S-parameters

Impact Ionization Analysis

o **Post-processing analysis:** **impact selb[or crowell]**

• The generation rate and the impact ionization current are calculated after each solution based on the electric field and current densities

• The generated carriers are not included in the solution

• Useful for calculating MOS substrate current or estimating long-term device degradation

q **Self-consistent calculation:** **MODELS IMPACT**

• The generated carriers are implicitly included in each solution

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• Useful for avalanche-induced breakdown or impact ionization-induced latchup

Usage : models…impact / impact selb

Gate Current Analysis

q **Post-processing capability** — the gate current is calculated for each bias or time point from electric field and current density after obtaining a solution

q **Models**

• **Lucky-electron model** (**HEI/HHI**) — calculates probabilities for certain scattering events to occur that will result in current being injected into the gate

• **Angle-dependent model** — based on the integral equation of the generation function derived from the Maxwell or Monte Carlo (non-Maxwellian) distribution

• **Carrier temperature-dependent model** — when energy balance model is used, the generation function can be calculated using an electron energy dependent model

Models and Coefficients

q **Models (physical and numerical)**

• **MODELS** {recombination, mobility, bandgap narrowing, tunneling, ionization, gate current, energy balance, …}

• **TRAPS** {energy level, lifetimes, trap charges, …}

• **PHOTOGEN** {injection spot, carrier type, spatial term, temporal term, …}

• **METHOD** {error tolerance, Gummel's parameters, Newton's parameters, energy balance parameters, …}

• **SYMBOLIC** {Gummel | Newton, carriers, …}

• **SOLVE** {initial guess, DC | AC | transient | continuation, …}

q **Coefficients**

• **MATERIAL** — associates physical parameters with the materials in the device

• **MOBILITY** — modifies parameters associated with the mobility models

• **CONTACT** — defines the physical parameters associated with an electrode

• **INTERFACE** — specifies interface parameters at any interface

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Regional Specification of Semiconductor Parameters

q **SPICES allows different semiconductor material parameters to be specified for different regions for structures that**
- contain more than one material
- have semiconductor properties which vary with position

q **Statements**
- `MATERIAL REGION=< n>` …
- `MOBILITY REGION=< n>` …

q **Example**
- Specify lower carrier ionization rates in the surface region than those used in the bulk region

Parameter Extraction

ø `EXTRACT` — extracts selected data for the solution over a specified cross section of the device

q **Extraction using names and expressions**
- w `EXTRACT name="idvg" curve(v."gate", i."drain")…`

q **Optimization using targets and expressions**
- w `EXTRACT ….-> see deckbuild's optimizer menu`

q **Extract physical quantities from solution**
- w `EXTRACT/PROBE ß from log file`
- w `OUTPUT wirte to solution outfile -> *.str`
- w `OUTPUT must be wriiten before SOLVE statement`

q **Extract MOS device parameters**
- `EXTRACT name="nvt" expr.`

`< see VWF Interfactive Volume 1. for Extract`

Simulation results and output expression

q **Output command : output e.field potential flowlines val.band con.band \ band.param à apply to structure file *.str**

q **Probe command: probe x=<> y=<> field n.mob… à apply to log file**

q **Measure command: not recommended. Use extract, output and probe instead**

Tonyplot has all of extraction features described above.

`< Extract/output/probe/*.str/*.log`

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Input and Output

q **Saving I–V and AC terminal data**

LOG OUTFILE=<>…

q **Saving solutions, structure, model and coefficients**

SAVE OUTFILE … master -à ascii

Solve outfile=sol_0 à bianry

q **Loading/saving solutions for continued simulations or post processing**

LOAD INFILE=<>

Interfacing with ATHENA/SSUPREM4

q **Significance**

• Meaningful device design and optimization based on real fabrication process

• Realistic device structure and impurity profiles

q **Key steps**

• Use mask information from MASKVIEWS

• Use the adaptive gridding in SSUPREM4 (automatic)

• Use the regrid facility in ATLAS/SPICES

• Require well calibrated process models and parameters

• Calibrate independently key device model parameters in ATLAS

q **Interface**

• In SSUPREM4: **STRUCTURE OUTFILE=mesh.str**

In ATLAS: **MESH INFILE=mesh.str**

Ex)

```
go athena ( or cutlines=2d_cut.str ß 2d mask from maskviews cutline)
line x …
line y …

deposit…
Implant…
Diffuse…
etch..
electrode…
structure outf=nmos.str
go atlas
mesh inf=nmos.str
```


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Discrepancies Between Simulation and Measurement

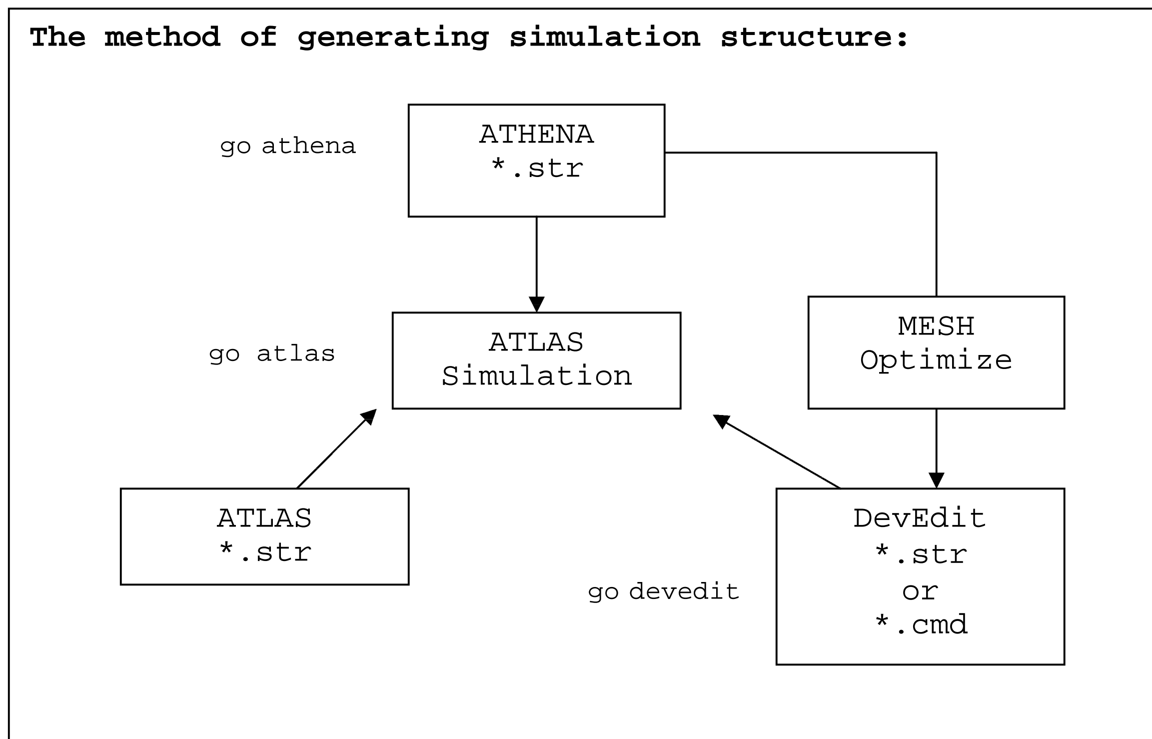
- **Simulation may be right, measurement may be "wrong"**
- **Device simulator unlikely produces incorrect results on correct structure**

ü First thing to check

- Accuracy of the doping profile: junction depths, peak concentrations, etc.
- Accuracy of the structure: gate oxide thickness, etc.

ü Other possibilities

- Inadequate grid (need to have vertical grid spacing in the channel of 15–25Å)
- Incorrect or incomplete specification of mobility and other physical models
- Incorrect workfunction (recommended value of 4.35 eV for n+ poly gates)
- Forgetting to specify fixed oxide charge (use values extracted from C–V)
- Forgetting to specify accurate lifetimes (use values measured on wafers)
- Is lattice heating important? (use GIGA) Does traps exist? (use TFT)
- Is your measured device typical when compared to others on the same lot



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