# Introduction to Process and Device Simulations with TSUPREM-4 and MEDICI

Dr. Zhou Xing and Mr. Low Wee Khng

February 5-7 and 12-14, 1996

# <u>Agenda</u>

DAY 1
A.M. Session (9:00 am—12:00 pm; break: 10:30—10:50 am)
Overview of Process and Device Simulation
Introduction to TMA TCAD Tools
P.M. Session (1:30—4:30 pm; break: 3:00—3:20 pm)
STUDIO Hands-On: Building an Input Deck
DAY 2
A.M. Session (9:00 am—12:00 pm; break: 10:30—10:50 am)
Process Simulation with TSUPREM-4
P.M. Session (1:30—4:30 pm; break: 3:00—3:20 pm)
TSUPREM-4 Hands-On
DAY 3
A.M. Session (9:00 am—12:00 pm; break: 10:30—10:50 am)
Device Simulation with MEDICI
P.M. Session (1:30—4:30 pm; break: 3:00—3:20 pm)
MEDICI Hands-On

# General Tips on Using CAD 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?
- $\hfill\square$  Device physics and modeling Will the device physics at 0.1  $\mu m$  still work?
- Processing technology
  - More complex/expensive processes and equipment, multilayer interconnect

### Lithography

• Electron, X-ray, and ion based techniques (0.1  $\mu$ m resolution)

#### □ 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

# **TSUPREM-4: 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

# **TSUPREM-4: 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.;

#### **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; ...

# **TSUPREM-4:** Input/Output

- □ Input A series of statements
  - Grid generation
  - Mask definition
  - Structure initialization
  - Process step specification
  - Output control
- Dutput 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 WorkBench, MEDICI/DAVINCI, LORENZO, MICHELANGELO

## **MEDICI: Simulation Capabilities**

- Electrical characteristics of arbitrary 2D structures under userspecified 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) as well as arbitrary use-defined materials
- □ Automatic regridding and I–V curve tracing
- **D** Parameter extraction ( $V_T$ ,  $I_{dsat}$ ,  $\beta$ ,  $f_t$ ,  $R_{SH}$ , ...)
- **Optimization for tuning device performance and model calibration**

# **MEDICI: Physical Models**

#### **D** 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 (CA, LT, TC, PD, HD, OD, AM) (sold separately :-)

# **MEDICI: 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
- Dutput 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 WorkBench, TSUPREM-3, TSUPREM-4, AURORA, DEPICT, MICHELANGELO

# **AURORA: 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

### Models

- MOS2, MOS3, BSIM2, BSIM3, Gummel–Poon, junction capacitance model, JFET model, diode model, user-defined model
- Up to 50 independent variables, 50 dependent variables, 500 fitting parameters
- Up to 60 parameters may be fit simultaneously
- □ Circuit simulator interface
  - HSPICE, PSpice, Spectre, Saber

# TMA WorkBench: 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 but <u>not automatic</u>! need your intelligent use of the embedded tools and the models

# Other TMA TCAD Tools

- □ STUDIO graphical TCAD environment
- □ MICHELANGELO structure editor and visualizer
- □ LORENZO layout interface
- □ TSUPREM-3 1D process simulation
- □ DAVINCI 3D device simulation
- **TERRAIN** 2D deposition and etch simulation
  - Use physically-based deposition/etch models for arbitrarily shaped structures
- □ DEPICT 2D photolithography (imaging, exposure and development)
  - Simulate photolithographic processes and aerial images affecting topography
- □ RAPHAEL 2D/3D interconnect analysis

- Simulate parasitics of interconnnect and 3D cell using field solver and RLC
- □ LIQUID liquid crystal display analysis
  - Physically-based electro-optical analysis of AMLCD's and TFT's

# Simulator Calibration

#### **D** Paramount importance

- Obtain meaningful simulation results related to your real process
- Provide <u>reliable</u> 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 TSUPREM-4**

- □ 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

# Grid in TSUPREM-4

#### □ 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}

# **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 ( $< n_i$ )
    - 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<sub>m</sub>* and *D<sub>n</sub>*) 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 enhancement factors *M/M* and *N/N* 
  - METHOD PD.FERMI M/M' = N/N' = 1 (no OED)
  - METHOD **^PAIR.SAT ^PAIR.REC** equilibrium concentrations

• METHOD {PD.TRANS | PD.FULL} — full equations

# **Choosing a Diffusion Model**

- METHOD {PD.FERMI | PD.TRANS | PD.FULL}
- Given that the special of the specia
  - 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  $\mu$ m), 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 (**AMBIENT STRESS.D**)

## **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
- □ 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 nonsemiconductor materials
- Point defects can participate in reactions at interfaces with silicon (suggested model: PD.FERMI)

### **Diffusion Simulation — Basic Statements**

DIFFUSION TIME TEMP PRES [IMPURITY I.CONC] {Ambient}

□ Temperature ramp

$$T_{C} = \begin{cases} \texttt{TEMP} + \texttt{T.RATE} \times t \\ \texttt{TEMP} + \frac{\texttt{T.FINAL} - \texttt{TEMP}}{\texttt{TIME}} t \end{cases}$$

□ Pressure ramp

$$P = \begin{cases} PRESSURE + P.RATE \times t \\ PRESSURE + \frac{P.FINAL - PRESSURE}{TIME} t \end{cases}$$

□ Ambient

- Specify a previously defined ambient with one of the parameters DRYO2, WETO2, STEAM, INERT, AMB.1, AMB.2, AMB.3, AMB.4, Or AMB.5
- 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

## **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

# lon 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

# 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

#### □ lon 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

#### □ 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

#### **U** When used with the analytic models

- **PD.TRANS** 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 **PD.FULL** diffusion model. Very small time steps are required in the initial stages of follow-up diffusion

#### **U** 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 IMPL.TAB MOMENTS | MONTECAR N.ION} +
CRYSTAL DAMAGE

- Gaussian model useful as a rough estimate only
- Dearson 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

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

#### **D** Relevant statements

MOMENT MATERIAL RANGE SIGMA GAMMA KURTOSIS

# <u>Epitaxy</u>

#### □ 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

#### □ Simulation statement

EPITAXY TIME TEMP THICKNESS IMPURITY

$$T_{C} = \begin{cases} \texttt{TEMP} + \texttt{T.RATE} \times t \\ \texttt{TEMP} + \frac{\texttt{T.FINAL} - \texttt{TEMP}}{\texttt{TIME}} t \end{cases}$$

□ EPITAXY is equivalent to DEPOSITION + DIFFUSION

# **Deposition**

#### □ 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

#### □ Capabilities

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

#### □ Simulation statement

DEPOSITION THICKNESS MATERIAL IMPURITY

#### 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<sub>2</sub> is inserted)

# Masking, Exposure and Development of Photoresist

#### □ Masking

- Masking information is read from a mask file created by LORENZO
- For each mask level, the starting and ending *z* coordinates of each opaque region are recorded

#### **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
- □ Simulation statement

```
MASK IN.FILE=fname \rightarrow EXPOSE MASK=name \rightarrow DEVELOP
```

# <u>Etching</u>

- □ Goal provide a means to generate the required structure for diffusion and oxidation, not intended to simulate a physical etching process
- □ Model and capabilities
  - *Trapezoidal etch model* dry etching with masked undercutting and angled sidewalls

ETCH TRAPEZOI THICKNESS ANGLE UNDERCUT

• 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**

#### □ 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., TSUPREM-4 parameters in the input statements)

- □ Choosing or executing models and setting coefficients
  - Choosing/executing models

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

• Setting coefficients

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

□ In TSUPREM-4, oxidation and diffusion models are saved with a structure, but coefficients are not

## **Electrical Calculation and Parameter Extraction**

#### □ 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

#### 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

#### **D** 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**

□ **ELECTRICAL** — extracts electrical characteristics by solving the 1D Poisson's equation

ELECTRICAL X V(start,stop,step) SRP RESISTAN JCAP + MOSCAP THRESHOL OUT.FILE ...

□ **MOBILITY** — defines or modifies the dependence of carrier mobility on impurity concentration and temperature

MOBILITY TAB.TEMP TAB.CONC TAB.E.MU TAB.H.MU ...

□ **MATERIAL** — sets carrier statistics and selects models and parameters

MATERIAL BOLTZMAN IONIZATI BANDGAP WORKFUNC AFFINITY

□ METHOD — selects mobility models

METHOD {MOB.TABL | MOB.AROR | MOB.CAUG}

### **Data Post-Processing**

#### **Quantity evaluation and extraction**

- **SELECT** evaluates the quantity to be printed or plotted
- **EXTRACT** extracts information about a structure

#### □ Print and plot

- **PRINT.1D** prints values of a quantity along a line through the structure
- **PLOT.1D** plots a quantity along a line through the structure
- PLOT.2D plots axes, boundaries, grids, etc. for 2D structure
- **PLOT.3D** plots a "bird's eye view" of the selected quantity
- CONTOUR plots contours in 2D

#### □ Others

- LABEL adds labels to a plot
- COLOR fills areas of a 2D plot
- **VIEWPORT** specifies a subset of the plotting surface to plot on

## Selecting a Quantity to be Printed/Plotted

- SELECT Z=<expression> TEMP LABEL TITLE
- □ The Z parameter specifies a mathematical expression for the quantity to be printed/plotted

#### □ Built-in quantities

antimony, arsenic, boron, phosphorus, doping, oxygen, interstitial, vacancy, ci.star, cv.star, trap, dloop, rloop, electron, x.v, y.v, Sxx, Sxy, Syy, x, y

#### □ Built-in functions

active, abs, diffusivity, erf, erfc, exp, log, log10, slog10, sqrt

#### □ Operators

+, -, \*, /, ^

## **Printing and Plotting 1D Information**

- PRINT.1D {X.VAL | Y.VAL} MATERIAL SPOT LAYERS ...
- PLOT.1D {X.VAL | Y.VAL} MATERIAL BOUNDARY ELECTRIC + IN.FILE ...

#### □ Print information

- A complete list of the values of the Z expression along the section
- The integral of the values of the Z expression through each layer along the section (LAYERS)
- The location along the section where the Z expression has a specified value (SPOT)

#### Plot information

- Values of a quantity along a 1D section (vertical or horizontal line, or an interface between two materials) through the device
- Parameters calculated by the **ELECTRICAL** statement
- Graphic device specified by "OPTION DEVICE"

### **Plotting 2D/3D Information**

- PLOT.2D X.MIN X.MAX Y.MIN Y.MAX BOUNDARY GRID FLOW ...
- PLOT.3D THETA PHI X.MIN X.MAX Y.MIN Y.MAX Z.MIN Z.MAX + BOUNDARY ...
- CONTOUR VALUE

#### Notes

- The plotted quantity is defined by the "SELECT Z" statement
- Values of contours of *log10*(concentration) should be specified as exponent:

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

END

### **TSUPREM-4: Strengths and Weaknesses**

#### □ Strengths

- Adaptive gridding algorithm
- Comprehensive diffusion and oxidation models to simulate 2D effects
- Accurate Monte Carlo and implant damage model
- Interface with device (MEDICI), layout (LORENZO), and TMA WorkBench

#### Weaknesses

- · Lack of good calibration and optimization facilities
- Too simplified etching, deposition, exposure and development models

□ Need a 3D process simulator to work with 3D device simulator DAVINCI for deep submicron process development

# **"Proper" Use of Process Simulator**

- □ Variable–result dependency (relative accuracy)
  - An inaccurate simulator *can* provide <u>relatively</u> accurate result in terms of variable–result dependencies
  - Vary <u>one</u> process parameter at a time the <u>difference</u> 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 TSUPREM-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!)

### **Device Simulation with MEDICI**

- □ Overview of device simulation
- □ Structure specification
- □ Major physical models
- □ Boundary conditions
- □ Solution specification

- □ Models and coefficients
- □ Parameter extraction
- □ Data post-processing
- □ Interfacing with TSUPREM-4
- □ 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
BOUNDARY	Modifies a mesh to conform to boundary interfaces read from a file

REGION	Specifies the location of material regions
ELECTRODE	Specifies the location of electrodes in the structure
RENAME	Changes the name of an electrode or region
PROFILE	Specifies impurity profiles for the structure
REGRID	Refines the simulation mesh

# Grid in MEDICI

#### □ 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

# **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 Reading from a File MESH MESH IN.FILE ELECTRODE X.MESH Y.MESH PROFILE ELIMINATE REGRID SPREAD BOUNDARY REGION ELECTRODE PROFILE REGRID

### 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**

#### □ Boundary conformation

- BOUNDARY IN.FILE TSUPREM4 ...
- □ Material type of a mesh region
  - REGION NAME X Y X.MIN X.MAX Y.MIN Y.MAX ...
- □ Impurity profiles
  - PROFILE N-TYPE P-TYPE REGION {UNIFORM | DOSE | X.ERFC} + {1D.PROC | 2D.PROC | TSUPREM4} IN.FILE ...

#### **Electrode definition and modification**

- ELECTRODE NAME REGION {X | Y} + {TOP|BOTTOM|LEFT|RIGHT|INTERFAC|PERIMETE} ...
- RENAME {ELECTRO | REGION } OLDNAME NEWNAME ...

# 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 (СОММОВ)
- Analytic mobility (ANALYTIC)
- Arora mobility (ARORA)
- Carrier–carrier scattering mobility (ССЅМОВ)
- Philips unified mobility (PHUMOB)

### Surface scattering

- Surface mobility (SRFMOB)
- Enhanced surface mobility (SRFMOB2)

#### High-field mobilities

- Parallel field-dependent mobility (FLDMOB)
- Caughey–Thomas mobility (FLDMOB=1)
- Gallium Arsenide-like mobility (FLDMOB=2)
- Hewlett-Parkard mobility (нрмов)
- Perpendicular field-dependent mobility (ркрмов)
- Lombardi surface mobility (LSMMOB)

# <u>Model Selection — Recommendations</u>

### □ For MOS I–V characteristics

• Use 1 carrier and:

- ANALYTIC, FLDMOB, PRPMOB; CONSRH
- □ For bipolar I–V characteristics
  - Use 2 carriers and:
  - PHUMOB, FLDMOB; CONSRH, AUGER, BGN
- □ For breakdown or SOI simulations
  - Use 2 carriers and:
  - PHUMOB, FLDMOB, PRPMOB; CONSRH, AUGER, BGN, IMPACT.I

# Advanced Application Modules (AAM's)

- □ Lattice Temperature (LT-AAM) Spatial-dependent heat equation
- □ Trapped Charge (TC-AAM) Time- and energy-dependent trapped charge
- **Programmable Device (PD-AAM)** FN tunneling & hot-carrier injection
- □ Heterojunction Device (HD-AAM) Composition-dependent band & material
- **Optical Device (OD-AAM)** Photogeneration & absorption
- **Circuit Analysis (CA-AAM)** Spice-like numerical-device circuit analysis
- □ Anisotropic Material (AM-AAM) Tensor dielectric constant & mobility

### **Boundary Conditions**

- **Ohmic contacts** (Dirichlet B.C.'s)  $(\psi_s, n_s, p_s)$  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
- □ Majority carrier contact
  - For simulating 1D BJT base contact
  - Injecting a majority carrier current at the contact

• ELECTRODE MAJORITY

## Solution Specification

#### □ Numerical methods

- Discretization
- Gummel's method (decoupled)
- Newton's method (coupled)
- Continuation method

#### □ Electrical analyses

- DC analysis
- Transient analysis
- 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</li>
- *dl/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

#### MEDICI control

- If MEDICI cannot converge in **ITLIMIT** = 20 iterations, the voltage or current step will be halved
- After **STACK** = 4 failed solutions, program will terminate

# Solution Specification Statements

#### □ Statements

- MODELS enables the use of physical models during solutions
- **METHOD** sets parameters associated with solution algorithm
- **SYMBOLIC** performs a symbolic factorization
- **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, while the previous solution elsewhere (P.LOCAL)

# **DC** Analysis

SOLVE ELECTROD {VSTEP | ISTEP } NSTEPS SAVE.BIA ...

```
□ Example
```

```
SOLVE V(gate)=0 V(source)=0 V(drain)=0
$ Bias up the gate
SOLVE ELECTROD=gate VSTEP=0.1 NSTEP=10 OUT.FILE=SOL01
$ Drain curves
LOOP STEPS=10
ASSIGN NAME=SFX C.VAL=01 DELTA=1
LOAD IN.FILE="SOL"@SFX
SOLVE ELECTROD=drain VSTEP=0.5 NSTEP=20
L.END
```

# **Transient Analysis**

● SOLVE {TSTEP TSTOP | NSTEPS} {RAMPTIME | ENDRAMP} ...

- □ 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)
- □ 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

- SOLVE AC.ANALY FREQUENCY FSTEP NFSTEP VSS TERMINAL + HI.FREQ ...
- □ **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

#### Capabilities

- Cutoff frequency f<sub>T</sub>
- S-parameters

# **Impact Ionization Analysis**

#### □ Post-processing analysis: SOLVE IMPACT.I

- 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
- □ Self-consistent calculation: MODELS IMPACT.I
  - The generated carriers are implicitly included in each solution
  - Useful for avalanche-induced breakdown or impact ionization-induced latchup

# Gate Current Analysis

- SOLVE GATE.CUR
- MODELS {GATE1|GATE2|GATE.TEM}
- □ **Post-processing capability** the gate current is calculated for each bias or time point from electric field and current density after obtaining a solution
- □ Models
  - Lucky-electron model (GATE1, default) calculates probabilities for certain scattering events to occur that will result in current being injected into the gate
  - Angle-dependent model (GATE2) based on the integral equation of the generation function derived from the Maxwell or Monte Carlo (non-Maxwellian) distribution
  - Carrier temperature-dependent model (GATE.TEM) when energy balance model is used, the generation function can be calculated using an electron energy dependent model

### **Models and Coefficients**

#### □ 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, ...}
- □ 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

### **Regional Specification of Semiconductor Parameters**

- MEDICI 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
- □ Statements
  - MATERIAL REGION=<n> ...
  - MOBILITY REGION=<n> ...
- □ Example
  - Specify lower carrier ionization rates in the surface region than those used in the bulk region

### Parameter Extraction

- EXTRACT extracts selected data for the solution over a specified cross section of the device
- **L** Extraction using names and expressions
  - EXTRACT EXPRESSI NAME UNITS CONDITIO INITAL.V ...
- □ Optimization using targets and expressions
  - EXTRACT TARGET WEIGHT MIN.REL MIN.ABS ...
- □ Extract physical quantities from solution
  - EXTRACT {NET.CHAR | NET.CARR | ELECTRON | HOLE | RECOMBIN | + IONIZATI | RESISTAN | N.RESIST | P.RESIST | METAL.CH | + N.CURREN | P.CURREN | II.GENER | SHEET.RE }
- □ Extract MOS device parameters
  - EXTRACT MOS.PARA DRAIN GATE IN.FILE I.DRAIN

### **Data Post-Processing**

#### Print

- **PRINT** prints specific quantities at points within a defined area
- Plot
  - **PLOT.1D** plots a specific quantity along a line segment through the device
  - PLOT.2D plots 2D characteristics, boundaries, junctions, depletion edges
  - **PLOT.3D** plots 3D physical quantities
  - 3D.SURFACE plots the projection of a 3D view of the specified data
  - CONTOUR plots contours of a physical quantity on a 2D area
  - **VECTOR** plots vector quantities over an area
  - E.LINE plots potential gradient paths and calculates ionization integrals

#### □ Others

- FILL fills material regions with specified colors
- LABEL plots character strings, symbols, and lines as part of a 1D/2D plot

### **Plot Quantities**

#### □ Structural

• BOUNDARY, JUNCTION, DEPLETIO, GRID

#### Physical

- Potential and energy levels (POTENTIA, QFN, QFP, VALENC.B, CONDUC.B, VACUUM)
- Charges (DOPING, ELECTRON, HOLES, NIE, NET.CHAR, NET.CARR)
- Currents (J.CONDUC, J.ELECTR, J.HOLE, J.DISPLA, J.TOTAL)
- Recombination and generation (**RECOMBIN**, **II.GENER**, **BB.GENER**)
- Carrier temperature and velocity (ELE.TEMP, HOL.TEMP, ELE.VEL, HOL.VEL)

### **Input and Output**

Saving I–V and AC terminal data

LOG OUT.FILE TIF AURORA ICCAP ...

□ Saving solutions, structure, model and coefficients

SAVE OUT.FILE SOLUTION MESH W.MODELS TIF ALL ...

□ Loading/saving solutions for continued simulations or post processing LOAD IN.FILE IN.PREV ASCII.IN OUT.FILE ...

#### **Data stored in a solution file**

- Potential and carrier concentrations at each node
- Information describing the setup used to obtain the solution (e.g., physical parameters, boundary conditions, physical model selection)

# □ When a solution is LOADed, the setup information will be used by default for all subsequent solutions unless modified

### **Documentation and Control**

#### □ Assigned variable

ASSIGN NAME {N.VAL DELTA C.VAL DELTA L.VAL}

□ Looping

```
LOOP STEPS {OPTIMIZE | SENSITIV}
```

L.MODIFY LEVEL STEPS {NEXT | BREAK }

L.END BREAK ALL

Conditional

```
IF COND=expression
```

ELSE COND=expression

IF.END

□ Statement inclusion

CALL FILE=fname

### Interfacing with TSUPREM-4

#### □ Significance

- Meaningful device design and optimization based on real fabrication process
- · Realistic device structure and impurity profiles

#### □ Key steps

- Use mask information from LORENZO
- Use the adaptive gridding in TSUPREM-4 (automatic)
- Use the regrid facility in MEDICI
- Require well calibrated process models and parameters
- Calibrate independently key device model parameters in MEDICI

#### □ Interface

• In TSUPREM-4: SAVEFILE <u>MEDICI</u> OUT.FILE=mesh.ts4 In MEDICI: <u>MESH TSUPREM4</u> IN.FILE=mesh.ts4

# **Discrepancies Between Simulation and Measurement**

- Simulation may be right, measurement may be "wrong"
- Device simulator unlikely produces incorrect results on correct structure
- □ First thing to check
  - Accuracy of the doping profile: junction depths, peak concentrations, etc.
  - Accuracy of the structure: gate oxide thickness, etc.
- □ 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 LT-AAM) Does traps exist? (use TC-AAM)
  - Is your measured device typical when compared to others on the same lot