The Essence of Process Simulation

***Semiconductors*: *How "semi" it is conducting the current*?**

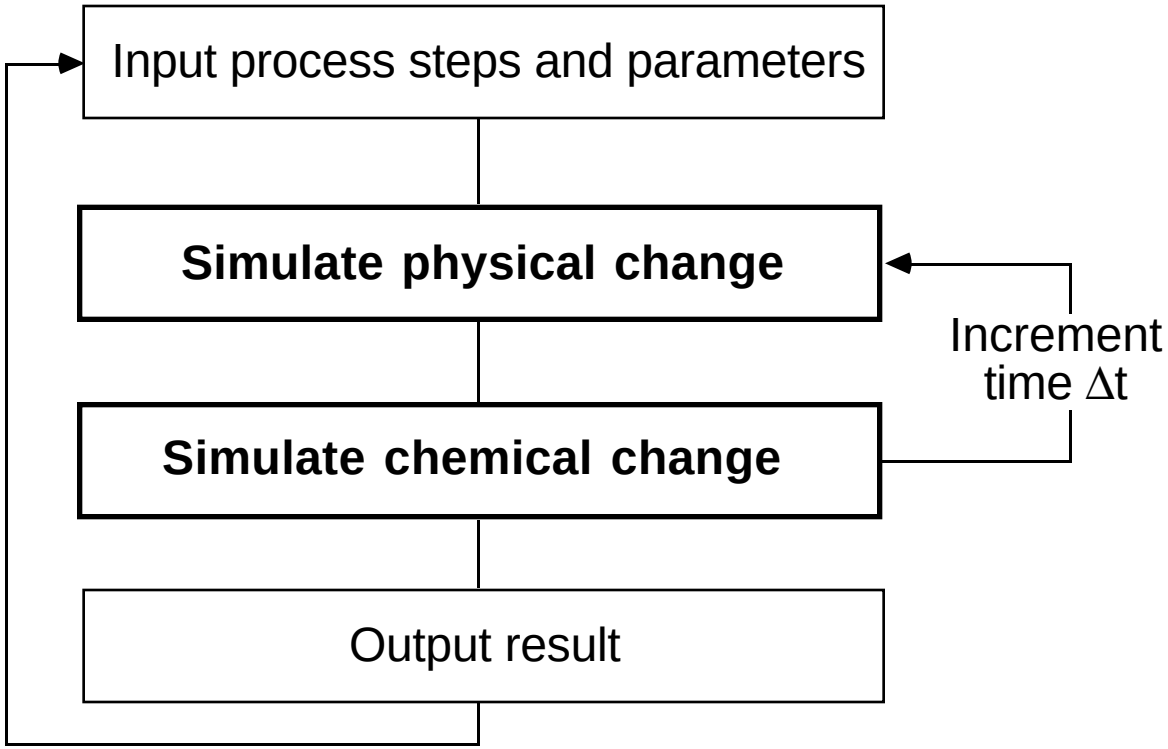
- **'Semi'-'conductor':** { **not a conductor** / **nor an insulator**

- **The fundamental principle** — the ability to incorporate impurities in a semiconductor to control its electrical conductance

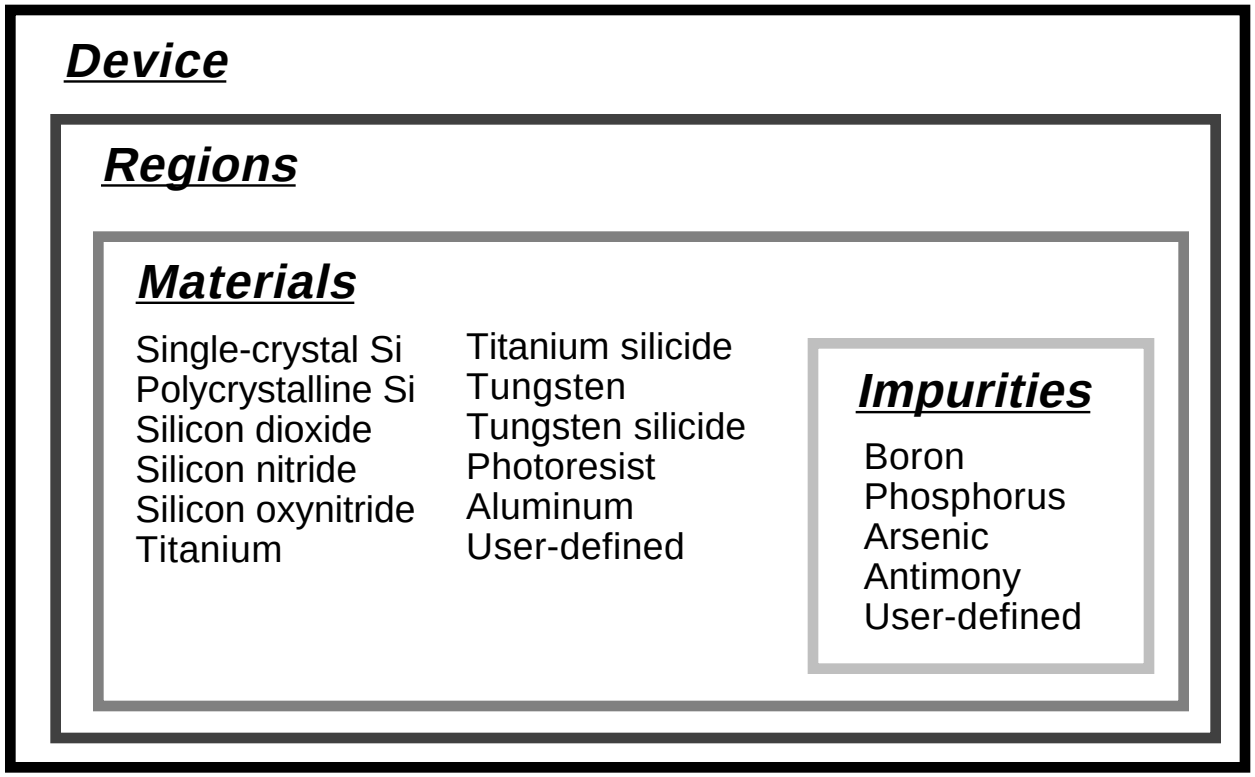
- **Major process variables and targets**
  - ***Variables***: temperature and time for diffusion and oxidation, energy and dose for ion implantation, …
  - ***Targets***: layer thickness, junction depth, threshold voltage, …

- **Question:** How to relate the process variables to the device/electrical parameters? (*Major goal of process simulation*)

Schematic Representation of Process Simulation



The Simulated Structure



TMA Command Language

- **TMA Command Language (TCL)** — the language used by TMA simulators

  COMMAND + PARAMETERS

- **Commands**
  - ***Declaration***: set parameters
  - ***Execution***: perform simulation process
- **Parameters**
  - ***Numerical***: **`Param`** = <value> (e.g., **`TEMP=900`**)
  - ***Logical***: **`Param`**, **`^Param`** (e.g., **`PD.TRANS`**, **`^CLEAR`**)
  - ***Character***: **`Param`** = "string" (e.g., **`"FILE.01"`**)
- **Example**

```
IMPLANT   BF2  ENERGY=40  DOSE=1E15  TILT=7
```

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

Structure Initialization

- **`INITIALIZE`** — sets up the initial structure (mesh, background doping, orientation, resistivity, etc.) for a simulation

❑ **Major functions**

- Sets up the initial grid

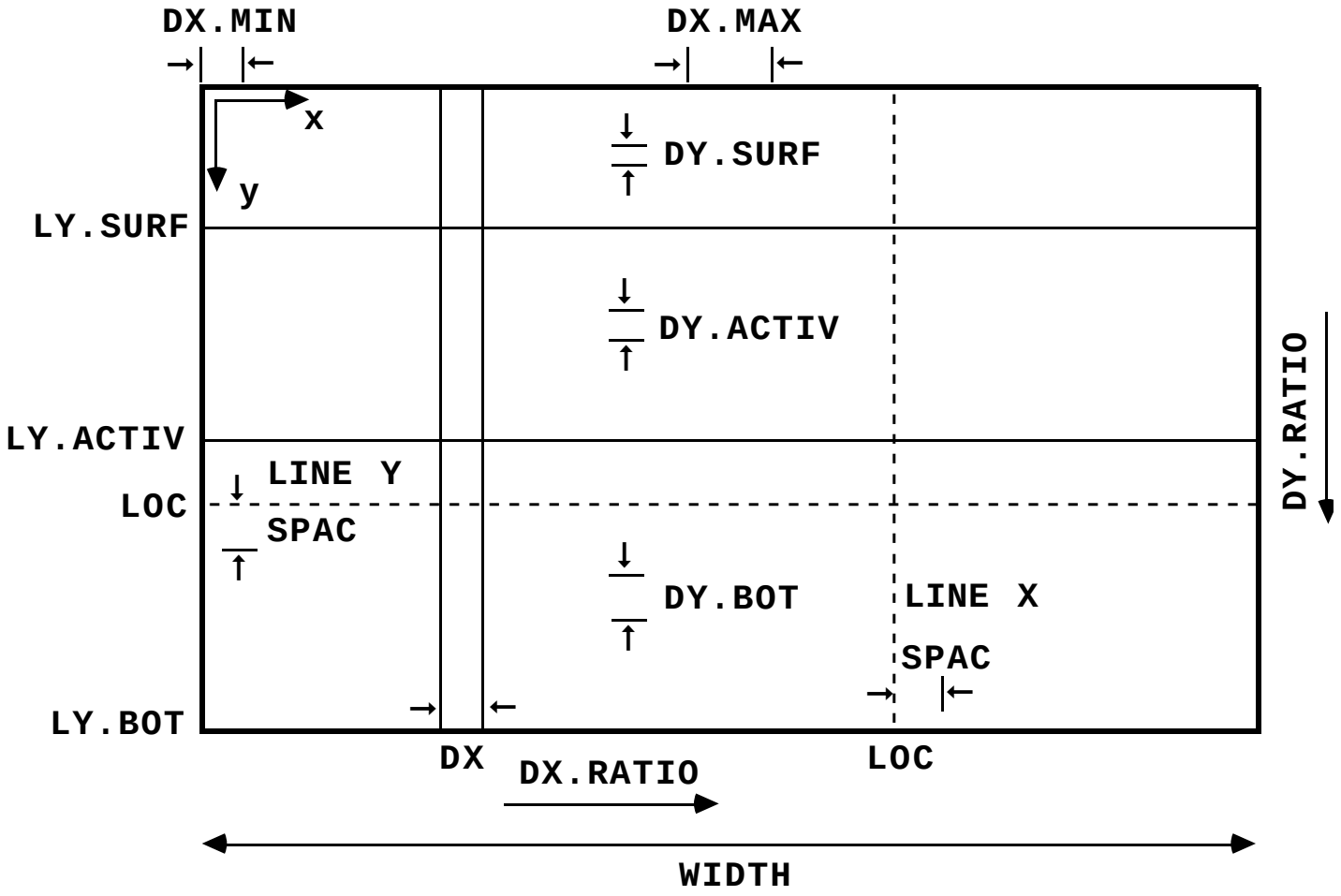
```
INITIALIZE  IN.FILE  SCALE  FLIP.Y  TIF  WIDTH  DX  RATIO
```

- Initializes the background doping, orientation, resistivity, …

```
INITIALIZE  IMPURITY  CONCENTR  I.CONC  I.RESIST  +
  ORIENTAT  X.ORIENT
```

❑ **A structure must be initialized before any processing steps (after setting up the mesh automatically, manually, or from a file)**

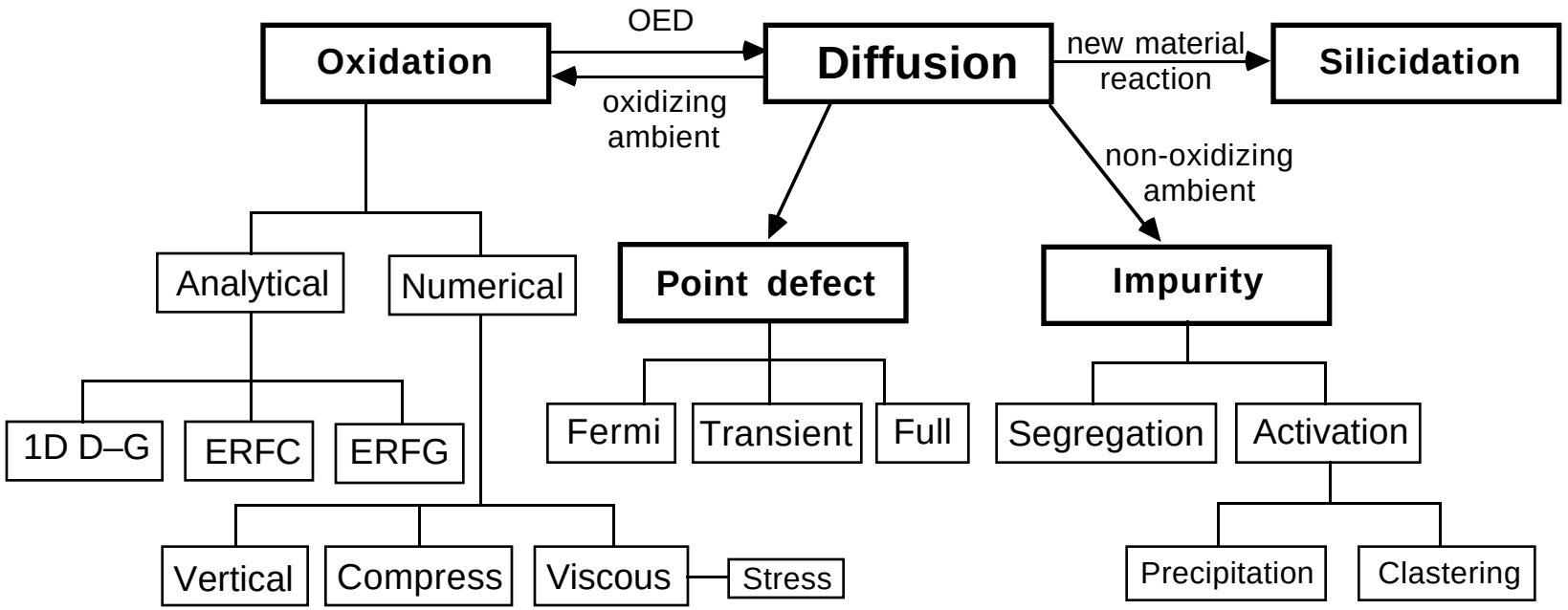
Summary: Mesh Generation Parameters



Major 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; thin-oxide 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; …

Diffusion, Oxidation, and Silicidation



- **TSUPREM-4: A single `DIFFUSION` statement to model:**
  - ***Diffusion*** — non-oxidizing ambient
  - ***Oxidation*** — oxidizing ambient
  - ***Silicidation*** — user-specified material, impurity, and reaction

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

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  THICKNES  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 — $TiSi_2$ is inserted)

Masking, Exposure and Development of Photoresist

❑ Masking

- Masking information is read from a mask file created by TMA LAYOUT
- 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* → **EXPOSE MASK=*name*** → **DEVELOP**

Etching

- **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 THICKNES 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

❑ Electrical parameters

- Threshold voltage
- Low-/high-frequency and deep-depletion MOS capacitances
- Spreading resistance profile and sheet resistances for all diffused regions

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**

  +, –, *, /, ^

“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 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!)