# ALAMODE: A Layered Architecture for Model Development

D.W. Yergeau, E.C. Kan, M.J. Gander, R.W. Dutton

Integrated Circuits Laboratory, Stanford University,
Stanford, CA 94305, USA

Abstract

To accurately simulate modern semiconductor process steps, TCAD tools must include a variety of physical models and numerical methods. Increasingly complex physical formulations are required to account for effects that were not important in previous generation of technology. As a specific example, the impurity diffusion mechanisms owing to point defects and damage kinetics are not well understood, and thus flexibility in definition of models is highly desirable. An object-oriented approach has been applied to implementing a 1-2-3D finite-element *dial-an-operator* [1] PDE solver. The control interface is based on Tcl [2] and allows layered access to model definitions and solution techniques.

## 1. Configurable TCAD Framework

To achieve a configurable and resuable TCAD framework, we have analyzed process simulation information flow carefully and separated the common functionalities such as the geometry/field server, the parameter/model library, and the visualization tools from the physical definition and numerical solvers (Figure 1) [3]. In this open framework, one can choose to use individual tools and any combination. For example, one has the choice of using SUPREM-IV diffusion code or the new ALAMODE dial-an-operator solver for impurity diffusion simulation. All tools communicate wafer representation through the geometry/field servers, and additional information for individual tools such as model and boundary condition setup can come from either the model library or the front-end controller.

This environment also provides several layers of access to the variety of users. A process engineer may need only to select a calibrated model appropriate for the process step (e.g. diffusion using the SUPREM "fermi" model) and specify the process conditions (e.g. time, temperature, and ambient). For calibration, one would need to modify the parameters used in a model to find the optimal set. At a lower level, the model developer may need to modify the equations used to implement the model, either by adding terms or even equations. Previous generation software provided user access to the first two levels, but any changes beyond altering parameters required access to and modification of the source code. By utilizing a *dial-an-operator* paradigm, we have provided access to the model definition layer.

## 2. Design of the ALAMODE PDE Solver

A portion of the information model for the ALAMODE PDE solver is shown in Figure 2 (see [4] for a more complete discussion). An *operator* is a dimensionally independent discretized representation of a term in a PDE such as $\nabla \cdot D\nabla C$ or $K_r\left(VI - V^{eq}I^{eq}\right)$. Operators generate residual vectors and tangent matrices for use in a nonlinear solver. Grouping operators via *equation* and *system in region* provides the coupled system of equations describing the homogeneous physical model within a *region*. Boundary and interface constraints are handled similarly by treating boundaries and interfaces as distinct regions and attaching operators to meet the constraint equations. Operators may be arbitrarily attached to any *field* and can utilize derived field quantities via *functions* such as is needed for the diffusion coefficient for the more compact diffusion models. Element interpolation is organized in the inheritance hierarchy shown in Figure 3, which provides the dimensional independence of the operators as well as the ability to solve equations mesh and field from a variety of sources.

The object-oriented data structure provides an efficient and versatile means to represent coupled systems of PDEs. To provide the user with access to the data structure, we have extended a Tcl interpreter with commands which mirror the information model objects. This allows the user to completely describe the physical model in a compact script, with nearly direct correspondence between the terms in the PDEs and the commands in the script. We will illustrate this mapping using the first example below.

## 3. Examples

For the first example, we use a previous generation model for boron diffusion with segregation at a stationary silicon/oxide interface to illustrate the Tcl interface in ALAMODE, and to show applicability to models in current simulation technology. This model is roughly equivalent to SUPREM's "fermi" diffusion model (without the electric field) and is described by $C_{B,t} = \nabla \cdot D_B \nabla C_B$, where $D_B$ is a constant in the oxide and $D_B = D_B(C_B) = D_B^x + D_B^+\left(p/n_i\right)$ in the silicon. Segregation of dopant between the regions is modeled by a segregation flux (flux $= \mathrm{Trn}(C_B^{\mathrm{outer}} - C_B^{\mathrm{inner}}/m)$). The Tcl script in Figure 4 directly maps the model's PDEs, interface conditions, and functional relationships into *equations* composed of *operators* and *functions* applied in the appropriate *region*. Figure 5 shows the initial and final boron profiles for a 15 minute, 1100°C anneal using SUPREM's defaults for diffusivities and the transport coefficient and value of 2.2 for the equilibrium segregation ratio ($m$).

Note that the model for the silicon diffusion coefficent is drawn from a function library while the oxide diffusion coefficient is a constant. Additional enhancements, such as vacancy and interstitial supersaturation effects (if the user adds equations for interstitials and/or vacancies), can be chained into the diffusion coefficient.

In the second example, we solve a system of reactive-diffusive equations for phosphorus diffusion [5]. The five-species model and the parameters used are shown in Figure 6. The profiles developed during a 10 minute, 900°C anneal are shown in Figure 7. Multi-species reactive-diffusive systems, similar to the one shown, are becoming increasing important to model low temperature and rapid thermal annealing as well as implant damage enhanced diffusion.

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## References


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[2] J.K. Ousterhout, *Tcl and the Tk Toolkit*, Addison-Wesley, 1994.

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[5] W.B. Richardson and B.J. Mulvaney, "Plateau and kink in P profiles diffused into Si: A result of strong bimolecular recombination?," *Appl. Phys. Lett.*, vol. 53, no. 20, pp. 1917-1919, 1988.


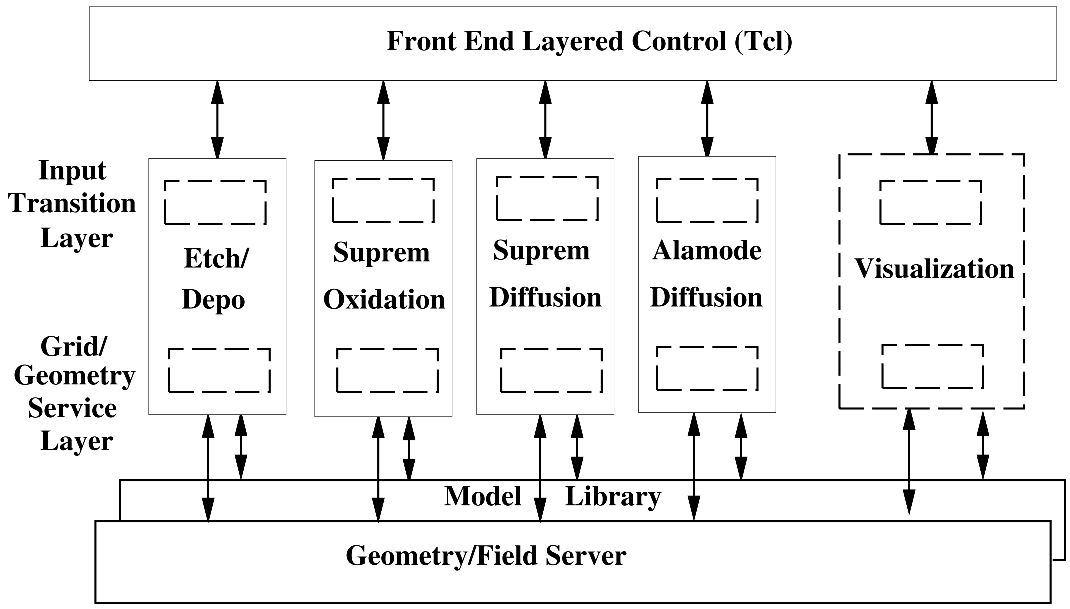


Figure 1: SUPREM OO7 architecture: an agent-based open framework for process simulation.

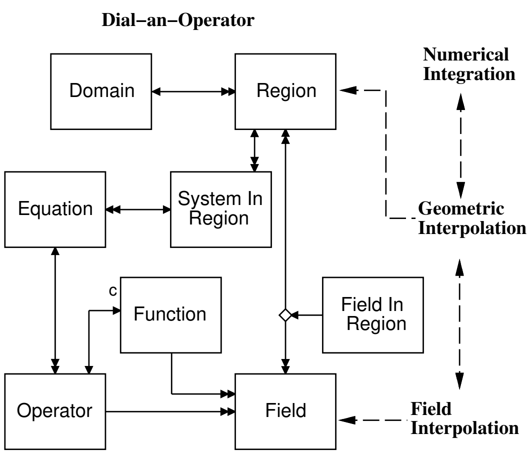


Figure 2: Information model for ALAMODE dial-an-operator solver.

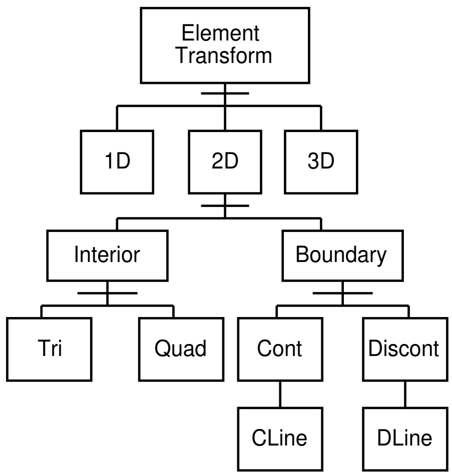


Figure 3: Inheritance structure of element transforms.

```
set DBSi [function fermi
  -parameters "B ni dbsi0 dbsip"]
set m 2.2
set modelDiff [model
 -systems [list
 [systemInRegion -region Si
  -equations [equation -parabolic
    -operators [operator diffusion
     -parameters "$DBSi B"]]]
 [systemInRegion -region Ox
  -equations [equation -parabolic
   -operators [operator diffusion
      -parameters "dbox B"]]]
 [systemInRegion -region {Ox/Si}
  -equations [equation
  -operators [operator segregation
   -parameters "B Trn m"]]]]]
```

Figure 4: TCL script for boron segregation example.

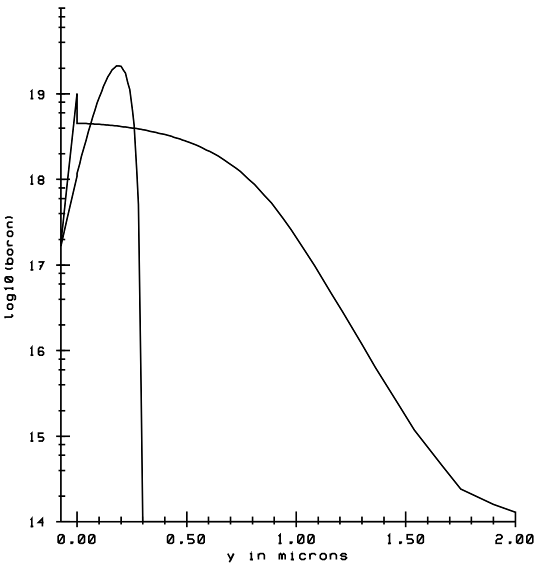


Figure 5: ALAMODE simulation of equations described by Figure 4.

$$V + I \leftrightarrow < 0 >, \ P + V \leftrightarrow E, \ P + I \leftrightarrow F$$

$$V_{,t} = \nabla \cdot D_V \nabla V - k_{for}^{E} PV + k_{rev}^{E} E$$
$$-k_{bi}(VI - V^{eq} I^{eq})$$

$$I_{,t} = \nabla \cdot D_I \nabla I - k_{for}^{F} PI + k_{rev}^{F} F$$
$$-k_{bi}(VI - V^{eq} I^{eq})$$

$$E_{,t} = \nabla \cdot D_E \nabla E + k_{for}^{E} PV - k_{rev}^{E} E$$

$$F_{,t} = \nabla \cdot D_F \nabla F + k_{for}^{F} PI - k_{rev}^{F} F$$

$$P_{,t} = -k_{for}^{E} PV + k_{rev}^{E} E - k_{for}^{F} PI + k_{rev}^{F} F$$

| | $C_{eq}$ $(cm^{-3})$ | $D_{def}$ $(\frac{cm^2}{s})$ | $D_{pair}$ $(\frac{cm^2}{s})$ | $k_{for}^{pair}$ $(\frac{cm^3}{s})$ | $k_{rev}^{pair}$ $(s^{-1})$ |
|---|---|---|---|---|---|
| V | $10^{14}$ | $10^{-10}$ | $10^{-13}$ | $10^{-14}$ | 10 |
| I | $10^{14}$ | $10^{-9}$ | $2 \cdot 10^{-13}$ | $10^{-14}$ | 12 |

Figure 6: Five species reactive-diffusive model for phosphorus.

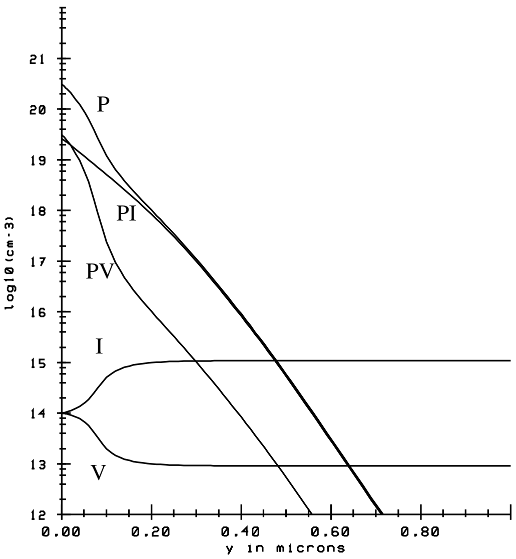


Figure 7: ALAMODE simulation of phosphorus plateau and kink as described by Figure 6. The results reproduce those in [5].