Living in an Expanding TCAD Space

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ABSTRACT

A substantial number of important industrial modeling and simulation problems lie outside of the scope of commercial TCAD (Technology Computer-Aided Design) software. The tools needed to solve such problems include a good PDE (Partial Differential Equation) package, reliable mesh generators, atomistic modeling capability and advanced numerical methods. A good opportunity may also exist in advanced visualization. These points are illustrated in the context of a specific problems drawn from reliability.

Keywords: modeling, numerical methods, TCAD

VARIETIES OF TCAD

By *traditional* TCAD will be meant the use of commercial device simulators to model the characteristics of a transistor design and the supporting use of commercial process simulators to model the underlying manufacturing processes that are used to create the device structure and doping profiles. The commonly used process simulation tools generally include point-defect models for dopant introduction and diffusion, viscoelastic or elastic models for silicon dioxide and silicide growth, and simple models for lithography, deposition and etching. This covers most of the common processing steps. Most simulators have 1D and 2D capability and a few now also support 3D, which is increasingly necessary to model the smallest leading edge devices. Since there is still controversy about the correct diffusion models and a persistent need to modify existing models or introduce new ones, there has also been a trend to provide a flexible PDE solving capability that allows one to define a model using a rather general set of diffusion-reaction equations.

The movement toward multidimensional process modeling codes with flexible model programming interfaces is very positive. However, in most new processes there are usually a few steps, often the most critical, for which the standard commercial simulators either fail to be predictive or are not even applicable. Examples of problematical steps include rapid thermal processing, electroplating, and chemical-mechanical polishing (CMP). The traditional tools also often fail to provide predictive capability and guidance when new materials are introduced, such as advanced gate dielectrics, when new elements are introduced or when the microstructure of a material is a critical factor, as in advanced metallization reliability. Sometimes the key roadblock in process development is not in understanding and modeling the desired feature scale effect of a process step, but in understanding how an expensive fab tool works and how to operate it in a stable, high throughput, high uniformity regime. For this reason, it is necessary to recognize traditional TCAD as just one compartment in a larger modeling and simulation domain that includes a significant volume of compelling *nontraditional* modeling.

TOOLS FOR NONTRADITIONAL TCAD

It will be helpful to discuss methods for addressing problems outside of traditional TCAD in the context of a recognized problem of exceptional difficulty whose solution would be of substantial benefit. Every company has a list of these. The problem chosen here, reliability, originated in needs identified at Motorola, Inc. and many of the associated tools have been developed internally, sometimes using freeware components.

A PDE Solver and Good Mesh Generators

We use a tool called ASSET that was constructed in 1989 around a sparse, stiff, variable time step, variable order Gear solver from Lawrence Livermore Laboratory [1]. The package externally looks very similar to a traditional process modeling tool. However, it supports the specification, parameterization and solution of fairly general systems of PDEs in 1D, 2D and 3D (without any changes) using finite element, finite difference and even combined FE/FD methods. Models are specified in a semiautomatically generated text file which is then compiled into the program. Model definition can be done wholly without reference to grids, problem dimensionality, or solution methods, thus allowing one to focus on the physics. One can choose to solve for all of the fields in a model or just some of them. Perhaps the biggest advantage of the tool is that even fairly complex models can be coded in a matter of a few hours or days (making them disposable, if desired), the formulation and quantification of the model generally being the most difficult step. The main disadvantage of such a solver is that it offers a high degree of flexibility, thus making it desirable to have the coding done by an experienced engineer. A second

disadvantage is that since it is very general, it is not usually possible to take advantage of the specialized structure of some models to optimize execution speed.

ASSET has been used to implement some of the latest dopant diffusion models in the literature, for modeling chip-level transient heating in Smart Power devices, for copper electroplating, for implementing various chemical vapor deposition models, solving the standard device equations, correcting carrier spilling in spreading resistance data, modeling metallization reliability, and many other applications. The reliability application is instructive, since it clearly distinguishes ASSET from traditional process tools.

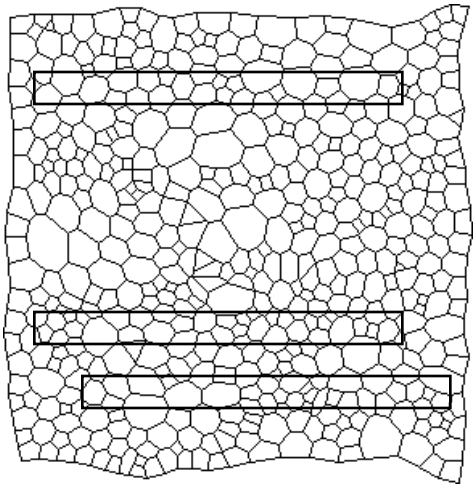

Figure 1: Creation of polycrystalline structures by random placement and cutting. Most of the work is done with a good mesh generator.

For the reliability application, ASSET takes as one of its inputs a finite element discretization of a polycrystalline metal line (Figure 1). For metallization with columnar grains that can be treated in 2D, large samples of such structures are generated automatically by randomly placing a pattern on a polycrystalline film model, then cutting and triangulating. The film models are generated using several methods, one involving random seeding of a planar region followed by the construction of the corresponding Voronoi polygons, a second involving the large scale optimization of the Voronoi network to match an experimentally measured grain size distribution. This sounds complex, but most of it can be done with a surprisingly small collection of software, the most important tool being a general and reliable Delaunay automatic mesh generator. We use the program *triangle* from Carnegie-Mellon University [2] for 2D structures. For 3D, one can use extrusion of 2D structure to form columnar grains, joining various metal levels together as necessary using a general 3D Delaunay mesh generator. A 3D utility from Los Alamos National Lab is used for this [3]. All such structures include both a volume discretization of the grains and an associated linear network or surface discretization of the grain boundaries. This allows the solver to discriminate between the two vacancy diffusion pathways, and to separately handle diffusion along them and exchange between them. One can readily imagine that instead of metallization, such structures could represent a polysilicon film overlying a transistor or a tin dioxide film in a chemical sensor, where the quantity of interest would be a diffusing impurity or a contaminant. Figure 2 shows the equations solved for the reliability model. Figure 3 shows the spherical part of the stress calculated in a long, polycrystalline metal line with ASSET. The equations and functionality are generally different for every application.

$$\frac{\partial c}{\partial t} = -\bar{} \quad \bar{q} + G$$

$$\frac{\partial \Sigma^{v}_{kk}}{\partial t} = \Omega\left(f^{-} \quad \bar{q} + f' G \right)$$

$$\mu \quad ^{2} u_i + (\lambda + \mu) \frac{\partial}{\partial x_i} (^{-} \quad \bar{u}) = B \frac{\partial \Sigma^{v}_{kk}}{\partial x_i}$$

$$\sigma_{ij} = -B\Sigma^{v}_{kk}\delta_{ij} + \lambda\Sigma_{kk}\delta_{ij} + 2\mu\Sigma_{ij}$$

Figure 2: A typical set of equations solved with the PDE solver in ASSET.

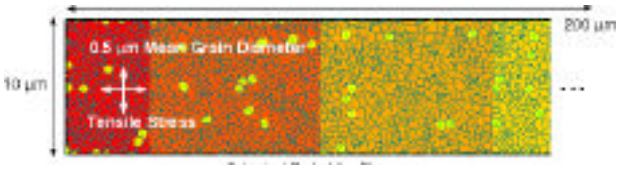

Figure 3: An example of a result calculated on a large polycrystalline structure, in this case the spherical stress in a metal line.

Ab Initio Tools

One of the most persistent problems in both traditional and nontraditional TCAD is that important model parameters are often unknown and the experiments needed to measure them are difficult or impossible to perform, especially in an industrial environment. Furthermore, in some systems, the fundamental mechanisms may not even be clear. For this reason, even experimentally calibrated models may have little validity or predictive power outside the calibration space.

In the last several years, commercial and university atomic-level modeling tools and methods based on quantum mechanics have been rapidly improving in accuracy, speed, and generality [4, 5, 6, 7, 8, 9; see also 10, 11 for reliability examples]. Such tools can claim to be predictive in a very strong sense. It is often practical to run *ab initio* codes now on a high-end workstation. Experienced users can, given enough time, accomplish such feats as working out and quantifying the chemistry mechanism and kinetics for a chemical vapor deposition process [12], elucidating and quantifying diffusion and void formation mechanisms in bulk material and in grain boundaries [13] including the effects of impurities or alloying elements, and calculating the electronic structure and physical properties of a totally new material. Figure 4 shows a result from a study of void formation morphology and energetics in aluminum and copper grain boundaries that was computed using the embedded atom method [14]. Energies predicted by the method for vacancies in the bulk were in good agreement with experimental data, lending some credibility to the grain boundary predictions. This is the kind of information that is very difficult to obtain experimentally but is essential for advanced modeling.

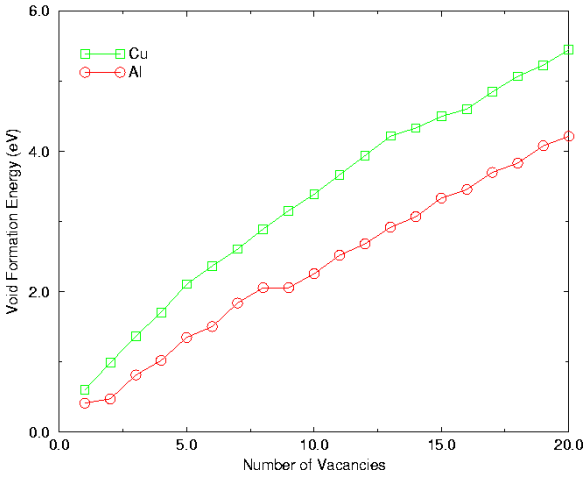

Figure 4: Void formation energies in aluminum and copper Σ5 [310] grain boundaries computed with the embedded atom method.

Advanced Numerical Methods

The most difficult classes of problems in process simulation are moving boundary problems. In 2D and particularly in 3D, the numerical solution of moving boundary problems can involve complex and sometimes unreliable computational geometry and mesh generation algorithms. *Level set* methods [15] are a particularly good alternative for many 2D and 3D problems. The simplest version of the method involves solving a Hamilton-Jacobi equation

$$\phi_t + F|\nabla\phi| = 0$$

for the evolution of a function whose ϕ=0 level set represents the surface of interest. The function F is generally an extension of the normal velocity field of the surface and thus contains all of the physics of the problem. Level set methods have been applied to moving boundary problems in many areas, including deposition [16], etching, plating, reliability and photolithography, where an extremely fast version of the technique can be used for resist development. A great advantage of the level set method is that it effortlessly handles complex changes in surface shape and topology while using a fixed, nonconformal grid. Because standard finite difference and finite element methods are unstable for the Hamilton-Jacobi equation, level set methods must use specialized upwinding schemes. Most popularly recognized as a finite difference method, finite element versions of the technique also exist. The latter eliminate problems with the accurate representation of thin layers. Level set codes are compact, reliable, and easy to write. Our internal utility has only 5,000 lines of code for both 2D and 3D, a consideration that considerably facilitates its application to non-traditional problems.

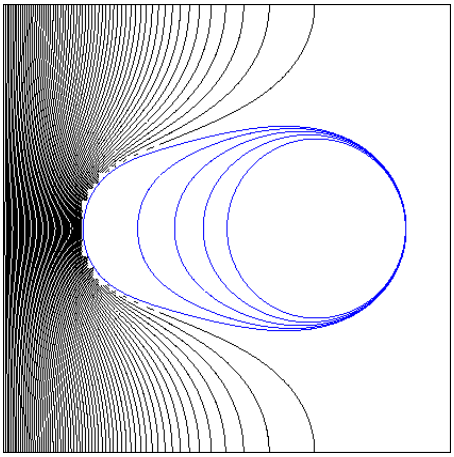
Figure 5: Shape change in a void due to vacancy absorption computed using the level set and immersed interface methods.

A second potentially useful technique is the *immersed interface method* [17]. Similar to a finite difference method, the basic idea is to discretize the operators in a PDE in a way that captures the influence of a boundary or interface. This complicates the setup of the discrete system and generally leads to non-symmetric, non-positive definite matrices, but as in the level set method, the interfaces need not coincide with grid points. It is possible to therefore combine the level set method with the

immersed interface method and solve a set of PDEs with a moving boundary on a fixed finite difference grid. For example, the Navier-Stokes equations have been solved in 3D to model blood flow in a beating heart [18]. Figure 5 [19] is an example from reliability. Here, a drift-diffusion equation for vacancy transport has been solved in 2D in the vicinity of a void, which grows as it captures vacancies. All of the calculations are done on a finite difference grid that does not conform to the void boundary. The combined method represents a substantial savings in complexity and programming effort compared with competing algorithms.

Advanced Visualization

This is a topic that should probably receive more serious consideration. In current TCAD interfaces, problems are defined with a series of menus, the basic computational tools are executed, and the results are displayed with visualizers that support graphical operations like rendering, transparency, rotation and slicing. The environment is essentially flat, with graphical objects being treated with a camera model. Although usually adequate, many potential users of process tools generally find the environment foreign and nonintuitive. There may be an alternative. Virtual reality (VR) hardware [20] has been steadily improving in price and performance. Within a VR environment, it is possible to construct an entirely different way of interacting with simulation tools. For example, instead of editing files and clicking menus to run a simulation of a rapid thermal processing tool, one could stand next to a realistic virtual model of the tool, interacting with it like one would interact with the real tool. The two could even be connected, so that a recipe developed on the virtual tool could be directly transferred to the real one and *vice versa*. However, the advantage of the virtual tool is that one could also see and explore flow and temperature fields from the inside, permitting greater, more concrete understanding of the connection between tool inputs and the dynamics of tool operation. Some thought is required to appreciate the benefits. VR is used as a collaborative design tool by General Motors, where it provides a relatively inexpensive alternative to building physical prototypes. It is also used by GM as a financial management tool. For many fab tools in the several million dollar range, investment in a related virtual tool that incorporates a process model may be beneficial. VR could provide the next generation of interfaces for advanced TCAD tools.

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