Moving Adaptive Unstructured 3-D Meshes in Semiconductor Process Modeling Applications

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The next generation of semiconductor process and device modeling codes will require 3-D mesh capabilities including moving volume and surface grids, adaptive mesh refinement and adaptive mesh smoothing. To illustrate the value of these techniques, a time dependent process simulation model was constructed using analytic functions to return time dependent dopant concentration and time dependent SiO₂ volume and surface velocities. Adaptive mesh refinement and adaptive mesh smoothing techniques were used to resolve the moving boron dopant diffusion front in the Si substrate. The adaptive mesh smoothing technique involves minimizing the $L_2$ norm of the gradient of the error between the true dopant concentration and the piecewise linear approximation over the tetrahedral mesh thus assuring that the mesh is optimal for representing evolving solution gradients. Also implemented is constrained boundary smoothing, wherein the moving SiO₂/Si interface is represented by moving nodes that correctly track the interface motion, and which use their remaining degrees of freedom to minimize the aforementioned error norm. Thus, optimal tetrahedral shape and alignment is obtained even in the neighborhood of a moving boundary. If desired, a topological "reconnection" step maintains a Delaunay mesh at all times. The combination of adaptive refinement, adaptive smoothing, and mesh reconnection gives excellent front tracking, feature resolution, and grid quality for finite volume/finite element computation.

Keywords: adaptive mesh refinement, adaptive mesh smoothing, mesh reconnection, multimaterial grids, moving grids, moving surfaces, unstructured grids

THE MULTIMATERIAL GRID CODE LaGriT

LaGriT, the Los Alamos grid code¹,², is a toolbox of multimaterial grid generation, adaptive mesh refinement, adaptive mesh smoothing, mesh reconnection, and mesh manipulation operations that are well suited to semiconductor process and device modeling. The toolbox commands operate on mesh objects that are user extensible and automatically sized; information stored within the mesh objects assures the correct attribute values are assigned to new nodes and elements as created and allow for time dependent geometric reconfiguration that can result from moving grid and moving surface applications.

To illustrate the capabilities of LaGriT, a time dependent process simulation model was constructed using analytic functions to return dopant concentrations and SiO₂ surface velocities. The model consists of layers of silicon, SiO₂, polysilicon, and nitride: a T-shaped mask is centered in the nitride. As the model is symmetric, only half the model was calculated. Initially all interfaces are planar (Fig. 1) and the dopant

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FIGURE 1 Initial planar surface and interface grids with T-mask

FIGURE 2 Boron concentration contours at t = 0

isosurfaces are highly curved (Fig. 2). Over time as the polysilicon is converted to SiO$_2$, the nitride region is pushed up; eventually the lower oxide surface penetrates the silicon at which time the dopant diffusion is effectively stopped at the silicon/oxide interface (Figs. 3, 4). LaGriT models the nitride region as a moving volume mesh, and models the lower oxide surface as a moving surface. At each time step the LaGriT tool, extract, is invoked to create a two dimensional mesh object, which is moved and then reinserted into the main three dimensional mesh object. By reinvoking the geometry definition, nodes and elements are assigned correct attributes.

SIMULTANEOUS GRID ADAPTATION TO DIFFUSION AND OXIDATION

In the lower Si portion of the model, an implanted boron dopant diffuses while at the same time a moving oxide boundary shrinks the Si. Complete grid adaption is accomplished by (1) refining the mesh based on the dopant concentration field, (2) smoothing the mesh to minimize the error in representing the concentration field, and (3) reconnecting the mesh to allow necessary topological changes to occur as the dopant field and problem domain deform.

The LaGriT redapt option invokes Minimum Error Gradient Adaption (MEGA) which is a 3D generalization of a 2D adaptive smoothing scheme of Bank and Smith$^3$, combined with the gradient weighting concept of Carlson and Miller$^4$. The idea is to adjust the positions of the vertices so as to minimize the functional

$$F = \int_\Omega \| \nabla (u - u_L) \|^2 w dx.$$  (1)

That is, the weighted $L_2$ norm of the gradient of the error between the true solution $u$ and its piecewise linear approximation $u_L$ on each tetrahedron. Minimizing the gradient of the error leads to optimal resolution of solution gradients which can be crucial
for correct calculation of diffusion profiles. A secondary benefit of minimizing the error gradient is that it works to prevent “tet collapse” as the mesh moves. This is because solution gradients are poorly represented on wafer-thin tetrahedra, and are thus avoided when minimizing this functional. For sufficiently large grids the gradient weighting factor $w$ can be omitted, and the grids produced become independent of the scale of $u$, thus eliminating fiddling with parameters.

Since the exact solution $u$ in (1) is generally unknown, the method is to approximate the error by the six quadratic “bump” functions associated with the edges of each tetrahedron. The “bump” functions are the pairwise products of the four linear "hat" functions associated with the four vertices of each tetrahedron.) To use the `redapt` command, all that is needed is an estimate of the error at each edge midpoint in the mesh. In our analytical model of boron diffusion, this data is exactly known, but this data can also be obtained as a posteriori error estimates which are routinely computed when numerically solving differential equations.5

In Fig. 5, we show the initial Silicon grid with boron contours of greatly exaggerated width. In Fig. 6 we show this grid after adaptive refinement; contour widths have been corrected but are highly irregular. A call to `recon` has been issued—the `recon` command is a novel 3D algorithm for re-establishing a Delaunay triangulation after mesh movement. `Recon` performs internal face swaps and boundary edge swaps in the mesh which typically modify a small proportion of the mesh connectivity during any given time step. As is well known, maintaining a Delaunay grid at all times is a crucial requirement for many finite volume PDE solvers. In Fig. 7, we show the effect of smoothing the grid via Minimum Error Gradient Adaption; the grid has now contracted and realigned to accurately resolve the boron contours.

In Fig. 8, we show the grid at $t = 4000$ when the oxide interface has partially collapsed the solution domain. Note how the front surface grid distribution
FIGURE 5 Initial unrefined, unsmoothed regular grid with boron contours

FIGURE 6 Refined, reconnected initial grid

FIGURE 7 Refined, reconnected and smoothed initial grid

FIGURE 8 MEGA smoothed grid at t = 4000
FIGURE 9 MEGA smoothed grid with 9765 nodes at $t = 0$

FIGURE 10 Grid at $t = 8000$ showing boron contours

FIGURE 11 MEGA smoothed grid with 9765 nodes at $t = 0$
(Close-up showing boron contours.)

FIGURE 12 Same close-up as Fig. 11, but using 206,500 node uniform hexahedral grid
has shown the remarkable ability to “deconcentrate” (through the repeated use of redapt and recon) as the boron diffuses.

In Figs. 9-11, we show a workstation run with 9765 nodes where we have chosen not to refine or reconnect the mesh, but to adapt the mesh solely with MEGA. Note the “triband” structure at $t = 0$ which indicates locations of large second derivative in the dopant function. Fig. 11 is a close-up of the front face of the smoothed $t = 0$ mesh and shows boron contours in a region of very high curvature. In contrast, Fig. 12 shows the same close-up on a much larger uniform hexahedral grid of 206,500 nodes. (The full hexahedral grid is not pictured.) The contours are more accurately resolved on the smaller MEGA smoothed mesh.

References

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Biographies

Andrew P. Kuprat received his Ph.D. in Mathematics from the University of California at Berkeley and is currently a staff member at Los Alamos National Laboratory. He is interested in moving adaptive mesh algorithms applied to problems in semiconductor process and device modeling, as well as to other convection/diffusion problems in physics. He is also interested in mesh generation and computational geometry.

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