11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

A 3D Moving Grid Algorithm for Process Simulation

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During the simulation of 3D oxidation and similar processes computation of geometry and topology changes requires construction of a valid 3D mesh at every time step.
During the past year significant progress has been made to improve the moving grid algorithm used in Synopsys' Sentaurus Process.
For each oxidation time step the oxygen diffusion/reaction and stress equations are solved in the appropriate regions of a static boundary fitted all-tetrahedron mesh.
The equations for the point defect and dopant diffusion are solved on a moving grid, using several smaller time steps if necessary. The displacements computed from the stress equations are used to deform the mesh elements and the geometry.
For each mesh element a cubic equation is solved to determine the time when the element degenerates. The minimum of these times for all mesh elements is used as grid limited step for the grid update and for solution of the diffusion equations. The box weights for the old and new positions of the mesh points are computed and used for the solution of the diffusion equations. During the diffusion step the mesh topology remains fixed.
This approach, which is very similar to the one used in the 2D simulator TSUPREM-IV eliminates the need for convective terms in the equations and only requires accounting for the discontinuous velocities at the reaction front.
At the end of each time step, a grid cleanup step is performed. Short edges and poorly shaped or small volume elements are removed. Several methods to remove such elements have been implemented:

- Face swapping
- Moving one node to the location of another
- Removing elements by breaking edges or faces for the degenerate cases of a node close to an edge or face and the case of two edges crossing at close proximity
- Re-assigning volume elements to another region.
- Local Laplacean smoothing

After removing poorly shaped mesh elements and too short edges, a refinement algorithm is used that checks for long edges "perpendicular" to a material interface.

With the given set of methods it is still not always possible to eliminate all elements of poor shape or small volume. As a backup method for these cases a global Delaunay reconnection algorithm is used, that allows constructing a new mesh from the set of all triangles on the material interfaces and the external surface and from the cloud of all (displaced) internal points that do not belong to a "bad" tetrahedron.

While the performance and robustness of the moving grid algorithm has been enhanced sufficiently during the past year, current and future work will be focused on the reduction of the geometric noise near moving ridges and corners and on maintaining a "nice" tessellation where an initially sharp ridge or corner becomes rounded e.g., along one axis. The identification of the root cause for such problems has been difficult due to the complex interaction of mesh element quality, computation method of box weights, iterative solution of large systems of equations, displacement of mesh points and local removal of "bad" elements. Test cases simulating isotropic deposition and etching with the same moving grid algorithm have been used to study the evolution and movement of such ridges and corners in the presence of “ideal” analytic velocity fields.

ISBN 3-901578-16-1

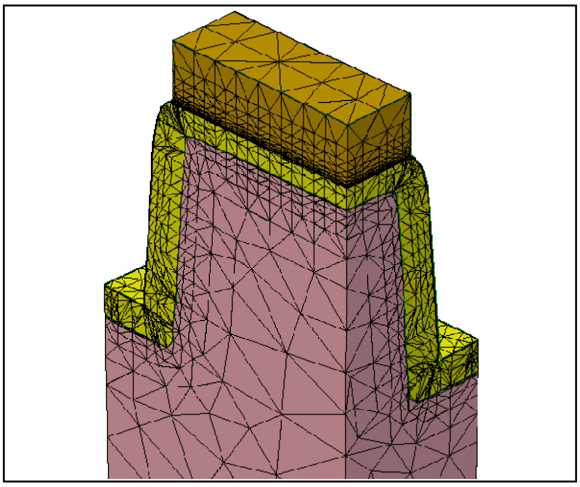

Fig. 1. Final mesh and structure after STI liner oxidation

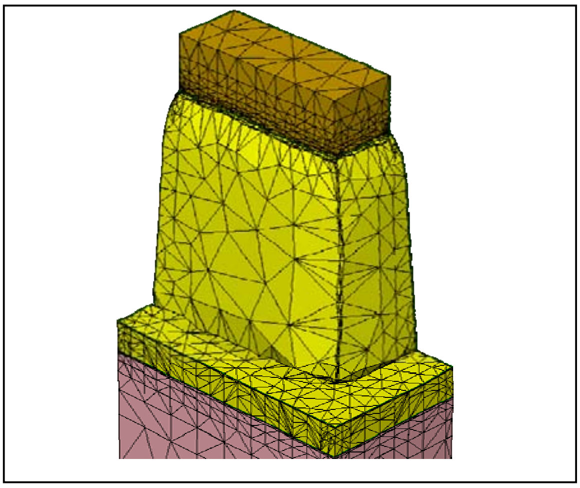

Fig. 2. 3D STI liner oxidation (opposite view)

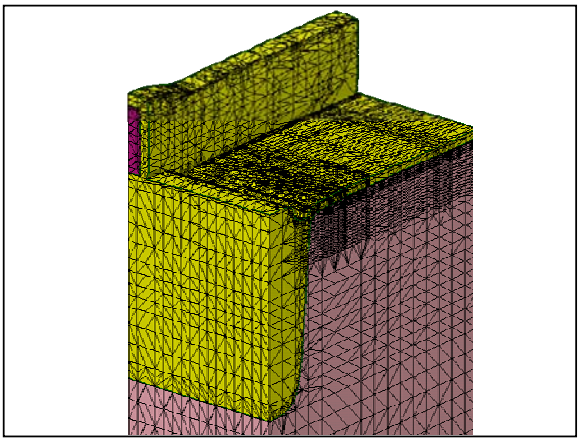

Fig. 3. Final mesh after 3D Poly gate re-oxidation

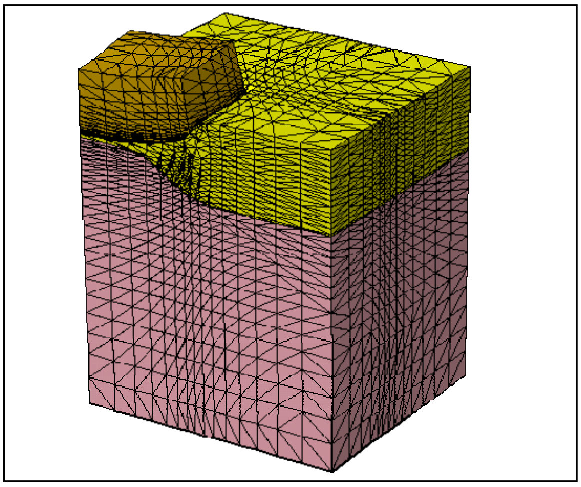

Fig. 4. Final mesh after long, conventional Locos simulation

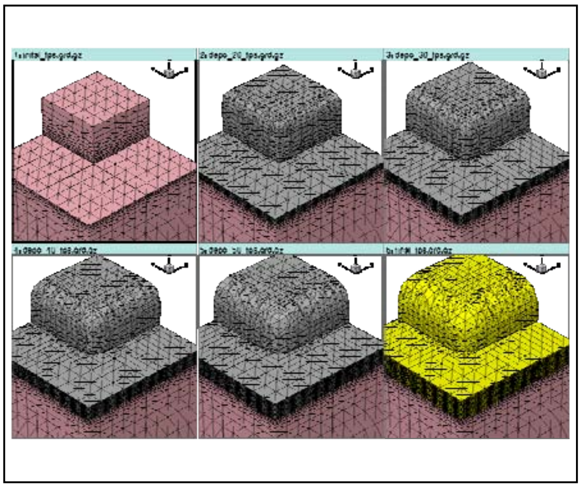

Fig. 5. Simulation of 3D isotropic deposition – test case

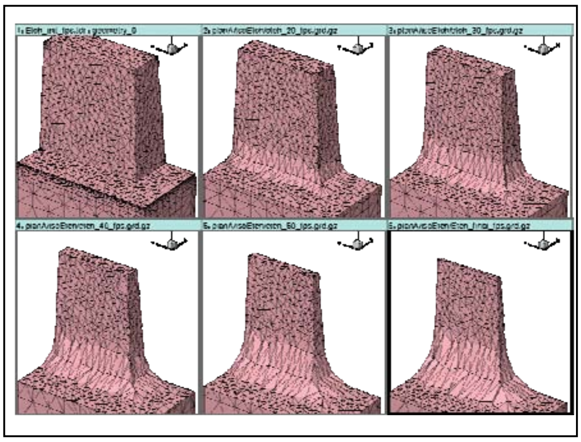

Fig. 6. Simulation of 3D isotropic etching – test case