2D/3D Etching and Deposition Simulation Tools Implemented with a General TCAD Geometry Server

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Abstract

Implementation and validation of 2D and 3D etching and deposition simulators using a general TCAD geometry server with both the boundary and level-set representation is performed. Advantages of our approach include not only enhanced functionalities such as accurate and robust boundary movement and smoothing, but also well-defined procedural interface for facile inter-tool communication. Accuracy in boundary movement is validated for various deposition and etching processes with the SPEEDIE physical models. Examples for sharing geometry information with adequate smoothing in nonplanar structures based on curvature are demonstrated between SPEEDIE (etching/deposition) and SUPREM (diffusion/oxidation).

I. Introduction

Computational prototyping with Technology CAD (TCAD) is gaining increasing importance in expediting VLSI technology design and fabrication optimization. Physical TCAD tools developed for different fabrication processes such as etching/deposition, oxidation, and lithography all require accurate and robust geometry movement. The moving boundary can be tracted geometrically (the boundary represented by moving surface grid points) or parametrically (fixed volume grid with parameter variables to record the boundary movement). The level set method [1] is a parametric boundary movement method by using the signed distance to the boundary as the tracking parameters, and has shown significant improvement on stability, accuracy and robustness in comparison with the geometrical methods [2,3]. Since the surface normal and curvature can be evaluated precisely, physical smooth surface evolution with high accuracy can be achieved. This is important for modeling the increasingly complex fabrication technology, such as high density plasma etching and deposition in deep submicron processes. Issues concerning accuracy validation for 2D/3D boundary movement and implementation of the geometry server will be discussed below.

II. Functionalities and Interface of the TCAD Geometry Server

The boundary movement and smoothing functions based on the level-set method are implemented into a geometry server with minimalistic pre-defined procedural interface [4], which also provides a consistent geometry representation for integration of various spatial discretization schemes such as volume, surface and Eulerian-type grids. Figure 1 illustrates the usage of geometry server calls in process simulation. The initial geometry is input from a file and handled by a global geometry object pointer “wafer”, which may be implemented as a C structure or a C++ class. Then, a typical APCVD process is simulated using the level-set boundary movement as illustrated in Fig. 2. To avoid spurious elements resulting from small surface line segments, the geometry is smoothed according to a curvature threshold before passing to FOREST [4], a conformal quad-tree gridder, for subsequent diffusion simulation. It is clear from Fig. 2(c) and (c) that adequate smoothing is very useful for reasonable tradeoffs between accuracy and efficiency [7]. The advantage of using the minimalistic geometry server procedural interface is clearly seen in fast integration of independently developed tools and easy inclusion of different boundary movement algorithms.

III. Technology Examples for Boundary Movement Accuracy Validation

The geometry server has been connected with the Stanford physical etching and deposition simulation SPEEDIE [5]. Accuracy in the physical models and level-set boundary movement has been validated in various fabrication processes in 2D and 3D. Figures 3-6 demonstrate the features captured by simulation for LPCVD, PECVD, PVD and self alignment contact formation [3], and the thinning and flattening at corners with PVD can also be accurately modeled without spurious geometrical effects from moving conformal grids due to grid sparsity and rule-based algorithms handling complex structures [8].

Acceleration of simulation is achieved by adaptive gridding according to the distance function itself with quad/oct-tree algorithms [3]. The data structure of the quad/oct-tree implementation reflects tradeoffs between memory usage and efficiency. Local connectivity information is required for spatial discretization schemes and boundary reconstruction from the quad/oct-tree volume mesh. Memory usage can be reduced by computing local connectivity on the fly, but this approach incurs a slowdown in execution time. In our implementation, a complete set of pointers to neighboring objects are precomputed and cashed during volume mesh generation. On Silicon Graphics Indigo 2 Extreme with Irix 5.3, a representative mesh (bounding square with side length of 2 μm, maximum adaptation level 7 and minimum grid size 0.03125 μm) with 3100 volume grid points takes 60 seconds in CPU time to generate, and uses 2.8 megabytes of memory. Evaluation of finite difference operators in spatial and temporal discretization schemes takes 24 seconds, and the actual boundary reconstruction takes 0.4 second. For 3D mesh generation, typical memory usage with maximum adaptation level 7 can reach over 30 megabytes. Memory should be properly de-allocated prior to grid regeneration. Reference counts are maintained in our implementation for this purpose.

IV. Conclusions

A TCAD geometry server with rich functionalities such as robust boundary movement and smoothing is very useful for tool development and integration. Computational prototyping of technology examples has demonstrated the accuracy and applicability of this approach.

V. Acknowledgment

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VI. References

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swrGeometry* wafer; // wafer is the common geometry throughout simulation

wafer = swrGeometryRead( "initial.geom" ); // input initial geometry from file
swrGeometrySetAttribute( wafer, "speedieModel", "APCVD" );  // pass to SPEEDIE
while( totalDepositionTimeNotAchieved ){
       timeStep = setVelocityFromSPEEDIE( wafer ); // SPEEDIE model evaluation
       lsGeometryMove( wafer, timeStep ); // level-set boundary movement
}
lsGeometrySmooth( wafer, curvatureThreshold ); // boundary smoothing
swrGeometrySetAttribute( wafer, "MaximumGridSize", 0.2 ); // pass to FOREST
qtGridGenerate( wafer ); // Lagragian quad-tree mesh generation for diffusion
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Figure. 1: Illustration of geometry server usage

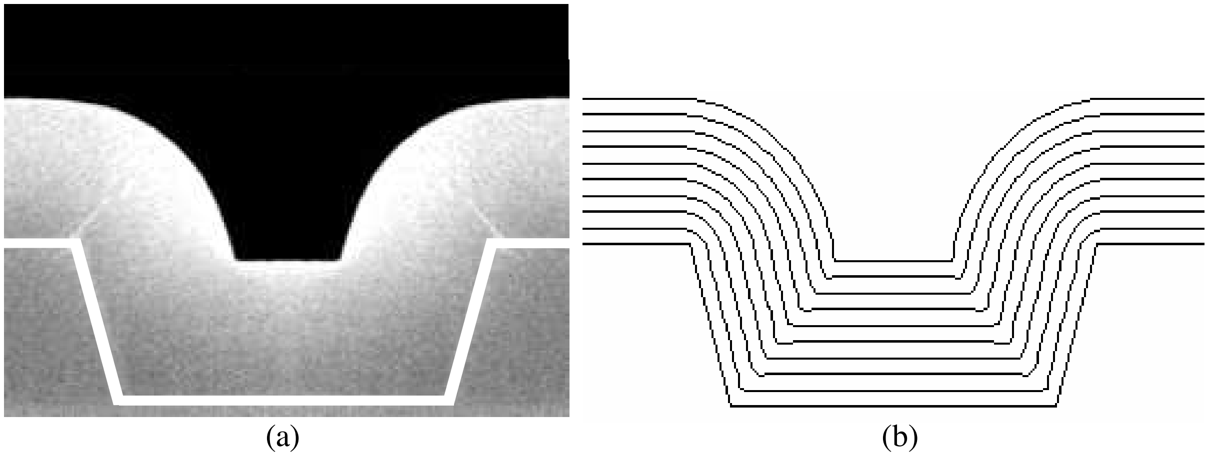


Figure. 2: A typical APCVD process over a shallow trench. Ozone concentration: 0.13% in the O_2 / O_3 stream. (a) The SEM. (b) shows the simulated profile evolution.

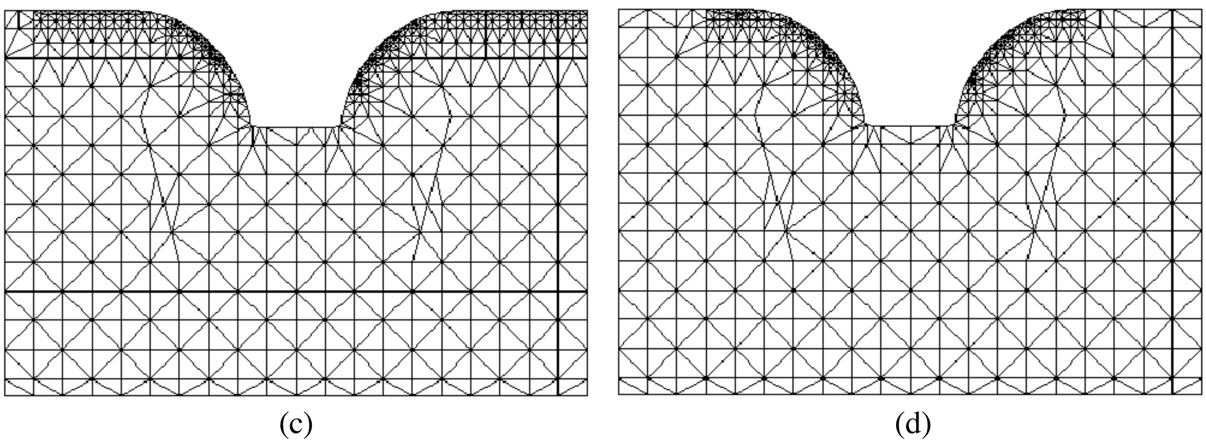


Figure. 2 (Continued): Conformal triangular meshes generated by FOREST for the geometry represented by the final surface profile in (b). (c) shows the resulting mesh with 1230 volume mesh grid points generated from unsmoothed surface. (d) shows the resulting mesh with 1058 volume mesh grid points generated from smoothed surface. The top flat surface contains much less grid points, while the mesh in the curved surfaces and interior regions remains roughly the same.

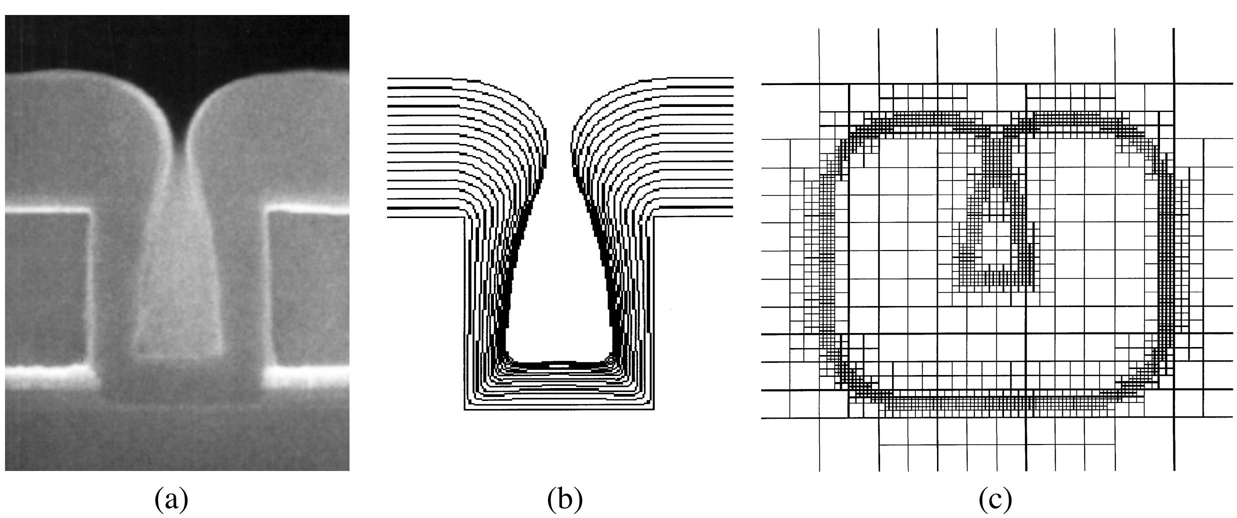
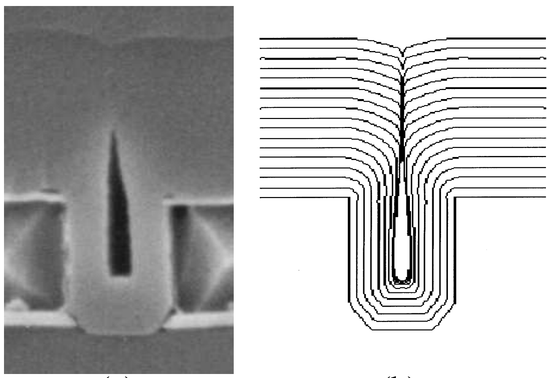
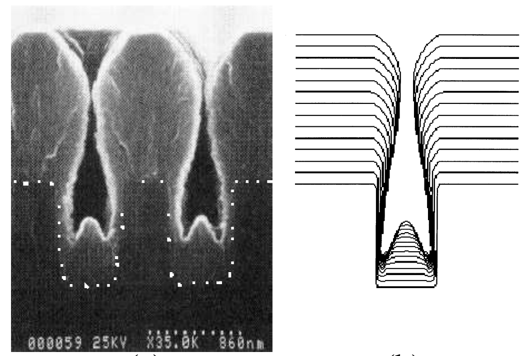


Figure. 3: LPCVD of SiO_2 from silane in a trench. (a) The SEM. Process conditions: $380^{\circ}C$, 250 mTorr, Sc = 0.35, $SiH_4 / N_2 / O_2 / PH_3$. (b) The simulated profile evolution. (c) The adaptive quad-tree mesh corresponding to the final profile.



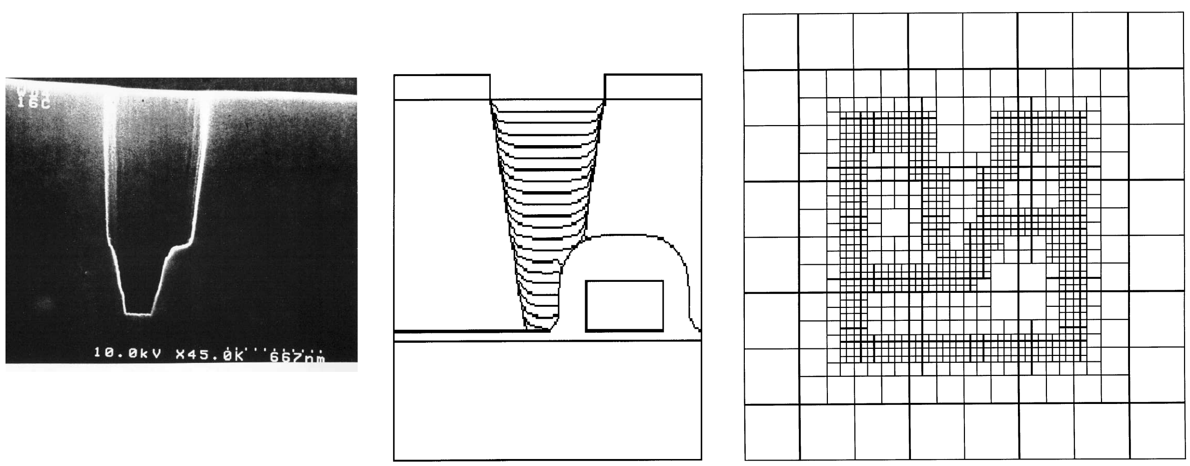
(a) (b)

Figure. 4: PECVD of SiO_2 from TEOS in a trench. (a) The SEM. Process conditions: $375^{\circ}C$, 2.1 Torr, Sc = 0.07, incoming ion impact-angle distribution: $\cos^{10}(\theta)$, ratio of neutral-to-ion component = 2, TEOS flow rate = 1.8 sccm, O_2 flow rate = 6.5 slm. (b) The simulated profile evolution.



(a) (b)

Figure. 5: Ionized magnetron physical vapor deposition (PVD) of aluminum in a trench. (a) The SEM. (a) The simulated profile evolution. Simulation conditions: temperature below $100^{\circ}C$, 35 mTorr, Sc = 1.0, unidirectional ion distribution, neutral-to-ion flux ratio = 7:3, sputter yield = 0.0.



(a) (b) (c)

Figure 6: Self Alignment Contact formation. (a) The SEM picture, courtesy of J. Nulty, Cypress Semiconductors. (b) The simulated profile evolution. (c) The adaptive quad-tree mesh corresponding to the final profile. This example also demonstrates the capability of the geometry server to handle multiple interfaces.