Modeling and Characterization of Three-Dimensional Effects in Physical Etching and Deposition Simulation

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INTRODUCTION: With the ever decreasing transistor feature sizes, scaling of interconnect has caused many new challenges in fabrication technology. Three-dimensional (3D) geometrical effects due to mechanical stress and electrical charge on short-length or sharp-corner conductors and dielectrics has become more prominent in analyses of IC process variation, leakage current and reliability. Calibration of etching and deposition simulation has been mostly performed on 2D geometrical profiles based on infinite-width approximation, not only because 3D simulation tools are much more computationally expensive and not widely available, but also because 3D profile characterization methodologies are limited by insufficient accuracy in positioning 2D cross-section measurements. 3D effects can alternatively be characterized by indirect electrical measurements such as dielectric breakdown voltage and enhanced electromigration at sharp corners, and resistance variation in 3D stringers and spacers. Modeling and characterization of 3D effects for etching and deposition, extended from physical models calibrated in 2D, will be discussed in view of boundary movement accuracy and robustness[1], and methodology for calibration with direct measurements. An L-shaped test structure will be used as a technology example[2].

3D GEOMETRY AND FIELD SERVER: For the next decade, it is still expected that many algorithmic improvements on numerical methods and computational geometry for 3D problems will be proposed. To benchmark and integrate these improvements under one software environment, recent advances in software engineering to maintain source code consistency and robustness such as object-oriented programming (OOP) are very helpful. The open architecture of SUPREM OO7 TCAD environment is designed to allow easy integration of new gridders[3], boundary movement methods[4], new physical definition and new solvers[5]. Communication with the SUPREM OO7 geometry/field server requires no specific data structure on either the tool or server side; only the access *methods* to wafer information and common geometry/field utilities such as boundary movement and error adaptation are specified in a restricted set of well-documented operational protocols named as the minimal semiconductor wafer representation (SWR) procedural interface. The TCAD open architecture is an ideal environment for characterization of 3D effects in etching and deposition, since various gridding and boundary movement methods can be tested and compared.

ACCURATE AND ROBUST BOUNDARY MOVEMENT: Owing to many special rule-based algorithms necessary to handle delooping and boundary collision, the Lagrangian type of boundary movement has shown accuracy and robustness problems when physical models and conservation laws are applied. This is especially serious in 3D since the number of grid points needs to be controlled more stingily to achieve engineering reasonable simulation time[2,4]. We have implemented the 3D level-set boundary movement method[1] using the oct-tree based adaptive Eulerian mesh in the SUPREM OO7 environment. Different conservation schemes such as Huygens' principle (deposition rate limited) and mass conservation (reaction rate limited) can be easily implemented. Curvature dependent boundary movement velocity and choice from multiple weak solutions at sharp corners can be accurately treated. In 3D, usually the deposition/etching rate calculation in physical models is most time consuming. Computational overhead in level-set function evaluation and extraction of boundary representation for visibility calculation is very small. Use of adaptive Oct-tree mesh has demonstrated good tradeoffs between efficiency and accuracy.

3D CHARACTERIZATION AND TECHNOLOGY EXAMPLES: An L-shaped test structure, with Ti/Al deposited over SiO_2 by physical vapor deposition (PVD), has been used for characterization of 3D effects. Figures. 1-2 show top views from SEM and simulation and Fig. 3 shows the location of 2D cross sections. The physical model for the depostion rate is from SPEEDIE 3D[2]. The infinite-width approximation where 2D simulation is used for 3D structures is quite acceptable for cross section 1, but poor for 2 and at corners. Comparison of the two initial-grove sizes at cross section 3 can give a reasonable estimate on the accuracy of the 45 degree cutting angle. The positioning of SEM at cross sections 4-6 can be reasonably obtained by comparing the initial grove sizes. Comparison of the two initial-grove sizes at cross section 6 can give a reasonable estimate on the accuracy of the cutting angle. The SEM and simulation results of the cross sections are shown in Figs. 4-9. Not only that 3D effects, such as the flattening and thinning of the bottom coverage going into the corners, can be clearly observed from comparing the cross sections, good match between SEM and simulation also shows the physical model and the boundary movement method are *accurate in 3D*. This is an important starting point for genuine 3D analyses on more complex structures. Other technology examples will be shown in the conference.

ACKNOWLEDGEMENTS: This work is supported by ARPA and SRC.

[1] D. Adalsteinsson and J.A. Sethian, *J. Comp. Phys.*, **122**, 348(1995).
[2] D.S. Bang, et. al., *IEDM*, 1995, p. 97.
[3] Z.H. Sahul, et. al., *IEEE Trans. Semi. Manu.*, **9**, 35(1996).
[4] Z. Hsiau, et. al., *IEDM*, 1995, p. 101.
[5] D.W. Yergeau, et. al., *SISDEP*, 1995.

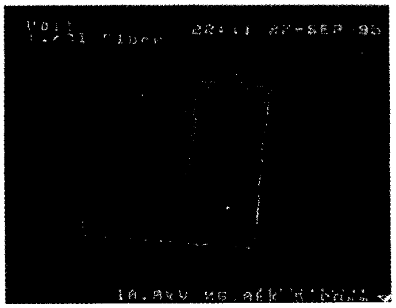

Fig. 1 Top view of elbow

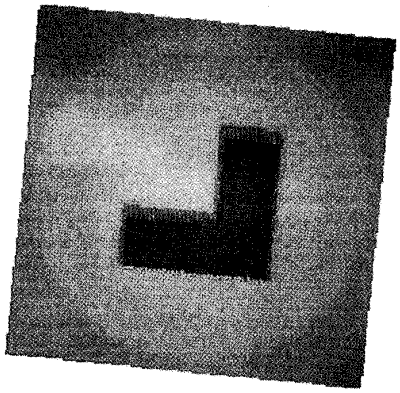

Fig. 2 Top view of simulation

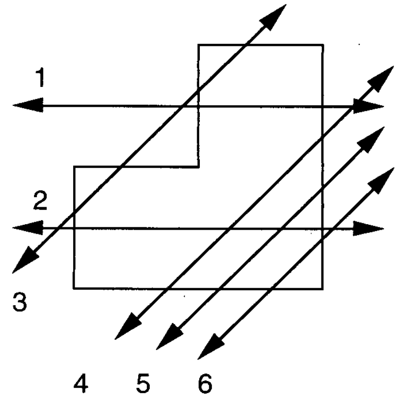

Fig. 3 Cross section schematics

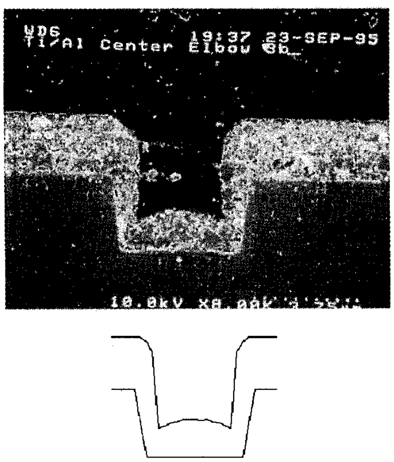

Fig. 4 SEM and simulation at cross section 1

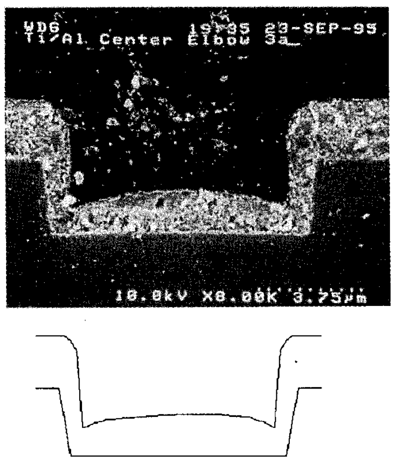

Fig. 5 SEM and simulation at cross section 2

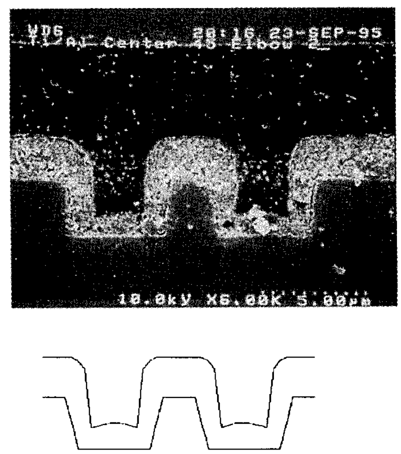

Fig. 6 SEM and simulation at cross section 3

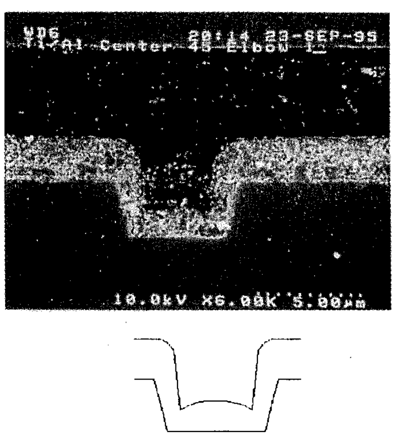

Fig. 7 SEM and simulation at cross section 4

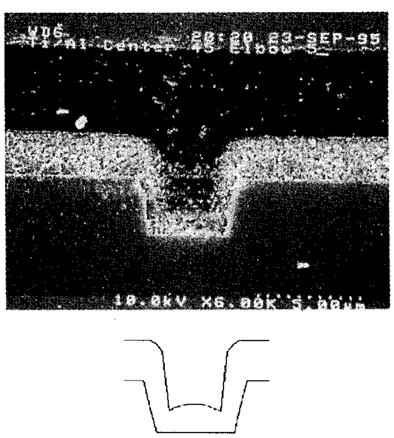

Fig.8 SEM and simulation at cross section 5

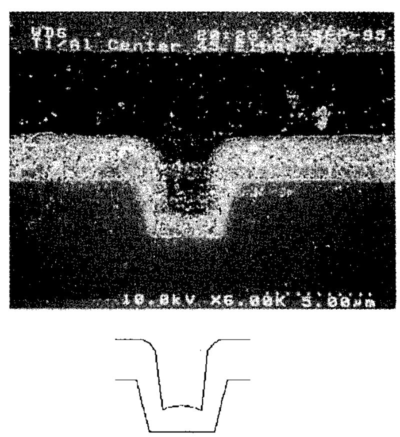

Fig. 9 SEM and simulation at cross section 6