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Three Dimensional Simulation for Sputter Deposition Equipment and Processes

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Abstract

A three dimensional sputter deposition simulator based upon the SPEEDIE topography simulator is presented. The simulator combines equipment models with topography evolution models in order to predict topography for VLSI metallization. Equipment scale simulation is used to determine 3D particle flux for specified wafer points. The particle flux is then used by a 3D topography simulator to determine profile evolution. The generality of the topography simulator allows deposition simulations to be performed on structures with asymmetries in the x, y, and z-directions. Examples of metal deposition simulations for contact and dual-damascene structures are presented.

1. Introduction

Sputter deposition is one of the most widely used techniques for metal deposition in VLSI fabrication. Previous approaches to modeling of sputter deposition either focused on equipment scale simulation or VLSI topography simulation [1,2]. More recent simulators combined equipment scale simulations with topography scale simulations, but continued to used symmetric VLSI topographic structures [3,4]. In this paper a 3D extension of the SPEEDIE process simulator is presented which combines equipment scale simulations with general 3D topography simulation [5].

2. Sputter Equipment Simulation

For sputter system modeling, the program uses target erosion, target emission, chamber dimensions, and analytic particle transport equations in order to determine 3D particle flux distributions for points across the wafer surface (Fig. 1). The analytic particle transport equations are generalized extensions of previous models [6-8], and are valid for chamber pressures below 2 mTorr, where the mean free paths for Al and Ti is comparable to a typical target to wafer throw distance of 5 cm [9]. Particle collisions may be considered with a Monte Carlo module which simulates collisional particle transport from target to substrate.

3. VLSI Topography Simulation

For thin film deposition process modeling, particle sticking coefficient, particle surface diffusion, and the calculated angular distribution at the substrate are applied to an initial substrate topography to determine the film's profile evolution (Fig. 2). The generality of the topography simulator allows deposition simulations to be performed on structures with asymmetries in the x, y, and z-directions (Fig. 3). Sticking coefficient is defined as the probability that a particle which strikes a surface remains at that surface. Previous experiments determined the Ti sticking coefficient to be 1.0 and surface diffusion to be negligible for sputter deposition at 250° C [9].

Film evolution is comprised of three parts: local flux calculation, surface velocity calculation, and surface regridding. Ray tracing algorithms which compares each grid's visibility versus every other grid are used to determine each surface element's visibility and direct particle flux. Surface velocity for each grid is proportional to its net flux, and the velocity of each surface node is calculated by averaging the surface velocities of each grid which surrounds the node. Initial and subsequent surface meshing is performed with ICEM [10]. The entire surface mesh is regridded after each iteration, eliminating grids which are too large, too small, or of a poor area to perimeter aspect ratio. Variable gridding size is implemented by defining subregions on the surface mesh. Surface loops are eliminated during regridding by meshing the volume above the surface topography and then keeping only those surface elements which border the meshed volume.

4. Summary

A three dimension sputter deposition simulator which combines 3D equipment scale models with 3D VLSI feature scale models to determine profile evolution for metal film deposition was presented. Examples of metal contact filling and a dual damascene liner depositions were presented with the simulator.

Acknowledgment

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References

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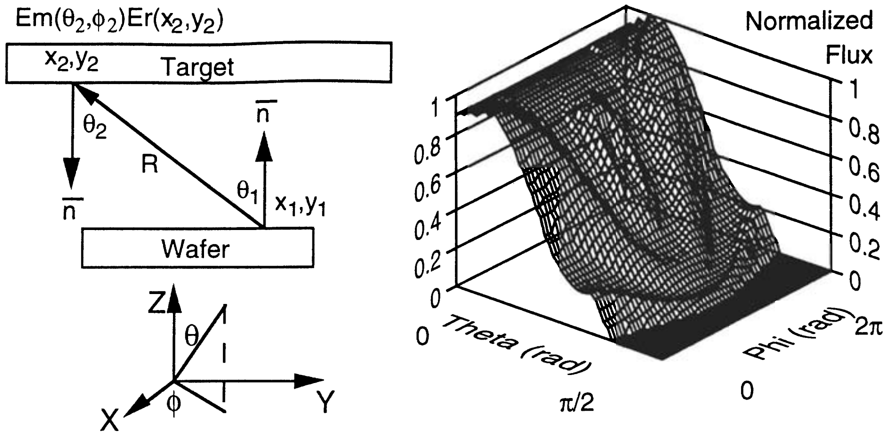
[10] ICEM is a commercial gridding program developed by ICEM CFD Engineering.



$$dFlux_{x_1,y_1}(\theta_1,\phi_1) = \frac{\cos(\theta_1)Em(\theta_2,\phi_2)}{\pi R^2}Er(x_2,y_2)dArea_{target}$$

Figure 1: The sputter system simulator uses target erosion data (Er), target emission data (Em), and chamber dimensions to determine 3D particle flux for specified wafer points. The analytic equations are valid for deposition below 2 mTorr. In this example, target erosion data and chamber dimensions for an Applied Materials system assuming cosine target emission was used to calculate the 3D flux for an off center wafer position.

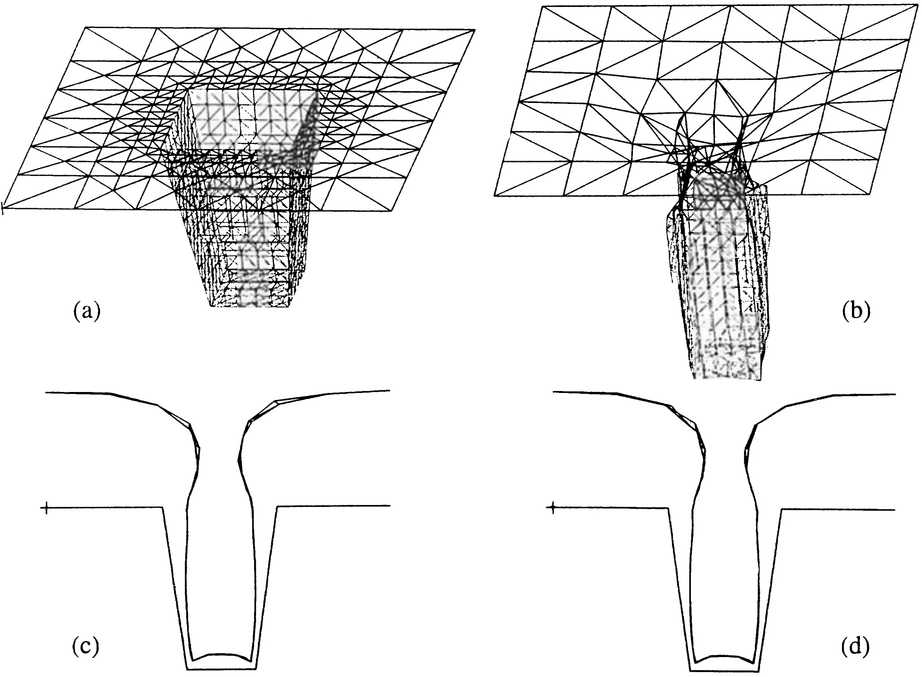


Figure 2: Simulation of 0.5 micron Ti into 0.5 micron square contact using sticking coefficient of 1.0, negligible surface diffusion, and distribution function from Fig. 1. (a) original surface mesh, (b) surface after deposition, (c) (d) two planer cross sections. Grid shading is for illustrative purposes and double grid lines in (c) and (d) represent grids which are not exactly perpendicular to the cross section plane.

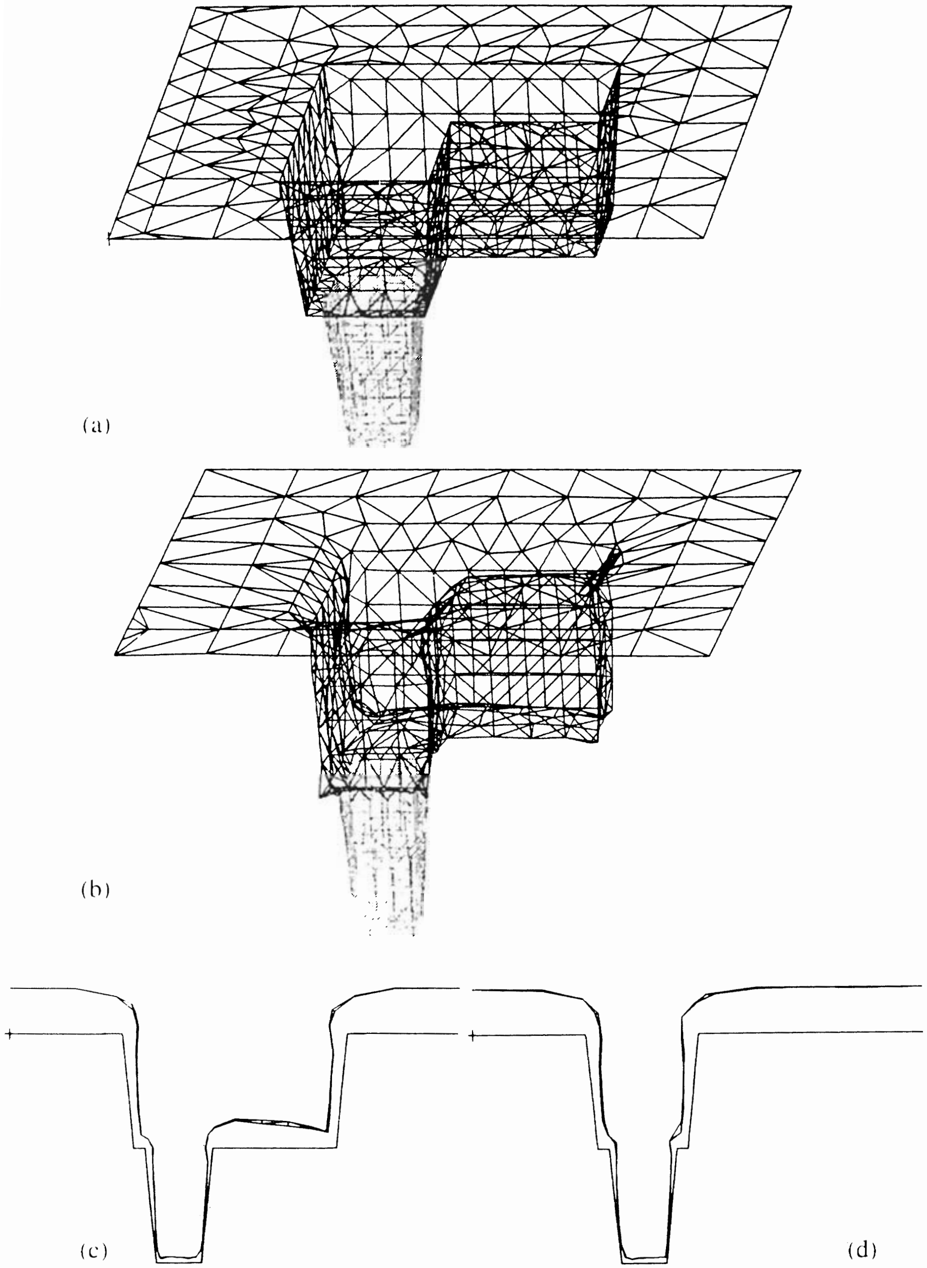


Figure 3: Simulation of 0.2 micron Ti deposition into a dual-damascene structure where the contact opening is 0.3 microns using sticking coefficient of 1.0, negligible surface diffusion, and distribution function from Fig. 1. (a) original mesh, (b) surface after deposition, (c) (d) two planer cross sections. The ability of the simulator to capture x, y, and z-axis asymmetries caused by surface asymmetries and off-center wafer position are shown in this figure. Grid shading is for illustrative purposes and double grid lines in (c) and (d) represent grids which are not exactly perpendicular to the cross section plane.