Numerical Simulations of Sputter Deposition and Etching in Trenches using the Level Set Technique

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ABSTRACT

We have performed 2D and quasi-3D numerical simulations of physical vapor deposition (PVD) into high aspect ratio trenches used for modern VLSI interconnects. The topographic evolution is modeled using (continuum) level set methods. The level set approach is a powerful mathematical/computational technique for accurately tracking moving interfaces or boundaries, where the advancing front is embedded as the zero level set (isosurface) of a higher dimensional mathematical function. The technique can be equally well applied to etching, including the incorporation of complex mask shapes. First, we study 2D cases for long rectangular trenches including the quasi-3D case in which the 3D target flux is mathematically reduced to an equivalent 2D flux. The 3D flux is obtained from molecular dynamics computations for Al(100), and hence our approach represents a hybrid atomistic/continuum model. We obtain good agreement with X-TEM data. Finally, we present results for etching problems of relevance to shallow trench isolation in electronic devices.

Keywords: sputter deposition, process simulation, level sets.

INTRODUCTION

The topographic evolution of moving interfaces has traditionally been simulated numerically using front-tracking (marker-particle/segment-based) methods. One major drawback in this approach is the formation of "swallowtails" when two adjoining line segments are advanced and cross one another. These overlapping segments (surfaces in 3D) must then be "de-looped" in order to obtain a single-valued surface. This de-looping involves complex decision rules and programming and requires excessive CPU time. The level set technique was introduced by Osher and Sethian (1) as a promising and fast alternative to front-tracking. In this paper we describe the implementation of this new mathematical technique to model back-end materials processes such as metal film sputtering and etching.

MATHEMATICAL APPROACH

Problem Statement

We are concerned with deposition into, and etching of, long rectangular trenches. In Figure 1 we plot a schematic drawing of the geometry for PVD from a finite target onto asubstrate with local surface normal **n,** inclined at an angle δ to the vertical. We denote the left- and right-hand side visibility angles β_L and β_R. The growth rate of the film at each point of the interace is determined by the "visible" area of the sputter target, which has to be computed by ray-tracing methods. The interface evolution is then computed using level set methods.

Level Set Technique

The level set approach embeds the interface, Γ (a curve in 2D), in a higher dimensional function, ϕ (a surface in 2D). In 2D, if we denote the co-ordinates as x and y, then the function $\phi = \phi(x,y) = \pm d(x,y)$ (where d is the signed distance from (x,y) to the nearest point on the interface, Γ), represents a single-valued surface in the (non-physical) z-direction. By this construction, the interface Γ is simply the zero level set of ϕ. The best analogy to visualize this mathematical construction is a lake shoreline. The shoreline is $\phi(x,y) = 0$; inside the lake $\phi(x,y) < 0$ and the (dry) shore is given by $\phi(x,y) > 0$. This analogy is depicted in Fig.ure 2. Continuing with this analogy, adding sand so that the water level rises causes the zero level set to propagate.

The evolution of ϕ, and thus of Γ, can be described by a partial differential equation, as described in Refs. (1,4). For brevity, we simply state here that if the level sets propagate normal to themselves with speed $F(x,y)$, then ϕ evolves according to

$$\frac{f\ddot{o}}{ft} + F\left|\quad \ddot{o}\right| = 0 \qquad (1)$$

This is a Hamilton- Jacobi type equation which can be solved relatively straightforwardly employing (standard) numerical techniques from the field of compressible gas dynamics. The tremendous over-arching benefit of this approach is that these numerical methods evolve $\phi(x,y)$

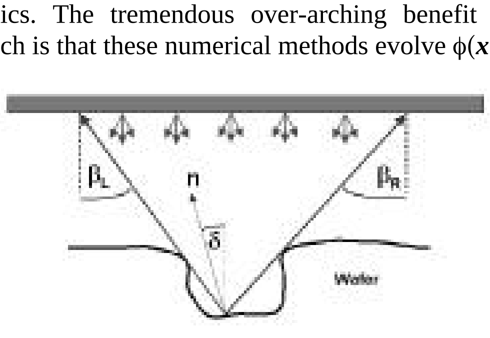

Figure 1: Schematic drawing of target/wafer sputter geometry with surface normal and target visibility angles indi

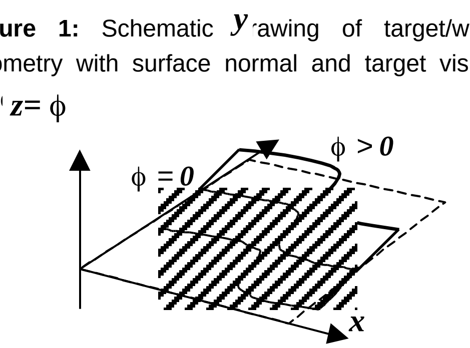

Figure 2: Schematic drawing of 2D level set function. The curve Γ is given by $\phi = 0$, $\phi < 0$ indicates regions beneath the wafer's surface and $\phi > 0$ indicates open space above the wafer.

correctly without the intricate task of de-looping. In particular, the zero level set, Γ (the curve of interest), can pinch-off, merg or undergo any complex morphological transitions while the level set function $\phi(x,y)$ remains well-behaved. See Ref [4] for a thorough introduction.

Quasi-3D Flux

In 2D models of PVD into trenches it is imperative to take into account full 3D (i.e. out-of-plane) flux sources. In this section, we outline a mathematical derivation for "re-normalizing" a fully 3D flux for such 2D simulations.

Figure 3 shows a schematic diagram for full 3D sputter deposition from an infinitesimal target area element $dA = dx\,dz$ which travels a distance r to reach a substrate location, taken to be at the origin. The angle between this ray and the surface normal is γ, while the angle between the ray and the downward normal from the target is θ.

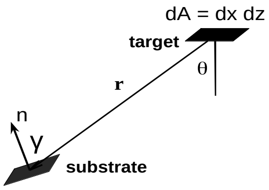

Figure 3: Schematic diagram for 3D sputter deposition

The material flux at the substrate depends both on γ (fixed for each location) and θ which depends implicitly on the (x,z) location of dA. The final net flux at the substrate (which determines the speed function, F, in Eq. (1)) is given by

$$F_{3D} = \int_{\substack{visible\\target}} \frac{f_{3D}(\theta)\cos\gamma}{r^2}\,dxdz \qquad (3)$$

where $f_{3D}(\theta)$ denotes the angular distribution of atoms leaving the target (namely, the target flux). It is common in sputter deposition to assume a cosine flux law for species emission from the target. However, it is well known that this is merely an approximation to real systems. Gilmer [2] has performed a 3D molecular dynamics (MD) simulation for Al(100) and obtained an appropriate target emission distribution as a function of polar angle, θ (averaged over the azimuthal angle, ψ), which differs substantially from the cosine law. We denote this flux as $f_{3D}(\theta)$ and plot it in Figure 4. In order to use the flux law derived from MD in our simulations, $f_{3D}(\theta)$ is approximated using the expansion

$$f_{3D}(\theta) = \sum_{k=1}^{M} A_k \cos^k\theta \qquad (2)$$

The coefficients, A_k, are determined by a (non-linear) least squares fit (using $M=8$).

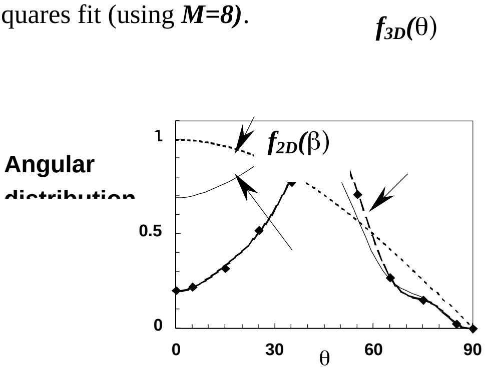

Figure 4: 3D MD emission flux (symbols+curve fit); equivalent 2D target flux (solid curve) and cosine target flux (dotted).

For a trench that is uniform in the z-direction and which has a flux as given by Eq. (2), the z-integration can be evaluated analytically. Hence, the equivalent 2D flux based on an <u>equivalent</u> line source is

$$f_{2D}(\beta) = \sum_{k=1}^{M} C_k A_k \cos^k\beta \qquad (4)$$

where β is the emission angle from the (2D/line) target. The coefficients are given recursively by

$$C_0 = 2, C_1 = \pi/2, C_n = \frac{n}{n+1}C_{n-2}, \text{ for } n \geq 2 \qquad (5)$$

This expansion in turn can be integrated analytically to obtain the total flux at the substrate. It should be noted that only in the case of a simple cosine distribution can the 3D flux be used directly in a 2D simulation. For more complex flux laws, the 3D flux must be re-normalized.

RESULTS

Deposition

Figure 5 shows results from a deposition simulation of 1500 Å of material into a trench using both the cosine flux (***M=1)*** and the MD flux (***M=8***). (Note: for all simulations we found that a 200x200 grid was sufficient for convergence and each simulation took less than 3 minutes to execute on a DEC Alpha 21164 machine). The most significant difference is in the bottom coverage where the MD flux predicts 18% lower coverage.

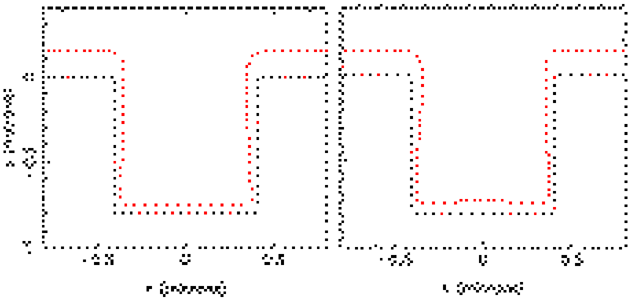

Figure 5: Simulated sputter deposition (1500 Å) into long rectangular (2D) trench. Left: using renormalized 3D MD flux law; right: using cosine flux law.

Etching

As a further demonstration of our 2D code's flexibility we have also performed simulations of wet chemical etching. In Figure 6 we have plotted numerical results of etching SiO_2 with a *HF*-based solution which does not attack *Si*. The *Si* substrate therefore acts as an etch-stop. This effect is implemented by prescribing a bounding curve for the *Si* and setting ***F=0*** if or when the interface (zero level set) crosses this boundary. We see "divot" formation in the SiO_2/*Si* junction region consistent with that observed experimentally by Chang et al. [3].

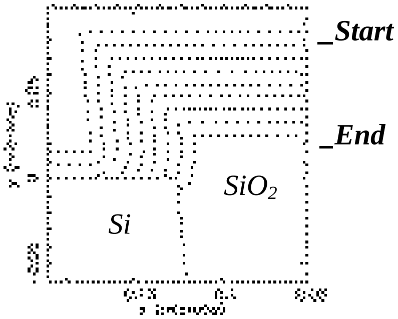

Figure 6: Simulation of wet chemical etching of SiO_2 shallow trench isolation.

Experimental Validation

We now compare our simulations to experimental data obtained from a cross-sectional transmission electron micrograph (X-TEM) of a 550 Å thick Ta barrier film which was sputtered onto trenches etched into SiO_2. Equation (1) is solved taking into account finite target visibility and shadowing effects for sputter deposition.

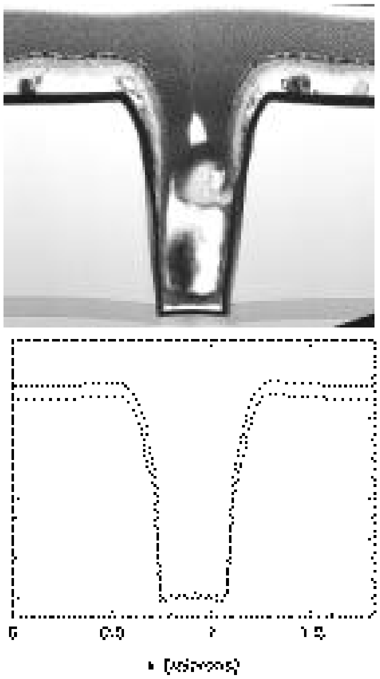

Figure 7: Deposition of 550 Å Ta barrier film. Top: XTEM; bottom: simulation.

The simulation was carried out using the same parameters for target radius and initial target-substrate distance as in the experiment (15 cm and 6.2 cm, respectively). We assume that the working material is a refractory metal with sticking coefficient of unity. The comparison of this numerical simulation with the TEM is shown in Figure 7, where we see good qualitative agreement.

CONCLUSIONS

Our numerical simulations indicate that we are able to capture the main aspects of deposition and etching with high accuracy using level set methods. Currently, we are extending our code's capability to 3D and also incorporating higher order physical effects.

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