Void Development in Plasma Enhanced CVD Models

D. Adalsteinsson
J.A. Sethian

Dept. of Mathematics, MailStop 50A-2152
Lawrence Berkeley National Laboratory, Berkeley 94720
510-486-5695/Fax=510-486-5101

and

Juan C. Rey
Technology Modeling Associates

Abstract

In this paper we describe the implementation of Plasma Enhanced CVD (PECVD) models. We show numerical results for a fully three dimensional structure using level set method techniques. The terms being simulated contain both an isotropic and a source deposition term, along with the effects of reflection and re-emission.

Overview

Void formation when depositing thin dielectric layers is a major contributor to reliability problems of integrated circuits. The experimental study of these voids in three dimensional structures is very expensive because of the large number of initial topographies and the time/equipment required to analyze the resulting data. Here, we describe an implementation of Plasma Enhanced CVD (PECVD) models and results for three-dimensional structures based on level set methods. Deposition simulations in full three-dimensional structures offer many challenges. Models and simulations developed for two-dimensional structures (such as very long trenches or cylindrically symmetric contact holes) require large computer resources when extended to general three-dimensional structures. In particular, (PECVD) processes require flux calculations of direct fluxes from the gas phase from isotropic as well as general angular distributions and re-emission fluxes characterized by a sticking coefficient.

Our implementation describes the modeling of PECVD based on the contribution of an Ion Induced Deposition component which is proportional to the direct ion flux arriving at every point of the structure and a chemical vapor deposition component characterized by a re-emission flux. To characterize the ion angular distribution we use an analytical expression given by a $\cos(\theta)^n$ where θ is the angle between the normal of the wafer and the incoming ion direction and n is an integer exponent.

This paper applies a robust simulation technique to investigate this problem, and explore the effects of each of the different physical mechanisms involved in this process. This technique allows for topological changes, and the combination of multiple simultaneous effects.

Level Set Techniques

Level set techniques [5, 4, 6] numerically approximate the equations of motion for a propagating front by transforming them into an initial value partial differential equation, whose unique solution gives the position of the front. In this setting, corners and cusps are naturally handled, and topological change occurs in a straightforward and rigorous manner.

Level set techniques, introduced in [4] on the basis of work in [5], have been used to simulate problems in the field of etching, deposition, and photolithography [1, 2, 3]. Our general level set etching/deposition methodology allows the combination of different physical terms, which include the effects of visibility, masking, non-convex sputter laws under ion milling, bulk diffusion, and reflection and reemission. This works is a continuation of previous work[1, 2, 3], and papers presented at the last two VMIC conferences.

A short description is as follows. To advance the front, we create a function ϕ, defined in all of space, which has the front as its zero level set, is positive on one side of the front and negative on the other side. For example, one such function is given by the distance function which at every point is equal to the shortest distance to the front, where the sign is positive/negative when the winding number is even/odd.

The movement of the front is translated into a movement of this function, such that the zero level set of the new function is the location of the new front. The benefit of this approach is that even though the points on the front move in a very complex manner, the change in the function is just a pointwise change of values. In this view, corners, cusps, merging and breaking do not pose any numerical difficulties.

More precisely, let γ be the initial front, and let ϕ be a function as described above. Assume further that ϕ is continuous and differentiable. Let F be a function defined on all of space such that if the front goes through the point x, the speed of the front in the normal direction is equal to $F(x)$. The movement of the ϕ function is then given by the partial differential equation

$$\phi_t + F|\nabla\phi| = 0$$

where $\phi(x, t = 0)$ is the initial surface. For the derivation of this PDE see [4]. Intrinsic geometric properties such as normals, curvature etc are easily determined from the ϕ function by using standard finite differences. This formulation is applicable to any number of space dimensions, and for arbitrary geometries. For details of how to evaluate the terms, numerical boundaries, time evolution etc, see [6].

A complete review of level set methods and its applications can be found in [6]

Numerical Aspects

In this paper we use analyze the effects of two types of deposition terms: isotropic deposition and source deposition. We allow some of the source deposition component to be re-emitted and redeposited on the front.

For the isotropic deposition the normal speed F is independent of the location and position of the front, and thus is constant. For the source deposition, it is necessary to include the effects of visibility. To do so, we discretize the source into individual directions, each direction representing a solid angle. The length is equal to the strength of the light source in that direction. In our case we use both a source distribution of $\cos(\theta)$ (uniform) and $\cos^5(\theta)$. To increase computational efficiency, the distribution of these directions is taken as proportional to the intensity of the lightsource, so that in the directions where the intensity is the most the angular domain is tightly discretized. A typical discretization involves around 400-1000 directions. The light intensity is the integral over the visible domain, which is approximated by a sum of the visible directions, where each direction vector is weighted with the solid angle that it represents.

The model for reflection and re-emission is as follows. Define I_0 to be the incoming intensity, I_R is the intensity reflected off the source, I_A the intensity arriving at the front. All these properties are functions defined on the front. Let β be the proportion that sticks on the front. Then we have the following equation

$$I_A(x) = I_0(x) + \int_{Visible} I_R(y) \frac{cos(\theta)cos(\theta')}{\pi r^2} dA$$

where θ and θ' are the angles between the normals and the line between the points x and y. r is equal to the distance between x and y. We also have

$$I_R = (1-\beta) I_A.$$

To discretize this, divide the surface up into small voxels. For each voxel we need to sum over the other voxels to get the incoming intensity. Define Ψ_{ij} to be 1 if voxels i and j are visible from each other, and 0 otherwise. The above integral changes into a sum over all the other voxels:

$$I_A(i) = I_0(i) + (1-\beta) \sum_{i \neq j} I_A(j) \Psi_{ij} \frac{\cos(\theta_{ij}) \cos(\theta_{ji})}{\pi r_{ij}^2} A_j$$

Where A_j is the area of voxel j. Define the matrix Ω by

$$\Omega_{ij} = \Psi_{ij} \frac{\cos(\theta_{ij}) \cos(\theta_{ji})}{\pi r_{ij}^2} A_j$$

Then the above equation can be written as

$$I_A = I_0 + (1-\beta) \Omega I_A$$

If I_S is the intensity that sticks, and leads to the surface advancement, $I_S = \beta I_A$ so that

$$I_S = \beta (I - (1-\beta)\Omega)^{-1} I_0$$

To solve this numerically, one can either use a matrix solver, or use a Taylors series expansion of the term $(I-A)^{-1}$, $A = (1-\beta)\Omega$. The sum is truncated when the remaining terms become less than some small fraction of the first term in the series.

This gives the source intensity and speed on the front. To compute the speed function F on the domain it is necessary to extend the speed off the front onto the gridpoints around the front. Once the intensity has been found on all of the domain, the speed function F follows directly from it.

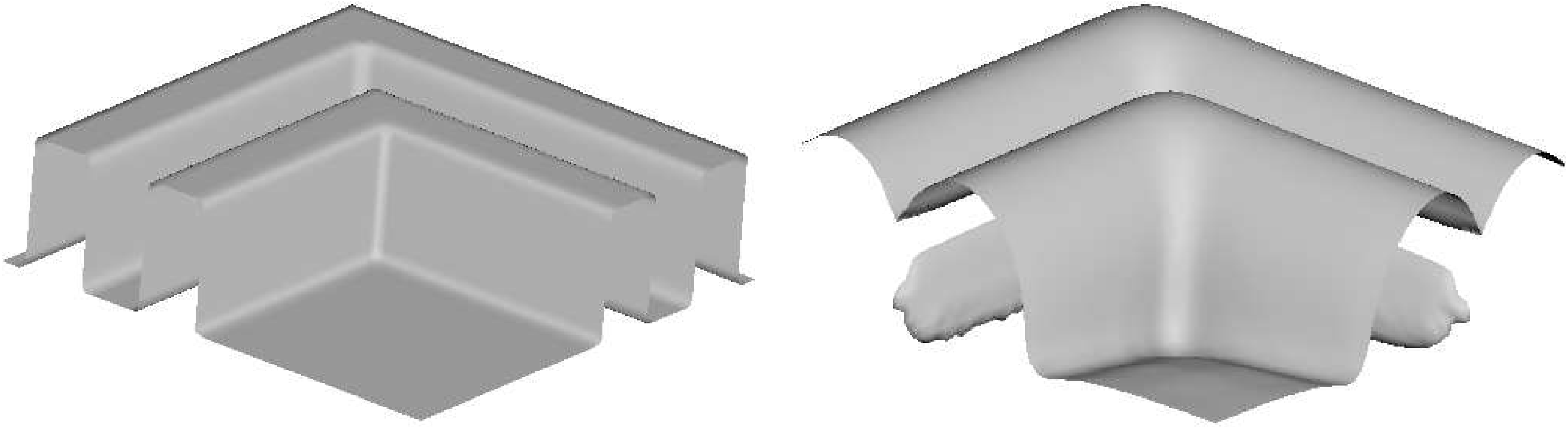
Results

A typical three–dimensional structure that offers challenges is the one shown in Figure 1, in which two long parallel aluminum traces bend in a square angle. The deposition of a non-perfectly conformal interlevel dielectric layer creates large voids between the parallel traces; in many cases, the voids are also formed in the larger area inside the 90 degree angle between the traces. While the void in the angle is usually smaller, it reaches higher and may be exposed later during a planarization step when using chemico-mechanical polishing. The void formation is controlled by both the ion angular distribution as well as the re-emission component (larger sticking coefficients produce larger voids), however in the case when the sticking coefficient becomes very low, the re-emission component is almost isotropic and the void is controlled only with the spread of the angular distribution. The example shown in Figure 1a,b is the result of a deposition term of the form $\cos(\theta)^5$ together with an isotropic deposition term to account for a very small sticking coefficient.

The isotropic deposition is 10% of the strength of the source deposition. In all of these tests, the light sources are normalized so that at 100% strength on a level surface the deposition rates are the same.

A more accurate simulation, especially for those with a larger sticking coefficient, includes the true effect of re-deposition which leads to a full 3D reflection problem. In Figure 2a,b we show results in which instead of the isotropic deposition term we have a source deposition term with sticking coefficient 0.1. In figure 2c we show one of the cross sections to display the time evolution.

This is a continuation of earlier work [1, 2], and related simulations can be found in [3].



Initial position

Final position

Figure 1: Evolving Structure:Note the developing void.

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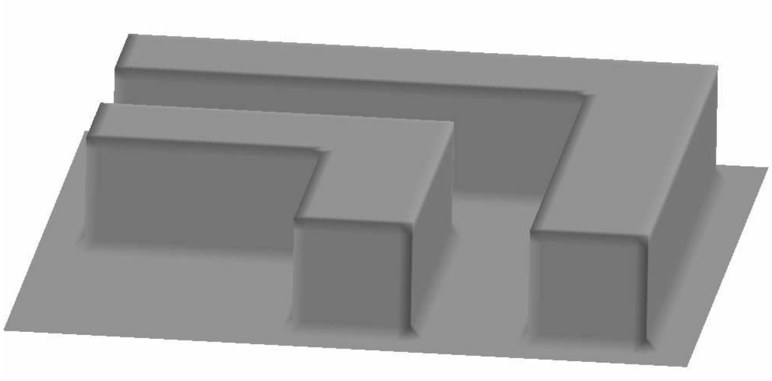

Fig. 2a: Initial Position

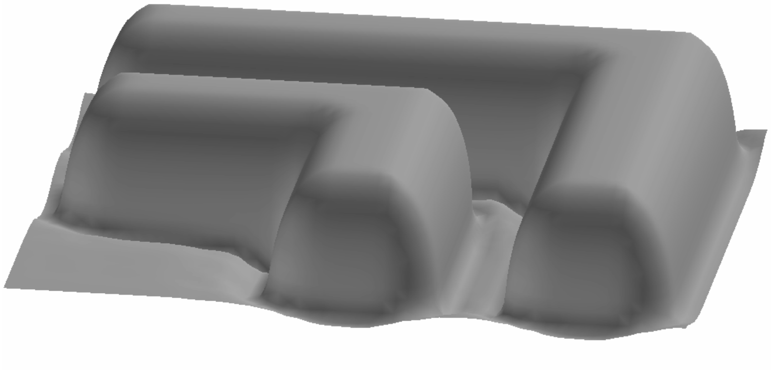

Fig. 2b: Time Evolution

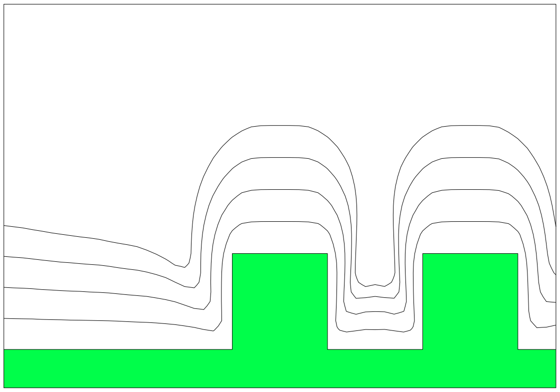

Fig. 2c: 2d Cross-Section

Figure 2: Three-dimensional Evolution under Cosine Source Distribution with Sticking Coefficient .1
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