Three–Dimensional Profile Evolution under Low Sticking Coefficient

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***Abstract*—This paper describes a careful numerical study of the effects of low sticking coefficient for two and three dimensional structures. The model for reflection is a cosine re–emission distribution with no dependence on the distribution of incoming particles. We calculate the limiting case for several different initial topologies. We conclude that the limiting profile can not in general be replaced by an isotropic deposition term, and demonstrate the effects of low sticking coefficient on complex structures.**

I. Introduction

In this paper we study re–emission for deposition. Throughout, we assume a problem where there is a source above a wafer. The particles either partially deposit on the surface or reflect off and deposit elsewhere. We assume a constant sticking coefficient with a cosine re–emission distribution, consistent with SiH desorption measurements from Si [5]. This paper focuses on this effect, and ignores secondary effects such as surface diffusion.

We consider primarily three dimensional problems. We analyze two types of problems, an axially symmetric problem which is simulated as a two-dimensional problem, and a full three dimensional problem. In both cases, we solve the same speed equation, and the numerical techniques are similar. Both calculations can easily be performed on a modern workstation, and we used Sun Ultra and Apple Power Macintosh workstations for our calculations.

II. Equations of motion

We begin by deriving the equation for the incoming intensity on the surface, which depends on the reflected dependencies off other parts of the front, and will lead to a integral equation. We will also derive the analytical limit when the sticking coefficient tends to zero.

A. General Equation

For a given surface Γ, define $S(x)$ to be the incoming source strength at a point x on Γ, and β to be the sticking coefficient. Let S^0 be the source strength arriving from the external sources. Since we are assuming a cosine re–emission distribution, we have that

$$S(x) = S^0(x)+(1-\beta)\int_{\Omega(x)} S(y)\frac{\cos(\theta(x,y))\cos(\theta(y,x))}{\pi|x-y|^2}dA,$$

where $\Omega(x)$ is the region of Γ which is visible from x, and $\theta(x,y)$ is the angle between the normal at x and the direction of the vector from x to y.

This equation can be written as

$$S = S^0 + (1-\beta)F(S),$$

where F is a linear function that maps functions on Γ into functions on Γ. Only a certain fraction (given by β) of this intensity leads to deposition on the surface, and if T is the deposition intensity, we then have that

$$T = \beta S^0 + (1-\beta)F(T)$$

B. Two-Dimensional Version

To formulate this problem in the axially symmetric case, we may rewrite the integral equation in terms of parameters given in the two–dimensional region.

We note that care must be taken, since even though the front motion can be assumed to be symmetric, visibility between pairs of points and information about the part of the source seen by each point must be computed using the full three–dimensional problem.

Define $Q_\alpha(x)$ as $Q_\alpha(x,y) = (x\cos\theta, x\sin\theta, y)$, which rotates a point around the z axis, and let P be the projection from a point on the surface onto the corresponding point in the two–dimensional section. The previous equation can now be written as.

$$S(x) = S^0(x) + (1-\beta)B(x),$$

where

$$B(x) = \int_{\Omega(Q_0(x))} S(P(y))\frac{\cos(\theta(P(x),y))\cos(\theta(y,P(x)))}{\pi|P(x)-y|^2}dA.$$

The surface can be parametrized by the two–dimensional path and the angle of rotation about the z axis.

$$S(x) = S^0(x) + (1-\beta)\int_{\text{Path}} S(y)G(x,y)y\cdot(1,0)dy,$$

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where

$$G(x,y) = \int \frac{\cos(\theta(Q_0(x), Q_\alpha(y)))\cos(\theta(Q_\alpha(y), Q_0(x)))}{\pi|Q_0(x) - Q_\alpha(y)|^2} d\alpha,$$

and the integral is over the angles α such that $Q_0(x)$ and $Q_\alpha(y)$ are visible to each other in the three–dimensional problem.

The normals at the points $Q_\alpha(y)$ can be written in terms of the two–dimensional normal to the path at the point y.

C. Low Sticking Coefficients

Consider the problem where the sticking coefficient is very close to 0. Normalize the problem so that βS^0 is constant independent of β, that is for a given β we are interested in the solution of the problem

$$T_\beta = T^0 + (1-\beta)F(T_\beta).$$

We wish to see how this behaves as β becomes arbitrarily small. Assuming continuity, the limit T_0 must satisfy

$$T_0 = T^0 + F(T_0).$$

In our simulations, we considered both problems, and analyzed the behavior as we reduced the sticking coefficient.

III. Numerical Implementation

Before discussing the results of the simulations, we describe the numerical methods that go into solving this problem. We must calculate the intensity on the front for both the two and three–dimensional problem and advance the front in time. To find the source intensity, we need to solve an implicit problem. We discretize the front into line segments in two dimensions and panels in three dimensions.

If $S = (S_i)$ is the discretization of the source strength along the front, the function $F(S)$ can be written as a matrix vector multiply of the form $F(S) = \Omega S$, since F is a linear function. Thus, the problem that needs to be solved is

$$(I - (1-\beta)\Omega)S = S_0.$$

This solution must be produced at each time step of the evolution since the front and the discretization will change. This matrix is solved using an iterative technique rather than a general linear solver since we know additional information about the properties of Ω. For details see [4]

A. The Level Set Method

Central to this numerical technique is the use of the Level Set Method, introduced in [7], based on previous work in [8]. For details about Level Set Methods, see [9]; for modeling and simulations applied to topography evolution see [2]–[4].

The Level Set Method is a front propagation scheme, which views the front as the zero level set of a scalar function defined in all of space. For a given speed function, a partial differential equation is constructed for this scalar function, such that the motion of the zero level set tracks the motion of the front under the given speed function. The benefits of this approach are that topological changes of the front are easily handled, since the scalar function needs no special consideration for those cases. The advection of the scalar function needs to be done in a upwind fashion, borrowing techniques from fluid mechanics. For more information see [2], [7], [9].

The extra cost of casting this into a higher dimensional problem can be countered by using adaptive methods, described in [1].

B. The Source

For three–dimensional simulations it is impractical to calculate at each point on the front the exact region of the source that is visible. A better approach is to adaptively decompose the source into a collection of unidirectional vectors. The decomposition is made such that each vector represents the intensity from its corresponding solid angle, and the length (strength) of each vector is approximately the same for each vector. That way we resolve the angle regions where the source has high intensity better than the regions where the intensity is low (angle with the z axis is very large).

For each point on the front it is necessary to find which vectors are visible, and add up their contributions. It is possible to determine the visibility very efficiently by scanning through the ϕ surface in the direction of the vector, looking for intersections with the zero level set. The line $(x+tu, y+tv+z+tw)$ starting at a point on the surface and heading in one of the source direction needs to be projected down to two–dimensional cross section, where its trace will be the path

$$(\sqrt{(x+tu)^2 + (y+tv)^2}, tw)$$

C. Three–Dimensional Problem

From before, the strength of the incoming intensity is given by

$$S(x) = S^0(x) + (1-\beta)B(x),$$

where

$$B(x) = \int_{\Omega(x)} S(y) \frac{\cos(\theta(x,y))\cos(\theta(y,x))}{\pi|x-y|^2} dA.$$

If the surface is split into panels (P_j), and the intensity is sampled at points (x_j) inside those panels, we get the approximation

$$S_j = S_j^0 + (1-\beta)B_j,$$

where

$$\sum_i \int_{\Omega(x_j)\cap P_i} S(y) \frac{\cos(\theta(x_j,y))\cos(\theta(y,x_j))}{\pi|x_j - y|^2} dA.$$

Define

$$\Omega_{i,j} = \int_{\Omega(x_j)\cap P_i} S(y)\frac{\cos(\theta(x_j,y))\cos(\theta(y,x_j))}{\pi|x_j-y|^2}dA.$$

This changes the problem into finding the solution to the linear system

$$S = S_0 + (1-\beta)\Omega S.$$

D. Two-Dimensional Problem

Similarly as before, we split the front into line segments (P_j), and create the linear system

$$S_j = S_j^0 + (1-\beta)\sum_i \Omega_{i,j} S_i,$$

where

$$\Omega_{i,j} = \int_{P_i} G(x_j,y)y\cdot(1,0)dy.$$

Special care needs to be taken when computing the visibility that goes into $G(x_j,y)$. This is because it is not enough to determine if two points are visible in the two-dimensional cut or not. For each pair (x,y) of points on the path, we must find the angles α such that the the point $Q_\alpha(y)$ is visible from $Q_0(x)$. This turns out to be the union of two intervals. These intervals can be found by scanning over the front. If N is the number of segments on the path, the cost of this visibility calculation is $O(N)$ and since there are N^2 points on the front, the cost of creating the matrix is $O(N^3)$.

E. Solving the Matrix Equation

When solving the system $(I-(1-\beta)\Omega)S = S_0$, the matrix is dense and non symmetric. General linear solvers are slow, especially in three dimensions, and since the matrix is generally dense, it is not possible to use sparse solvers. However, we note that the matrix norm is strictly less than 1. This follows from the observation that the matrix describes how much gets redeposited after a single reflection. Since the front does not contain any closed voids the sum of material will always decrease after the reflection since something will escape. Therefore

$$(I-(1-\beta)\Omega)^{-1} = \sum_{k=0}^{\infty}(1-\beta)^k\Omega^k$$

We note that the series converges for all values of β, including $\beta = 0$.

IV. Numerical Results

A. Reflection effects

First, we present in Fig. 1 simulations on the shape that led to this consideration, that of a cylindrical via and the source above the surface has a cosine distribution as a function of the angle from vertical. A similar simulation was done in [6].

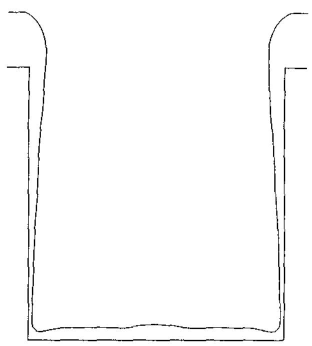

Fig. 1. Source Deposition (2D), Sticking coefficient is 1.0

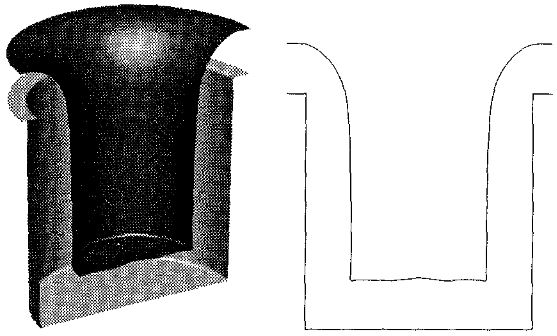

Fig. 2. Source Deposition (2D), Sticking coefficient is 0.01

This simulation might lead to the conclusion that the limiting case is an isotropic deposition; however the result is a little more subtle.

To try to isolate what effects redeposition has, consider the case of a via where the deposition source is compleatly vertical. Therefore all deposition on the sides is started by particles reflected off the bottom of the via. The incoming intensity will translate everything in the z direction. The result is shown in Fig. 3 This is a 2D simulation, simulating only the right half of the cave shown in the two-dimensional drawing.

For some problems, it is obvious that the ending shape will not resemble an isotropic deposition. Consider the case of a cave-like structure, where the shape is a cylindrical hole, but the radius of the opening is larger at the bottom. The result is shown in Fig. 4.

Lastly, In Fig. 5 we present results from three-dimensional simulations. This is a T-junction, and the source above it has the same cosine distribution as in the problem before. This problem could not be modelled as a two-dimensional problem.

V. Conclusion

We have done a careful study of the effects of small sticking coefficient. We conclude that for some special topology and source distribution the resulting deposition will look isotropic. But in general this is not the case. We have described a robust numerical technique for two and three-dimensional problems. This paper only focused on the re-emission process, but previous work [2]-[4] has included other types of processes such as surface diffusion,

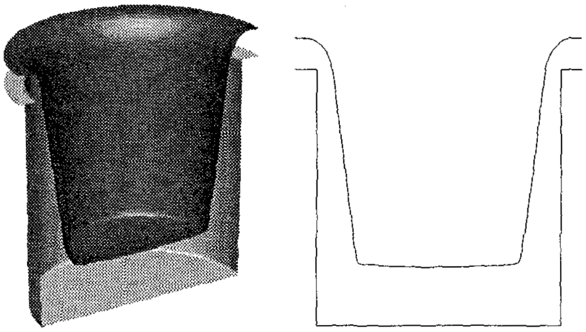

Fig. 3. Unidirectional etching (2D), Sticking coefficient is 0.01

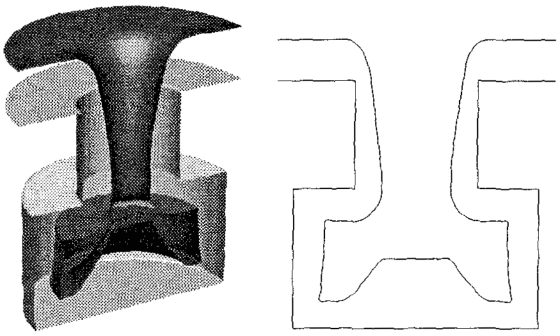

Fig. 4. Unidirectional etching (2D), Sticking coefficient is 0.01

masking, sputtering, both for two– and three–dimensional problems.

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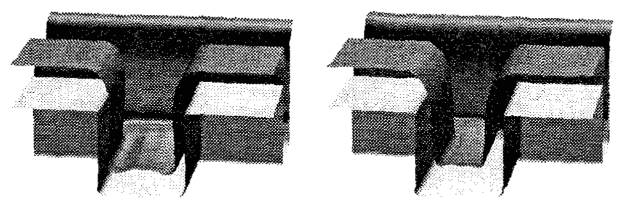

Fig. 5. Source Deposition in 3D, Sticking coefficient 1.0 and 0.01