HIGH DENSITY PLASMA DEPOSITION MODELING USING LEVEL SET METHODS

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Abstract

Several silicon dioxide chemical vapor deposition processes using high density plasma sources have been recently proposed in the literature [11, 7] for deposition of self-planarizing inter-level dielectric deposition. All these processes exhibit the competitive effect of simultaneous deposition and etching mechanisms. This paper describes the use of a robust simulation technique that can include all physical mechanisms involved in these processes.

The techniques rely on level set methods [20] for tracking evolving interfaces. These techniques are based on solving a Hamilton-Jacobi type equation for a propagating level set function, using techniques borrowed from hyperbolic conservation laws. Topological changes, corner and cusp development, and accurate determination of geometric properties such as curvature and normal direction are naturally obtained in this setting. The equations of motion of a unified model, including the effects of isotropic and unidirectional deposition and etching, visibility, surface diffusion, reflection, and material dependent etch/deposition rates are presented and adapted to a level set formulation. In the case of isotropic etching/deposition, a particularly fast marching level set method can be employed.

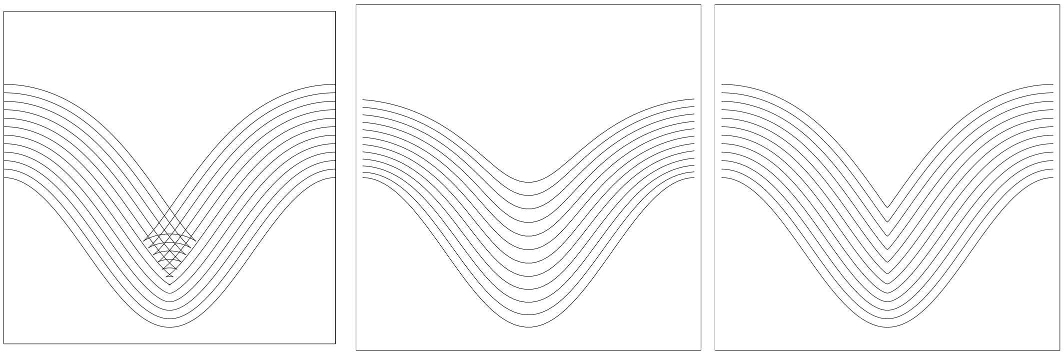
Using these techniques, we demonstrate results applied to two and three-dimensional problems analyzing isotropic deposition, ion milling, simultaneous etching and deposition, and multiple effects of re-emission and redeposition.

1 Introduction

Several silicon dioxide chemical vapor deposition processes using high density plasma sources have been recently proposed in the literature [11, 7] for deposition of self-planarizing inter-level dielectric deposition. All these processes exhibit the competitive effect of simultaneous deposition and etching mechanisms. This paper describes the use robust simulation techniques based on level set methods that can include all physical mechanisms involved in these processes.

2 Level Set Techniques

Level set techniques [15, 12, 20, 21] 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. Complex motion, particularly those that require surface diffusion, sensitive dependence on normal directions to the interface, and sophisticated breaking and merging, result from a straightforward implementation of the scheme, with no user intervention.



$Swallowtail(F = 1.0)$ $F = 1. - 0.25\kappa$ $Entropy\,Solution(F = 1.0)$

Figure 1: Cosine Curve Propagating with Unit Speed

2.1 Background

Consider a boundary, either a curve in two dimensions or a surface in three dimensions, separating one region from another, and imagine that this curve/surface moves in its normal direction with a known speed function F. The goal is to track the motion of this interface as it evolves. We are only concerned with the motion of the interface in its normal direction, and shall ignore tangential motion.

As shown in [14, 15, 17], a propagating interface can develop corners and discontinuities as it evolves, which require the introduction of a weak solution in order to proceed. The correct weak solution comes from enforcing an entropy condition for the propagating interface, similar to the one in gas dynamics. Furthermore, this entropy-satisfying weak solution is the one obtained by considering the limit of smooth solutions for the problem in which curvature plays a regularizing role.

As an example, consider the initial cosine curve propagating with speed $F = 1$ shown in Figure 1. As the front moves, a corner forms in the propagating front which corresponds to a shock in the slope, and a weak solution must be developed beyond this point. If the motion of each individual point is continued, the result is the swallowtail solution shown in Fig. 1a, which is multiple-valued and does not correspond to a clear interface separating two regions. Instead, an appropriate weak solution is obtained by considering the associated smooth flow obtained by adding curvature κ to the speed law, that is, letting $F = 1 - \epsilon\kappa$, see Fig. 1b. The limit of these smooth solutions as ϵ goes to zero produces the weak solution shown in Fig. 1c; this is the same solution obtained by enforcing an entropy condition, similar to the one for a scalar hyperbolic conservation law, which selects the envelope obtained by Huygens principle as the correct solution, see [14]. This weak solution corresponds to a decrease in total variation of the propagating front and is irreversible [15]. For details, see [15].

As a numerical technique, this suggests using the technology from hyperbolic conservation laws to solve the equations of motion, as described in [16]. This leads to the *level set* formulation introduced in [12], which we now describe.

2.2 The Level Set Method

Given an initial position for an interface Γ, where Γ is a closed curve in R^2, and a speed function F which gives the speed of Γ in its normal direction, the level set method takes the perspective of viewing Γ as the zero level set of a function $\phi(x, t = 0)$ from R^2 to R. That is, let $\phi(x, t = 0) = \pm d$, where d is the distance from x to Γ, and the plus (minus) sign is chosen if the point x is outside (inside) the initial hypersurface Γ. Then, by the chain rule, an evolution equation for the interface

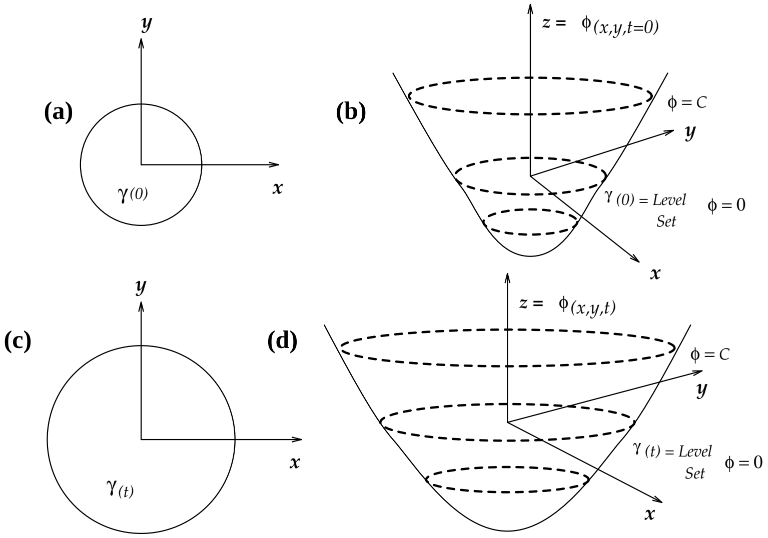


Figure 2: Propagating Circle

may be produced [12, 17], namely

$$\phi_t + F|\nabla\phi| = 0, \tag{1}$$

$$\phi(x, t = 0) = given. \tag{2}$$

This is an initial value partial differential equation in one higher dimension than the original problem. In Figure 2 (taken from [18]), we show the outward propagation of an initial curve and the accompanying motion of the level set function ϕ.

There are several advantages to this level set perspective:

1. Although $\phi(x, t)$ remains a function, the level surface $\phi = 0$ corresponding to the propagating hypersurface may change topology, as well as form sharp corners as ϕ evolves (see [12]).

2. Second, a discrete grid can be used together with finite differences to devise a numerical scheme to approximate the solution. Care must taken to adequately account for the spatial derivatives in the gradient.

3. Third, intrinsic geometric properties of the front are easily determined from the level set function ϕ. The normal vector is given by $\vec{n} = \frac{\nabla\phi}{|\nabla\phi|}$ and the curvature of each level set is $\kappa = \nabla \cdot \frac{\nabla\phi}{|\nabla\phi|}$.

4. Finally, the formulation is unchanged for propagating interfaces in three dimensions.

Since its introduction in [12], the above level set approach has been used in a wide collection of problems involving moving interfaces. Some of these applications include the generation of minimal surfaces [5], singularities and geodesics in moving curves and surfaces in [6], flame propagation [13, 23], shape reconstruction [10, 9], as well as etching, deposition and lithography calculations in [2, 3]. Extensions of the basic technique include fast methods in [1], level set techniques for multiple fluid interfaces [19], and grid generation in [18]. The fundamental Eulerian perspective presented by this approach has also been adopted in many theoretical analyses of mean curvature flow.

2.3 Numerical Approximation

As mentioned above, a careful approximation to the gradient in the level set equation (Eqn. 1) is required in order to produce the correct weak solution. One of the simplest such schemes is given in [12], namely

$$\phi_{ij}^{n+1} = \phi_{ij}^{n} - \Delta t \, (\max(D_{ij}^{-x}\phi, 0)^2 + \min(D_{ij}^{+x}\phi, 0)^2 \max(D_{ij}^{-y}\phi, 0)^2 + \min(D_{ij}^{+y}\phi, 0)^2)^{1/2}, \tag{3}$$

where here we have taken the speed $F = 1$ and employed difference operator notation that, for example, $D_{ij}^{+x}\phi = (\phi_{i+1,j} - \phi_{i,j})/(\Delta x)$. The crucial point in this (any such appropriate) numerical scheme is the correct direction of the upwinding and treatment of sonic points.

2.4 Fast Level Set Methods

2.4.1 Narrow Band Methods

The above method can be made fast in two ways. First, one can restrict the update of the level set function to a small neighborhood around the zero level set. This is known as the *narrow band approach*, see [1]. In this case, the operation count in three dimensions for N^3 grid points drops to $O(kN^2)$, where k is the number of cells in the width of the narrow band, providing a significant cost reduction. This “narrow band method” method was introduced in [5], used in recovering shapes from images in [10], and analyzed extensively in [1].

2.4.2 Fast Marching Level Set Methods

A second fast version can be applied when the speed function F is only a function of position; such is the case in isotropic etching/deposition, in which the speed function is constant. This results in the *fast marching level set method*, introduced by Sethian [21, 20], in which the problem is converted to a stationary solution, and the level sets correspond to positions of the front at various times. The key to this fast approach lies in a marriage of the above narrow band method and heapsort algorithm with back pointers, which, together with the entropy-satisfying schemes presented above, produce a very fast technique.

In more detail, suppose the speed of the front is given as $F = F(x)$ (this is the case in photolithography resist development). Then start with the level set equation given by

$$\phi_t + F|\nabla\phi| = 0, \tag{4}$$

Let T be the time at which the curve crosses the point (x). The surface $T(x)$ then satisfies the equation

$$|\nabla T|F = 1. \tag{5}$$

Eqn. 5 simply says that the gradient of arrival time surface is inversely proportional to the speed of the front. Thus, we have replaced a time-dependent partial differential equation with a stationary equation in this particular case. We can then march through the grid points in an orderly upwind fashion, updating the values from smallest to largest, to obtain the solution in one sweep. This method, for this particular case, is extremely fast. For example, a complete three-dimensional propagation isotropic deposition/etching or lithograhic etch problem can be computed on a 150x150x150 grid in less than 45 seconds on a Sparc 10.

For details of these and many other level set schemes, see [20, 22].

3 Level Set Methods for Etching, Deposition, and Lithography

Using these versions of level set methods, in [2, 3, 21], problems in etching, deposition, and photolithography development were analyzed. The model allows for physical mechanisms which include the effects of visibility, masking, non-convex sputter laws under ion milling, bulk diffusion, and sensitive flux integration laws.

3.1 Isotropic Deposition

First, we consider the case of simple isotropic deposition above a trench, with corresponding speed function $F = 1$, using the fast marching level set method introduced in [20, 21]. In Figure 3, taken from [21], we show a two-dimensional trench being filled in with a deposition layer; we note the sharp corner that develops when the entropy condition is invoked.

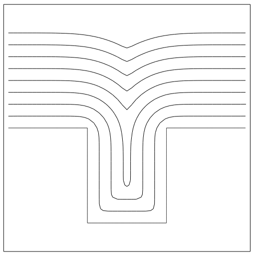
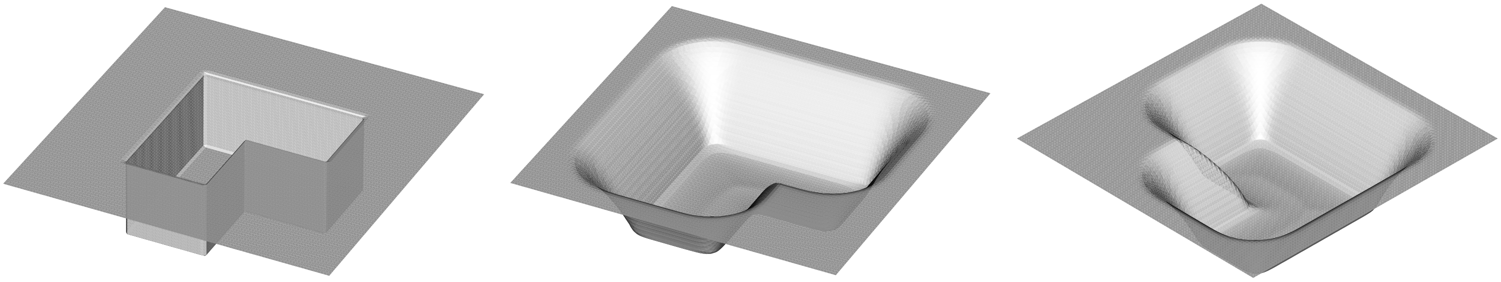


Figure 3: Isotropic Deposition Above Trench

3.2 Sputter Deposition: Non-convex flux laws

In Figure 4, taken from [3], we show etching of a saddle surface under ion milling with a non-convex speed law, where θ is the angle of the surface normal with the vertical.



Initial Shape : $T = 0$ $F = [1 + 4\sin^2(\theta)]\cos(\theta)\quad T = 8$ *Final Rotated*

Figure 4: Downward Saddle Under Ion Milling

We note the interesting effects at the the convex corners, the concave corners, and the saddle surfaces. The non-convex yield law means that special versions of our schemes must be used, see [2, 3].

3.3 Combined Effects: Simultaneous Etching and Deposition

Recently reported evidence [8] strongly suggests that the deposition process can be modeled by a deposition rate mainly composed by ion induced deposition, low pressure chemical deposition, re-deposition from material back-scattered from the gas phase, and direct re-deposition from material sputtered from the surface. Furthermore, it is shown that the etch component as predominantly due to physical sputtering. This last component introduces instabilities in the simulation result when using surface advancement techniques such as string algorithms producing artificial roughness.

We include results to show the application of the level set technique using a deposition rate as a combination of direct deposition from the gas phase (to emulate the contribution of re-deposited material) and a perfectly conformal contribution (as in the case of a small sticking coefficient contribution), and an ion-milling component for the etch rate. Figure 5, taken from [4], shows the robustness of this technique when varying the individual contributions over a wide range of parameters.

No artificial roughness is observed on the surface, and additionally, under certain conditions the material is etched through the interface.

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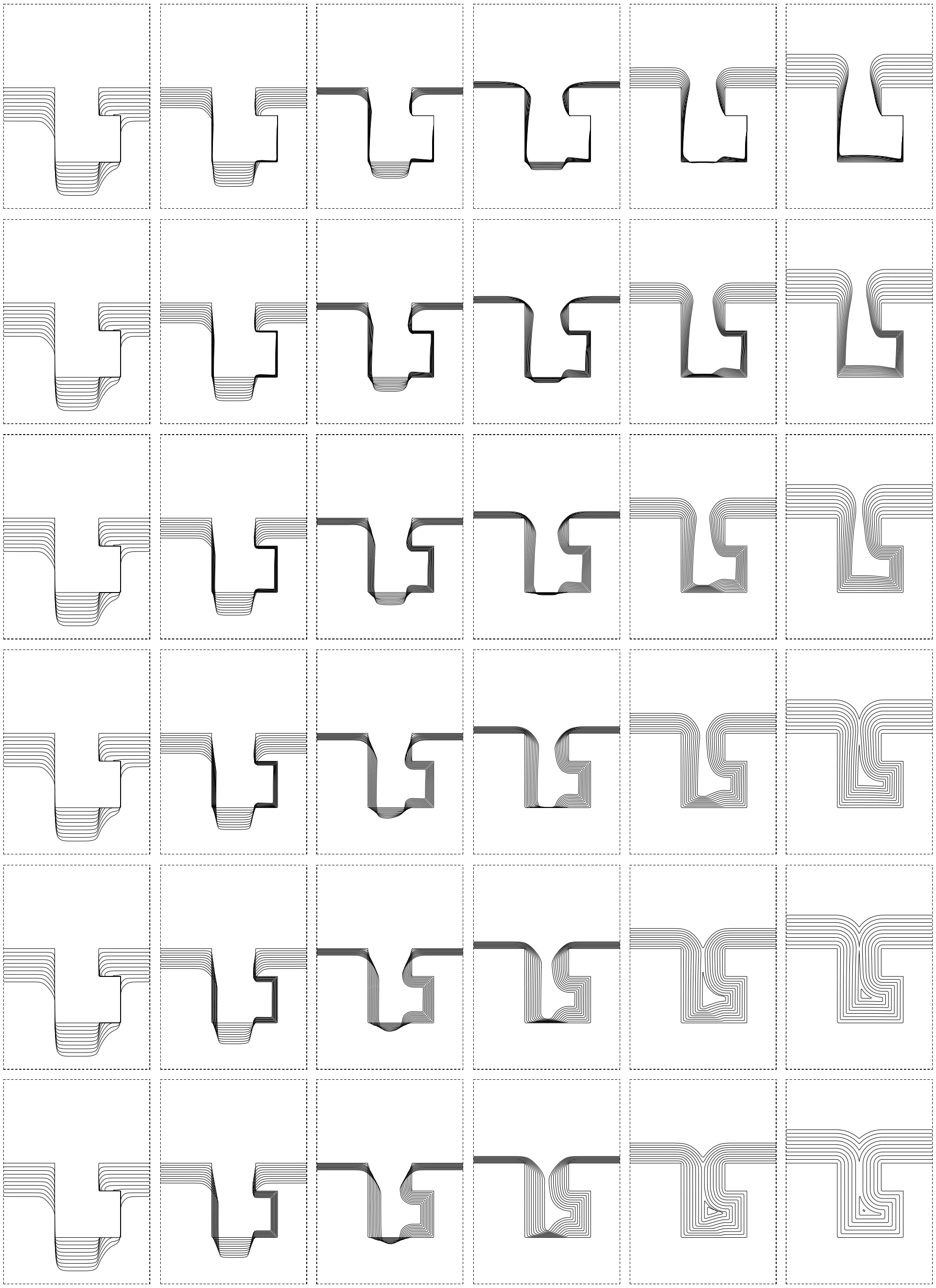

$$F = (1-\alpha)F_{etch} + \alpha F_{Deposition}$$

$$F_{etch} = (5.2249\cos\theta - 5.5914\cos^2\theta + 1.3665\cos^4\theta)\cos\theta$$

$$F_{Deposition} = \beta F_{Isotropic} + (1-\beta)F_{Source}$$

α Increases From Left to Right

β Increases From Bottom to Top

Figure 5: Simultaneous Etching and Deposition