Proceedings of the 36th
Conference on Decision & Control
San Diego, California USA • December 1997

Toward Real-Time Estimation of Surface Evolution in Plasma Etching: Isotropy, Anisotropy, and Self-Calibration

Jordan M. Berg
Department of Mechanical Engineering
Texas Tech University
Lubbock, TX 79409-1021
jberg@ttu.edu

Anthony Yezzi and Allen Tannenbaum
Department of Electrical Engineering
University of Minnesota
Minneapolis, MN 55455
tannenba@ee.umn.edu

Abstract

Level set methods are proving to be an effective tool for simulating surface evolution during chip manufacturing processes such as etching, deposition, and lithographic development. These methods can be implemented using extremely fast and robust algorithms, making them ideal for real-time model-based control applications. An approach for isotropic etching is developed, and demonstrated in simulation. Modifications necessary to address certain anisotropic processes and self-calibration of the estimator are sketched.

1 Introduction

Applications of the theory of curve evolution to modeling surface development in etching processes have been considered by several authors, in a number of papers beginning in the late 1960's [4, 7, 8, 18]. Adalsteinsson and Sethian generalize and extend this methodology, culminating in a unified approach to modeling etching, deposition, and lithographic development of semiconductor chips This approach allows the treatment of a host of important effects, including position-dependent and angle-dependent speed laws, convex and non-convex speed functions, masking and visibility, re-emission and surface diffusion—alone or in combination [15, 16]. Most importantly for our purposes, the approach of Adalsteinsson and Sethian is amenable to numerical solution techniques which are fast and robust. The speed and dependability of these algorithms lead us naturally to consider them as a basis for real-time estimation of surface profile evolution.

Given such a real-time process model, our general approach is as follows: Where possible, we relate available measurements to *geometric* properties of the wafer surface, such as length, curvature, and area. We then write a least-squares cost function involving the predicted value of those geometric quantities and the actual measurements. Estimates of process parameters are generated to minimize that cost function. This results in a corresponding estimate of the surface profile evolution as well.

The key to successful implementation of this strategy is the rapid and reliable minimization of the cost function. The advantage of basing the calculations on fundamental geometric objects is the immense store of results on the dynamics of these objects available in the literature. In an earlier study [1, 2] we demonstrated this procedure on a simulated isotropic etching. This is the simplest etching process, with a single free process parameter. In this paper we extend those earlier results in several directions.

A number of studies have investigated incorporating feedback control into the plasma etching process [3, 11, 13, 6, 19, 20]. The focus of these studies has been on the plasma itself. We are interested instead in using *in situ* measurements in real-time to estimate the evolving features. This work is completely complementary to other process control tasks, such as the control of plasma variables. One can imagine, for example, adjusting plasma inputs in response to changing etch rate estimates. Or, one might use the area of the active surface generated by the estimator as an input to the plasma model.

2 Curve Evolution in the Plane

In two dimensions surface motion is described by the equations of *curve evolution.* Here, the moving interface is described by a family of parameterized curves, $C(p,t) := (x(p,t), y(p,t))$; $p \in [0,1], t \in [0,t_f]$. The curve describing the interface evolves according to, $C_t = \beta(p,t)\mathcal{N}$, where p parametrizes the curve, $\mathcal{N}$ is the outward normal vector and β is the velocity function.

[1]This work was supported in part by grants from the National Science Foundation ECS-9122106, by the Air Force Office of Scientific Research AF/F49620-94-1-0058DEF, and by the Army Research Office DAAH04-94-G-0054, DAAH04-93-G-0332s, and by the Institute for Mathematics and its Applications.

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Numerical solution of curve evolution problems can be difficult, for several reasons. One is that, if curvature terms are absent or small, the solution will typically develop corners, or "shocks," even if the initial data is smooth. Once such shocks occur, one must be careful in defining precisely what is meant by a "solution," since the curve is now non-differentiable and so cannot satisfy a differential equation. Many problems with shocks can be handled by the Huygens principle, which defines the propagating front as the *envelope* of a continuum of circles (or other shapes, in more general formulations), centered on the initial front.

Another difficulty arises in treating topological transitions of the evolving curve, such splitting or merging. A series of algorithms that successfully address both these problems has been developed by Osher and Sethian, and their coworkers [12]. These algorithms employ a *level set* representation of the interface. In this description, the evolving curve is treated as a level curve of a scalar-valued function on the plane (or on $\mathbf{R}^3$, for surface evolution in 3-D), called the *level set function.* As clearly and thoroughly explained by Osher and Sethian [12], topological transitions of the level surface are absent from the higher-dimensional surface formed by the graph of the level set function.

2.1 Standard Nomenclature and Results

In what follows, $g(p,t)$ will denote the Euclidean metric $[x_p^2 + y_p^2]^{1/2}$. θ is defined to be the angle between the tangent $\mathcal{T}$ and the x-axis. The tangent, $\mathcal{T}$, curvature, κ, and outward normal, $\mathcal{N}$ are defined in the standard way [5]. Further, we let $K(t) := \int_0^1 \kappa g\, dp$ denote the *total curvature.* The following formula, a derivation of which may be found in several places [9, 12], expresses the rate of change of the length of $C(t)$: $L_t = \int_0^1 \beta\kappa g\, dp$. If C is a *closed* curve, then the area enclosed by $C(t)$ is given by Green's Theorem, $A(t) = \frac{1}{2}\int_0^1 \langle C, \mathcal{N}\rangle g\, dp$. The rate of change of area is $\dot{A}(t) = \int_0^1 \beta g\, dp$.

2.2 Piecewise Constant Normal Velocity

The relations in the previous section give $L_t(t) = \beta K(t)$ for a smooth curve with constant β. However, the cases to be considered below will only be *piecewise* smooth. We will need an expression for L_t for a continuous curve made up of smooth segments, with the segments joined at corners, or shocks, at which the curve fails to be differentiable. In the case to be considered the normal velocity will be *piecewise constant*, that is, constant on a given segment, but possibly varying from segment to segment. In particular, it may take one of two values; either zero, or a positive value which will be denoted β. The underlying notion is that the curve is propagating through an "active" medium in which it has a uniform, isotropic, normal velocity, β. This medium has imbedded in it inert inclusions, through which the curve cannot pass.

Corners in the curve may arise in three ways. First, shocks may form in the evolving curve, as described in [12]. We will refer to these as active-active shocks or fans. Second, an active portion of the curve may encounter an inert inclusion, forming an active-inert shock or fan. Third, the inert inclusion may have a corner, which, as it becomes part of the evolving curve, forms an inert-inert shock. At any such corner the curve undergoes a discrete jump in orientation. This jump is denoted $\Delta\theta$. To derive the necessary expression for L_t, consider an arbitrary arrangement of such segments at time t. Then propagate each segment for small time Δt at the appropriate normal velocity, ignoring the effect of the corners. The result will be a series of segments that no longer meet at their endpoints. Then *shock correction terms* are applied at each corner to enforce continuity. The specific form of the correction term will depend on the type of material on either side of the corner, and on whether the segments are converging or diverging—that is, on whether the corner is a shock or a fan. The shock correction terms all have the form $\beta\ \chi(\Delta\theta)$. The specific functions χ are listed in [2]. Then the corrected expression for rate of change of length is $L_t(t;\beta) = \beta K(t;\beta) + \beta X(t;\beta)$, where $X := \sum_{\text{shocks}} \chi$, and the dependence on the value of the constant β is indicated explicitly.

3 Numerical Implementation

Consider the class of curves evolving so that the normal velocity never changes sign. Then once the curve has passed through a point, it never returns. Thus at each point we may assign a unique value, equal to the time at which the curve passed through it. If the curve never reaches that point, a value of ∞ may be used. The resulting *crossing-time* function $T(x,y)$ is in fact a time-invariant level set function. Note that the crossing-time function stores the complete evolution. No information is wasted, because only the level set values corresponding to the actual curve at some time are computed. The corresponding time-invariant governing PDE is $\beta\|\nabla T\| = 1$. Sethian has presented a *fast marching* (FM) algorithm for evolving this equation; see [17].

3.1 Contour Tracing

The total shock correction term, $X(\beta;t)$, mentioned in Section 2.2 is easy to write down, but its numerical implementation requires extreme care. In particular, it is difficult to compute the change in tangent direction, $\Delta\theta$, accurately. Although the level set function may be used to directly generate this information through computation of the unit normal (which is simply $\nabla T/\|\nabla T\|$), these estimates are most precise when

T is *smooth*. Unfortunately, we also require these values when T is *non-smooth*. In pursuing this research, we first applied a simple pixel-based algorithm for recovering the level set itself [1]. This technique is quite crude, and provides a fast, but rough sketch of the evolving feature. The next version of the algorithm used bilinear approximation in each grid cell to estimate the curve length, and, as suggested in [15], averaged the unit normal vector estimates at neighboring grid points to obtain the change in orientation. The resulting length estimate was reasonable, but the contour orientation was not satisfactory for our purposes near the shock points.

Siddiqi *et al.* [14] compare techniques for recovering contours from a level set function, with subpixel resolution through interpolation. They develop a method that is similar to standard contour tracing algorithms found in computer vision applications, with the addition of *shock placement* logic. The algorithm first detects zeros along the grid lines of the mesh. It then uses geometric interpolation based on lines, arcs, and Euler spirals (curves of linearly varying curvature) to approximate the entire contour. Threshholding logic determines whether the contour contains a shock. The scheme presented in [14] detects shocks by abrupt changes in the *orientation* or *curvature* of the contour. If two shocks occur in a row, they are "relieved" by placing a single new shock with subpixel resolution. The curves on either side of that single point will have smooth orientation and curvature. We refer to [14] and the references therein for more details. The version implemented here, as described in [2], is similar, but only first order. That is, shocks are detected by a large change in orientation only, and when consecutive shocks are relieved by placing a single subpixel shock, the orientation is smoothed, but the curvature may not be.

4 The Estimator Structure

If the surface evolution is to be estimated directly from *in situ* measurements, then some of those measurements must relate to properties of the surface. For example, the rate at which by-products of the chemical component of a plasma etch are released into the plasma is related to the exposed area of active material. In a 2-D planar etch, the area is replaced by the length of the active surface in a planar cross-section. Another example is the particle flux to the surface in molecular beam epitaxy. That flux is related to the rate of change of volume (area, in a 2-D planar approximation) of deposited material on the surface. In both cases the relation is through a fundamental geometric quantity, either the length or the area. Note that in either case the functional relationship may be quite complicated.

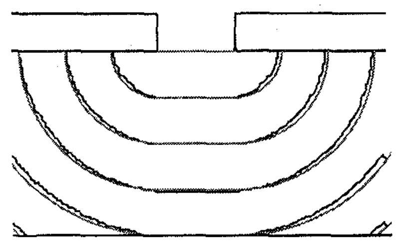

Figure 1: Feature evolution: estimated vs true, $h = 0.10$. Dark: Estimated; Light: Exact.

Denote the measurements by the function $Y(X, \lambda)$, where X is the surface, and λ is the vector of unknown parameters, and use a static level set model:

$$\beta(X(t), \lambda)\|\nabla T\| = 1, \tag{1}$$

$$\{X(t) \in \mathbf{R}^2 : T(X) = t\}, \tag{2}$$

$$y(t) := Y(X(t), \lambda). \tag{3}$$

The level set simulation plays the role of the plant model. The estimated process parameters are used to propagate the estimated feature. For our present purpose, "best" will be in a least squares sense.

The nature of $Y(X, \lambda)$ largely determines the details of the identification scheme. The remainder of this section describes how two different schemes are applied to surface tracking of an isotropic etch. The first postulates that the *rate* of material removal can be sensed. This case gives a measurement that involves the *curve length*. The second postulates that the *total* amount of material removed is known. This case gives a measurement that involves the *area swept by the curve*.

4.1 Estimation Based on Curve Length

Under the assumption of piecewise constant β, in the case of measurement of the rate of material removal, the predicted measurement is $\beta L(t; \beta)$. It is understood that $L(t; \beta)$ refers only to the portion of the surface that is exposed silicon, not resist or substrate.

The cost function is then

$$J(\beta) = \frac{1}{2} E(\beta)^T E(\beta) \tag{4}$$

where $[E(\beta)]_i = \beta L(t_i; \beta) - y(t_i)$. Generally, efficient solution of minimization problems requires analytical expressions for the first derivative of the cost function with respect to the unknown parameters. Here that is not straightforward, because it is not obvious

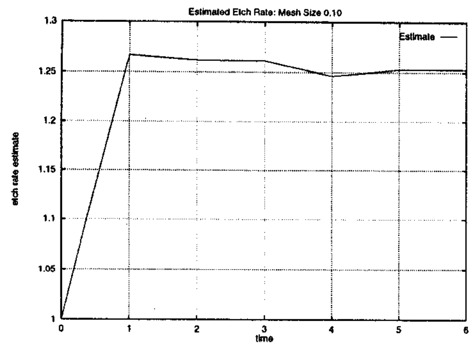

Figure 2: Etch rate estimate, $h = 0.10$. True value 1.25.

how to take derivatives through the set operation in Eq. (2). We now show how the necessary expressions can be obtained. The derivative of the cost function is $J_\beta(\beta) = E(\beta)^T \nabla E(\beta)$. The necessary derivative is given by $[\nabla E(\beta)]_i = L(t_i;\beta) + \beta L_\beta(t_i;\beta)$. At any time t_i, given some value of β, $L(t_i;\beta)$ can be found using a forward solve. It then remains only to find $L_\beta(t_i;\beta)$. Recall that $L_t(t;\beta) = \beta K(t;\beta) + \beta X(t;\beta)$. We make the following observation: The shape of the evolving feature may be expressed as a function of the variable $R := \beta t$ only. This may be seen from Huygens' principle, which states that the front is the envelope of the set of circles with radii R centered on the initial active surface. Thus we can write $L = L(R)$, $K = K(R)$, and $X = X(R)$, and $L_t = L'(R)R_t = L'(R)\beta$. Then $L'(R) = K(R) + X(R)$. Finally, $L_\beta = L'(R)R_\beta = L'(R)t$, or

$$L_\beta(t;\beta) = (K(R) + X(R))t \tag{5}$$

For any time t and etch rate β the values of $K(R)$ and $X(R)$, and therefore $J_\beta(\beta)$, can be found via a forward solve.

4.2 The Length Method: Simulation results

An exact solution to the feature evolution question is easily obtained for a single-trench etching using the Huygens principle. The exact solution was used to generate measurement data, and the algorithm of the preceding section applied. The height of the active layer is 5 units, and the width of the periodic cell is 10 units. The true etch rate was set to 1.25, and the initial guess given to the estimator was one. The etch rate was estimated at intervals of 1 time unit, and the corresponding surface drawn. The process was carried out for an estimator mesh size of 0.1. Figures 1 and 2 show the results.

Consider a mask pattern which repeats after three trenches. Again, the height of the active layer is 5 units, but the periodic cell now has a width of 20 units. In this case the truth model used is an FM simulation with a mesh size of 0.1. Again, a true etch rate of 1.25

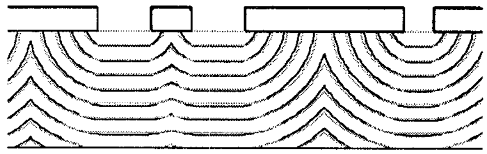

Figure 3: Three-trench feature evolution: estimated vs true, $h = 0.25$. Light: Estimate; Dark: Truth model.

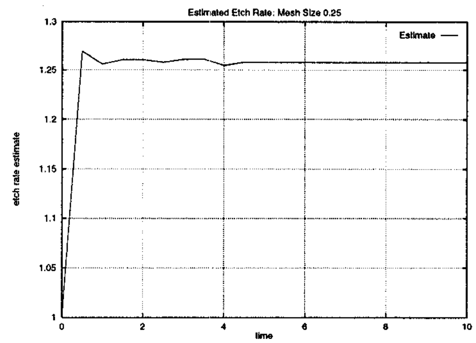

Figure 4: Three-trench etch rate estimate, $h = 0.25$. true value 1.25.

is used, and an initial guess of 1.0 is supplied to the estimator, which updates an etch rate estimate at 0.5 time unit intervals. Figures 3 and 4 show the results for an estimator mesh size of 0.25.

4.3 Estimation Based on Total Area

Now consider the case where the measurement is based on the total amount of material removed. Then the etch rate estimate is based on minimizing the least-squares cost function

$$J(\beta, T) = \frac{1}{2}\int_0^T (A(\beta,t) - y(t))^2\, dt \tag{6}$$

That is, the measurement is assumed to be exactly the total area swept out by the evolving curve in time T. Such a measurement might be available directly, or it might be obtained by integrating a measurement such as described in Section 4.2. For the isotropic case we can prove certain important properties of J.

Given an underlying material geometry then, the curve is completely defined by the parameter $R := \beta t$, and we write $C(R)$ for the curve itself, and $L(R)$ for the length of the curve. Now, the rate of change of the area swept by the curve can be computed to be $\dot{A}(t) = \beta L(R)$. So, the area itself is $A(t) = \int_0^{\beta t} L(\beta t) d(\beta t)$. Therefore, adjusting the notation $A(R) = \int_0^R L(\rho)d\rho$. Because

$L(R)$ and β are nonnegative, $A(R)$ is nondecreasing.

Let the true isotropic etch rate be γ. Then $J(\beta,T) = \frac{1}{2}\int_0^T (A(\beta t) - A(\gamma t))^2 dt$ We seek the value for the parameter β that will minimize this function. Since $A(R)$ is differentiable, $J(\beta,T)$ will be as well, and so any such minimizer will satisfy

$$\begin{aligned} J_\beta(\beta,T) &= \int_0^T (A(\beta t) - A(\gamma t))L(\beta t)t\,dt \\ &= 0 \end{aligned} \tag{7}$$

Since L and t are both nonnegative, and L is not identically zero for any interesting process, the sign of J_β is determined by $A(\beta t) - A(\gamma t)$. The nondecreasing property of $A(R)$ then gives $\text{sign}(J_\beta) = \text{sign}(\beta - \gamma)$. This shows that the correct estimate of etch rate is the unique global minimizer.

It is also of practical interest to examine $J_{\beta\beta}$. We can write

$$\begin{aligned} J_{\beta\beta} = \tfrac{1}{\beta}T^2(A(\beta T) - A(\gamma T))L(\beta T) + \\ \tfrac{\gamma}{\beta}\int_0^T L(\beta t)L(\gamma t)t^2 dt - \\ \tfrac{2}{\beta}\int_0^T (A(\beta t) - A(\gamma t)L(\beta t)t\,dt \end{aligned} \tag{8}$$

We see that the second derivative is not continuous, because $L(R)$ is only piecewise continuous. On the other hand, if T is chosen sufficiently large, then $J_{\beta\beta}$ is continuous for an arbitrarily large range of β. Then since $J_{\beta\beta}(\gamma,T) = \int_0^T L(\gamma t)^2 t^2 dt$, $J_{\beta\beta}(\beta,T) > 0$ in some neighborhood of γ. This raises the question of whether $J_{\beta\beta}(\beta,T) > 0$ everywhere it is well-defined. The answer in general is no. This can be seen by considering a planar etch, for which $L(R) = L_0$ when $R < R_f$, $L(R) = 0$ when $R \geq R_f$. Then $J_{\beta\beta}(\beta,T) > 0$ for $\beta < (3/2)\gamma$, $J_{\beta\beta}(\beta,T) = 0$ for $\beta = (3/2)\gamma$, and $J_{\beta\beta}(\beta,T) < 0$ for $\beta > (3/2)\gamma$.

The preceding discussion suggests the following approach to minimizing the cost function. Given an etch rate estimate, calculate the first and second derivatives. If the second derivative is positive, use a Newton-type method to update the estimate. If the second derivative is negative, take a gradient-descent step.

4.4 Self-Calibration for Isotropic Etching

The total-area cost function assumes that the measurement $y(t)$ is exactly the area swept out by the evolving curve. We now treat the case where the measurement is merely *proportional* to that area, and the constant of proportionality is not known *a priori*. Physically the unknown constant is usually determined in a *calibration* step. Calibration may be extremely time-consuming (and therefore expensive). Furthermore, the process must be periodically recalibrated as process parameters drift. In a production setting this may severely impact productivity. Therefore it is desirable to eliminate the calibration step. As we will now show, this can be done in some, possibly most, circumstances.

Denote the constant of proportionality by μ, its estimate by σ, and consider the case of an isotropic etch. Then the cost function becomes

$$J(\beta,\sigma,T) = \frac{1}{2}\int_0^T (\sigma A(\beta t) - \mu A(\gamma t))^2 dt \tag{9}$$

The first partial derivatives are given by $J_\sigma = \int_0^T (\sigma A(\beta t) - \mu A(\gamma t))A(\beta t)dt$ and $J_\beta = \int_0^T (\sigma A(\beta t) - \mu A(\gamma t))\sigma A'(\beta t)t\,dt$. These are differentiable. The second partials are given by

$$\begin{aligned} J_{\sigma\sigma} &= \int_0^T A(\beta t)^2 dt \\ J_{\beta\beta} &= \int_0^T \sigma^2 A'(\beta t)^2 t^2 dt + \\ &\quad \int_0^T (\sigma A(\beta t) - \mu A(\gamma t))\sigma A''(\beta t)t\,dt \\ J_{\sigma\beta} &= \int_0^T (2\sigma A(\beta t) - \mu A(\gamma t))A'(\beta t)t\,dt \end{aligned} \tag{10}$$

Let H denote the Hessian. Then at the solution $\sigma = \mu$ and $\beta = \gamma$,

$$\begin{aligned} \det H = \left(\mu^2 \int_0^T A(\gamma t)^2 dt\right)\left(\mu^2 \int_0^T A'(\gamma t)^2 t^2 dt\right) - \\ \left(\mu^2 \int_0^T A(\gamma t)A'(\gamma t)t\,dt\right)^2 \end{aligned} \tag{11}$$

By the Cauchy-Schwarz inequality $\det H \geq 0$. It would be nice if the inequality were strict for every problem geometry $A(R)$. Unfortunately, this is not the case. For example, in a planar etch, for which $A(R) = L_0 R$, equality holds, and the Hessian is not full rank. In fact it is easy to see physically that the etch rate and the calibration coefficient cannot be distinguished independently for this case. On the other hand, equality holds *if and only if* $A(\gamma t) = cA'(\gamma t)t$, that is, if and only if $A(R) = L_0 R^c$, for some constants L_0 and c. The planar etch is of this form, but in fact, we expect that most processes will not be. Then the Hessian will be positive definite, at least in some neighborhood of the solution. In [2] it was observed that the isotropic etching of a long trench may be self-calibrated. We therefore propose a conjugate gradient method, switching to Newton's method when the Hessian is positive definite.

4.5 Angular Dependence

Up to this point, we have considered only isotropic etching. However, most of the interesting plasma etching processes are anisotropic. Sources of anisotropy include the directionality of incoming molecules, the crystal structure of the material to be etched, and visibility effects. Here we treat an important class of anisotropic processes, namely those in which the surface normal velocity is a function of the surface orientation. The angular dependence is expressed using a *yield function*, $F(\theta)$. In many cases of interest this yield function is *non-convex*. These cases require special algorithms for propagating the level set equations. We begin our examination of this class of functions by considering the case $\beta = \beta_0 F(\theta)$. For now, we restrict $F(\theta)$ to be nonnegative, continuous, and not identically zero.

As we remarked above, from Green's theorem, the area enclosed by a closed curve is given by $A = \frac{1}{2}\int_0^1 \langle C, \mathcal{N}\rangle g\, dp$. The rate of change of area is $\dot{A} = \int_0^1 \beta_0 F(\theta) g\, dp$. Huygens' principle applies to this class of systems as well. We can consider the evolving curve to be generated by the envelope of a continuum of plane shapes—the so-called *structuring elements*, no longer necessarily circular—expanding with rate $\beta_0 t$ [10]. Then, as before, the area can be written as $A(R) := A(\beta_0 t)$. Here $R := \beta_0 t$ is some characteristic dimension of the structuring element at time t. β_0 will play the role of the unknown process parameter. An analysis similar to the one in Section 4.3 gives $A'(R) = \int_0^1 F(\theta) g\, dp$. The quantity A' no longer has the interpretation of length, but it is still non-negative, and may be found by integrating around the contour at any time. We then proceed as above.

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