

Real-Time Control of Etching Processes: Experimental Results

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ABSTRACT

A unified approach to the modelling, simulation, and control of thin film processing is presented. The focus of this approach is to combine in-situ sensing with a model that deals directly with evolving surfaces. Using this method, and an in-situ process modelling technique (e.g., plasma emission spectroscopy during reactive ion etching) is used as a source of in-out data for a model which deals exclusively with interface evolution. In this way, in-situ monitoring gives predictive process control capability, rather than simple end-point detection.

Keywords: etching, curvature driven flows, control, estimation, in-situ monitoring

1 INTRODUCTION

In this paper, we will consider the experimental verification of some procedures that we developed for the control of certain semiconductor manufacturing processes using mathematical models based on interfacial physics in [4, 5]

The process designer seeking to optimize the manufacture of modern thin film based devices faces a difficult task. Both the reacting flows in the transport phase, and the surface physics in the solid phase, are complex and often poorly understood. Critical events at the atomic scale of the growing lattice may profoundly influence the properties of the finished product, but these events must be typically sensed and controlled at the macroscopic level. The situation is worse when electromagnetic effects are included, as in the production of giant magnetoresistive (GMR) devices.

Numerical simulations provide the designer a valuable tool with which to confront these problems. Ideally, such software enables extensive parametric studies, or even numerical optimization, at a fraction of the cost that experiments would require. The most straightforward approach to developing suitable numerical models is exhaustive; every potentially important effect is described with its own PDE, and coupled to the whole. The codes produced by this method are often massive, with significant maintenance and reliability problems. Most notably, results may take days to obtain, even on the fastest computers available. Thus the

code is extremely limited as a design aid, and useless for any kind of real-time control.

In this paper, our focus is directly on the evolving interface—that is, on the film surface, or at phase boundaries. The motion of such an interface is described completely by its velocity along the outward surface normal. The explicit solution of surrounding fields is necessary only when they directly influence this velocity. In a remarkable number of situations, the underlying physics (which may be quite complex at the atomic or molecular level) manifests itself in the normal velocity as a function only of intrinsic properties of the curve—such as the mean curvature. Examples include grain growth, dendritic solidification, phase boundary motion, Hele-Shaw flow, flame propagation, and thermal grooving. For brevity, we refer to the class of evolving interfaces with motion governed by intrinsic properties as *curvature flows*.

Propagating a curvature flow requires knowledge only of the evolving surface. Therefore, these models require much less computation to solve than do the full equations of the underlying phenomena. The reduction in complexity is great enough to make these models candidates for real-time process controllers. Curvature flows also have a direct geometric interpretation, giving the designer a deeper intuitive feel for the qualitative behavior of the process.

Although curvature flows can incorporate many important physical processes, there will be cases when they can not adequately capture the full effect of non-local variables. Then field equations for those variables must also be solved. If the relevant time-scale is not much faster than the interface motion, the field equations must be coupled to the interface evolution equations. Even in these cases, the use of curvature flows offers several advantages. The first is efficiency. A savings in computation results from eliminating some of the field variables. The second is as a framework for homogenization. Microscopic variations in local properties are important only in their effect on the normal velocity of the interface, averaged over a much larger surface element. Finally, the curvature flow model, because it can be efficiently solved, is implementable in a real-time control scheme. The normal velocity is parametrized by the effect of the non-local field variables. *In situ* measurements are made, and an inverse problem solved, to determine the proper values for the parameters, which may vary in time and space. The second and third features may be combined, in a real-time controller that uses knowledge of the interface motion to estimate microscopic parameters, such as lattice defect density.

2 CURVE FLOWS

In this section, we will sketch some of the relevant theory from curve evolution theory, which we will need to describe the mathematical models of thin-film growth and etching to which we will apply our simulation and control methods. (This

discussion is informal, so we will be rather loose with the hypotheses put on the families considered here. See [12, 13, 26] for the formal mathematical treatments.)

We will consider families of curves $C : S^1 \times [0, T) \rightarrow \mathbf{R}^2$ evolving according to functions of the curvature, where S^1 denotes the unit circle. More precisely, the general deformation of a curve in the plane of interest in semiconductor manufacturing problems may be given by

$$\frac{\partial C}{\partial t} = \alpha(s, t)\mathcal{T} + \hat{\beta}(s, t)\mathcal{N} \quad (1)$$

where \mathcal{N} is the (inward) normal, \mathcal{T} is tangent, and $\alpha, \hat{\beta}$ are smooth functions. Notice that since we are only interested in shape we may take $\alpha = 0$. (Changing α changes only the curve's parametrization, and not its shape.) Furthermore, we constrain the deformations to be determined by the local geometry of the curve, i.e., $\hat{\beta}(s, t) = \beta(\kappa)$ where $\kappa(s, t)$ denotes the curvature of the curve $C(s, t)$. Thus we are led to the following equation:

$$\frac{\partial C}{\partial t} = \beta(\kappa)\mathcal{N}. \quad (2)$$

In the mathematics literature, a number of cases for the function β have been explored. For example, there has been a great deal of work in connection with the geometric heat equation in which $\beta(\kappa) = \kappa$. In the problems of interest to us in process control, a key function is $\beta(\kappa) = a\kappa + 1$, where $a \geq 0$. The case $a = 0$, i.e., $\beta \equiv 1$ is very important, and here equation (2) becomes an equation that has been studied in relation to problems in geometric optics, flame propagation [27], and shape morphology. The κ part gives a diffusive effect, while the constant part gives a wave (hyperbolic) effect which tends to create singularities.

3 LEVEL SET REPRESENTATIONS

We now briefly discuss some of the numerical algorithms developed for curve evolution. This work is based on writing the approximations in *conservation form* and applying the *Godunov method* [17]. For more details, see the fundamental work of Osher and Sethian in [21, 22, 27].

Let $C(p, t) : S^1 \times [0, \tau) \rightarrow \mathbf{R}^2$ be a family of curves satisfying the following evolution equation:

$$\frac{\partial C}{\partial t} = \beta(\kappa)\mathcal{N}. \quad (3)$$

There are a number of problems which must be solved when implementing curve evolution equations such as (3) on computer. For example, singularities may develop. The question is how to continue the evolution after the singularities appear. For example, in case $\beta = 1$, from all the *weak* solutions corresponding to (3), the one derived from the Huygens principle is *unique*, and can be obtained via

the entropy condition constraint given in [27]. In numerical implementations, the evolving curve is embedded in a two dimensional surface, and then the equations of motion are solved using a combination of straightforward discretization, and numerical techniques derived from hyperbolic conservation laws and Hamilton-Jacobi theory.

The embedding step is done in the following manner: The curve $C(p, t)$ is represented by the zero level set of a smooth and Lipschitz continuous function $\Phi : \mathbf{R}^2 \times [0, \tau) \rightarrow \mathbf{R}$. Assume that Φ is negative in the interior and positive in the exterior of the zero level set. We consider the zero level set, defined by

$$\{X(t) \in \mathbf{R}^2 : \Phi(X, t) = 0\}. \quad (4)$$

We have to find an evolution equation of Φ , such that the evolving curve $C(t)$ is given by the evolving zero level $X(t)$, i.e.,

$$C(t) \equiv X(t). \quad (5)$$

By differentiating (4) with respect to t we obtain:

$$\nabla \Phi(X, t) \cdot X_t + \Phi_t(X, t) = 0. \quad (6)$$

Note that for the zero level, the following relation holds:

$$\frac{\nabla \Phi}{\|\nabla \Phi\|} = -\mathcal{N}. \quad (7)$$

In this equation, the left side uses terms of the surface Φ , while the right side is related to the curve \mathcal{C} . The combination of equations (3) to (7) gives

$$\Phi_t = \beta(\kappa) \|\nabla \Phi\|, \quad (8)$$

and the curve C , evolving according to (3), is obtained by the zero level set of the function Φ , which evolves according to (8).

The second step of the algorithm consists of the discretization of the equation (8). If singularities cannot develop during the evolution, as in the geometric heat equation flow, a straightforward discretization can be performed [22]. If singularities can develop, as in the case of $\beta = 1$, a special discretization must be implemented. In this case, the implementation of the evolution of Φ is based on a *monotone* and *conservative* numerical algorithm, derived from the theory of hyperbolic conservation laws [17, 22]. For a large class of functions β of this type, this numerical scheme automatically obeys the entropy condition, i.e., the condition derived from the Huygens principle. For velocity functions such as $\beta = a\kappa + 1$, a combination of both methods is used [22].

4 ESTIMATION AND CONTROL OF THIN-FILM PROCESSES

Thin-film manufacturing processes are well-suited for the level set techniques described above. There is a natural physical interpretation of the entropy conditions in this context [1, 2]. For deposition, this would be, *material deposited is never removed*. For etching, *material that is removed is never restored*.

The main alternative to a level set description of the surface is a “Lagrangian” approach, such as a string method, where a moving mesh is attached to the surface, and used to discretize a parametrization of the curve. These methods exhibit poor numerical stability, however, when the interface is not convex [27]. Even greater difficulties are posed by topological transitions, as when two interfaces, growing towards one another from separate nucleation sites, touch and merge. The morphology of thin film devices may involve many complex geometric features and singularities of this type. The “volume of fluid method” is related to the level set approach, and has been used in a number of free-boundary problems. However, interface properties such as length and curvature, which are easily computed from the level set function, are very awkward to extract using the volume of fluid approach. There are also time step limitations, imposed to prevent “over-filling” of boundary cells.

Some other features of level sets are the ease with which they can be extended from two space dimensions to three, and the potential for capturing effects like surface diffusion in a curvature term. These issues, and others, are discussed extensively in [1, 2]. See also [14, 28, 29].

Equation (8) is a general description of curve or surface evolution. The physics of the underlying process is entirely contained in the function β . So far, β has been given as a function of curvature only. A realistic description of manufacturing processes for thin-film devices may require that β have a more complicated functional dependence. One possibility is that it will depend on other quantities intrinsic to the interface, such as the direction of the unit normal, or derivatives of the curvature. These flows can be treated by similar methods. It also may occur that the interface normal velocity is determined in part by inherently non-local effects. Some non-local contributions that play a role in low pressure deposition and etching processes are treated by Adalsteinsson and Sethian [1, 2].

The remainder of this section discusses the application of curvature flow models to problems of estimation and control. A number of studies have shown that incorporating feedback control into the the manufacture of electronic devices can improve the result [3, 7, 8, 11, 18, 19, 23, 24, 25]. In the context of the process control problem as discussed in [25], we are interested in using *in situ* measurements for real-time and run-to-run control of process parameters. The central problem we address is estimating the evolving shape of the surface features from available measurements. This is a challenging task, but the potential benefits are large.

Ultimately, the performance of the finished device will be heavily determined by the surface morphology.

Note that it may be possible to relate macroscopic properties, such as growth rate and surface morphology, which are estimated by the numerical model, to atomistic quantities, such as impurity concentrations or lattice defects. This level of modeling, which is our goal, would allow direct, real-time control (or at least diagnostics) of these critical quantities.

The steps in the process are illustrated by the following example, developed in a related study [4]. Although the process is etching, rather than growth, the principles are clearly demonstrated.

5 ISOTROPIC ETCHING OF A LONG TRENCH

The evolution equation (8), along with an appropriate β , define a plant model. The estimation scheme also requires a representation of the measurement. Here we consider a measurement of the *total* etch rate, that is, the total quantity of material removed, per unit time. Note that it is impossible to relate this to the surface velocity without knowledge of the surface shape. Then a complete model of the system is,

$$\Phi_t = \beta \|\nabla\Phi\|, \quad (9)$$

$$\{C(t) \in \mathbf{R}^2 : \Phi(X, t) = 0\}, \quad (10)$$

$$y(t) := \int_{C(t)} \beta dl = \int_0^{2\pi} \beta \rho(p, t) dp. \quad (11)$$

The expression (11) is just the normal velocity, integrated over the entire surface. Thus, (11) is the amount of material being removed per unit time. Therefore, it is also the amount of material being released into the surroundings per unit time, and so can be related to the rate of change of concentration.

We consider a simple feature geometry. A uniform layer of silicon sits on an inert substrate. The silicon is masked with a thin layer of resist, except for a narrow gap. At $t = 0$, a reactive substance, in this case chlorine gas, is introduced at the surface. This substance etchs silicon, but not the resist or the substrate. For the purposes of this simulation, the model is simply $\beta = 1$ for Si, and $\beta = 0$, otherwise.

Our concern in [4] is plasma etching, so a plasma process is assumed here. Although isotropic plasma etching is relatively rare, we begin with the isotropic case because an analytical solution is available as a truth model. We have recently worked out a much more realistic anisotropic model in [5]. Preliminary experimental work using a chlorine etch of a crystalline silicon wafer suggests that the appropriate concentration can be measured, via optical emission spectroscopy.

We now treat a simplified isotropic etching. Here β is a positive constant for the material to be etched (silicon), and zero for the masking resist and the inert

substrate. We assume that the initial geometry is known exactly, but that the etch rate, though constant, is not known. Then we try to choose an etch rate that causes our predicted measurements to “best” match the actual process values. For our present purpose, “best” will be in a least squares sense. The estimated etch rate is then used to propagate the estimated feature morphology. The estimated etch rate, and the surface morphology, will be updated at an interval, τ . An observer is constructed of the form (9)–(11). The predicted measurement is now $\beta L(t; \beta)$ where $L(t; \beta)$ is the length of the estimated surface, and the dependence of the time history of L on β is explicitly indicated. Since β is zero on the mask and substrate, $L(t; \beta)$ is understood to refer only to the portion of the surface that is exposed silicon.

We express this objective as a minimization problem,

$$\min_{\beta} J(\beta) = \min_{\beta} (1/2) \sum (\beta L(t_i; \beta) - y(t_i))^2 = \min_{\beta} (1/2) R(\beta)^t R(\beta) \quad (12)$$

where $[R(\beta)]_i = \beta L(t_i; \beta) - y(t_i)$.

Ordinarily, such a problem would be treated using a Newton or Gauss-Newton approach. Here that is not straightforward, because it is not obvious how to take derivatives through the set operation in (10). We now show how the necessary derivatives can be obtained, using results from the mathematical literature.

Following the Gauss approximation to the Hessian often used in least-squares problems, we have,

$$J(\beta)_{\beta} = R(\beta)^t \nabla R(\beta), \quad (13)$$

$$J(\beta)_{\beta\beta} = \nabla R(\beta)^t \nabla R(\beta) + R(\beta)^t \nabla^2 R(\beta) \approx \nabla R(\beta)^t \nabla R(\beta). \quad (14)$$

The necessary derivative is given by,

$$[\nabla R(\beta)]_i = L(t_i; \beta) + \beta L_{\beta}(t_i; \beta). \quad (15)$$

At any time t_i , given some value of β , $L(t_i; \beta)$ can be found using a forward solver. It then remains only to find $L_{\beta}(t_i; \beta)$. This is done as follows: from [12, 13, 16],

$$L_t(t; \beta) = \int_0^{2\pi} \beta \kappa \rho dp = \beta \int_0^{2\pi} \kappa \rho dp = \beta K(t; \beta), \quad (16)$$

where $K(t; \beta) := \int_0^{2\pi} \kappa(p, t; \beta) \rho(p, t; \beta) dp$ is the *total curvature*.

Then,

$$L_{\beta t}(t; \beta) = L_{t\beta}(t; \beta) \approx K(t; \beta). \quad (17)$$

The total curvature is independent of β , and the approximation (17) is exact, when the exposed silicon surface meets the mask or substrate at a right angle. Then,

$$L_{\beta}(t_i; \beta) = \int_0^{t_i} K(t; \beta) dt. \quad (18)$$

This expression is now applied throughout the etch. The total curvature is generated at any time, for a given value of β via a forward solve.

The surface at $t_0 = 0$ is assumed known. A standard Gauss-Newton algorithm can now be applied to find the surface at any subsequent time. The same technique could be used in a batch mode to do run-to-run control of process parameters. See [4] for numerical results using this method.

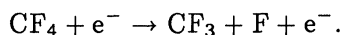
6 IN-SITU MONITORING

For this experiment, reactive ion etching (RIE) of silicon with the $\text{CF}_4 - \text{O}_2$ system was studied. It was chosen because of the well characterized relationship between the optical emission of the plasma and the corresponding etch rate. In particular, the etch rate of the silicon can, under certain conditions, be proportional to optical emission intensity due to electrically excited, but neutral, fluorine atoms. While plasma emission spectroscopy has been extensively studied as a means of process control, it has primarily been proposed and used as an end-point detection scheme. In that case, one generally looks for a step increase or decrease in the optical emission intensity indicating completion of the etching. This generally works quite well if the underlying layer has a drastically different etch rate or a different etching mechanism, resulting in significantly different concentration of F atoms in the plasma bulk.

In order for the plasma emission spectroscopy technique to work for our purposes, the following conditions must be met:

1. The concentration of the neutral species whose optical emission is being observed must be proportional to the rate of material removal.
2. The concentration of excited neutrals must be proportional to the overall concentration of neutrals.
3. The emission intensity of the excited neutrals must be proportional to the concentration of the excited neutrals and sufficiently bright to be accurately measured.

In the $\text{CF}_4 - \text{O}_2$ system, the concentration of neutral atoms in the plasma bulk is primarily due to the following reaction in the plasma bulk:



This process is followed by either the oxidation of the CF_3 radical in the plasma bulk, forming CO and three F atoms, or a similar surface process. In either case the four F atoms required for the removal of one Si atom are created. In this way, the first condition seems to be satisfied as long as the etching chamber is not excessively loaded. Even if the first condition is satisfied, the second two

conditions can be quite problematic. Since any real-time control system needs reliable data which does not depend on plasma conditions, simply observing the emission intensity from the excited F atoms is not reliable. Instead, an actinometric approach is used whereby the ratio of the emission intensity of excited F atoms ($\lambda=703.7$ nm) is compared to the emission from a small concentration of relatively inert Ar atoms, introduced expressly for the purpose of the actinometric measurement. Even though the Ar concentration is maintained at a relative low level, its emission intensity ($\lambda=720.7$ nm) is the dominant line in the entire plasma spectrum from 200 nm to 1000 nm. Since the excitation mechanisms of these two states are similar, and since the partial pressure of the Ar atoms is known (within the accuracy of the various mass flow controllers in the system), the ratio of the two intensities can be taken to be proportional to the partial pressure of F atoms in the bulk, thereby satisfying all three of the criteria listed above. Using the above procedure, actinometric measurements were made for the following etching conditions in a standard parallel plate RF etching system set up for 6" wafers with top shower head gas delivery:

Power: 100W

Pressure: 250 mTorr

CF₄: 50 SCCM

O₂: 5 SCCM

Ar: 2 SCCM

Using these conditions 3" silicon wafers were placed on 6" carriers and 5 μ m stripes were etched into the silicon using photoresist as an etch mask. This ensured that less than 1% of the area on the etching surface was actually exposed silicon. During etching, an initial etch rate of 15.4 Angstrom/s was observed. This rate decreased over the course of the first 90 seconds of etching to a final steady state rate of 8.8 Angstrom/s. During this same time the observed ratio of emission at 703.7 (due to excited F atoms) to emission at 720.7 nm (Ar atoms) decreased from 39% to 28%. The baseline value of this ratio for an unloaded etching chamber was 25%. The trends of the two measured quantities (etch rate vs. time and emission ratio vs. time) are similar: as etch rate decreases, so does relative emission intensity of excited F atoms, implying that immediately after plasma ignition the F atom concentration is at its highest level, and the etching proceeds at a comparably high rate until the concentration of F atoms reaches steady state. This explanation is unfortunately not consistent with the high baseline value of F atoms observed in an unloaded chamber. In addition, it is not expected that the plasma conditions take 90s to reach steady state. Instead, the data suggests that the first condition above (that the concentration of F atoms in the plasma bulk is proportional to the rate of material removal) is not met; instead any dependence of the rate of material removal on relative emission intensity must include a correction. This correction is thought to be due to the masking effect of the gradual accumulation of carbon atoms on the surface. Since the surface

is initially clean, the etch rate is initially high. As carbon atoms accumulate the etch rate slows, until steady state is reached between adsorption/dissociation of CF_3 and conversion to CO and CO_2 by the oxygen in the plasma. While these transients are of little concern when using plasma optical emission as an end-point detection scheme, any predictive or control application must take them into account as the initial rate of material removal has a profound effect on the final depth and profile of the feature being etched. This is a fundamental problem when the monitored species is the etchant, rather than an etching product species (such as SiF in the case of $\text{CF}_4 - \text{O}_2$ etching). It is important to remember that there is a fundamental difference between monitoring of an etchant species, such as F atoms, and an etching product species, such as SiF. In the case of monitoring the etchant concentration, the resulting data is proportional to etch rate (assuming a lightly loaded system, etc.). In the case of monitoring an etching product, the resulting data is proportional to the rate of material removal - *which is the product of etch rate and surface area* (assumed to be evolving with time in the case of an isotropic etch). While monitoring etching products is more desirable from a process control standpoint, it has the disadvantage that the various etching product species are generally molecules. Since molecular species generally have different excitation mechanisms than atomic species, a reliable actinometric ratio involving a molecular etching product and an inert gas such as Ar has not yet been demonstrated.

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