A Semi-Empirical Resist Dissolution Model for Sub-micron Lithographies

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ABSTRACT

In this paper, we present a new resist dissolution model suitable for large range of application domains – from memory devices employing $\leq 130nm$ design rules to MEMS devices with design rules exceeding 10s of microns. The proposed model uses empirical data such as "bulk" dissolution rate, and can be further tuned by other resist characterization studies such as depth and feature-size dependence of dissolution rate. The model can also take into account "local" properties such as developer concentration during the development process. The model uses the *Fast Marching Level Set* technique to track the developer-resist interface.

We discuss the dissolution model and its numerical implementation in detail and present the experimental techniques used to characterize the resist dissolution process, the data from which is then used to tune the dissolution model. We also present modeling results for a wide range of feature sizes and aspect ratios. We also present a "virtual development tool" that animates the 3D development process via an interactive graphical user interface shown in Figure 1.

Keywords: dissolution, lithography.

INTRODUCTION

Emerging lithographic technologies such as XRL and EUVL depend heavily on modeling tools to characterize and optimize process parameters [1], [2]. The published studies tend to focus on just the image formation, but the ever shrinking feature size and the resulting tighter error budget demand that resist dissolution be included in the process studies as well. The resist dissolution model chosen must meet at least the following criteria: be experimentally verified; be numerically robust; and, work in a wide range of application domains – from very small features ($\leq 70nm$) to high aspect ratio structures ($\geq 10\mu$) such as those used in MEMS, and from soft to hard x-ray regimes.

In this paper, we present a new "bulk" dissolution model that meet the three requirements stated above; in addition, the model can be "tuned" with empirical data obtained from resist characterization studies. At the most basic level, it uses bulk dissolution rate data obtained from resist characterization studies and propagates the resist front using a variation of the *Fast March*ing Level Set algorithm [3]–[6], and is proven to be numerically stable even under arbitrarily complex geometries. At a more complex level, the model can be tuned to the process parameters via empirical data such as depth and feature-size dependence of dissolution rate. This empirical tuning is the key to a good agreement between simulated and experimental profiles.

MODEL SPECIFICATION

Our specification for a dissolution model include the following criteria:

- **Correctness** Correct prediction; at the very least, the model must be able to correctly predict "trends".
- **Robust Implementation** As important as correctness for anything involving process exploration and optimization studies. This also specifies that the model must be able to handle arbitrarily complex geometries.
- **Cross Lithographic Techniques** Must be able to bridge multiple lithographic techniques such as synchrotron and point source based $1 \times$ x-ray proximity, $4-5 \times$ EUV projection Lithographies, etc.
- **Cross Application Domains** From DRAMs to logic to MEMS to novel applications such as Fresnel Zone Plates used for microscopy.
- Short "Time to Usability" Minimal turn-around from acquisition of a new resist to getting reliable results from the model.

CURRENT STATE OF THE ART

Most of the current dissolution models fall into one of the two following categories:

1. Local models: Physical models that takes into account local characteristics, such as Y. Zhu *reactiondiffusion* model [7]. These *physically-based* models have the potential for the most accurate modeling of the dissolution process, but the downside is that the chemical reaction is extremely complex to characterize, making it difficult to obtain the data needed for the simulation. Moreover, the software implementation of these models tend to be numerically very complex and CPU-intensive, and the CPU time required to model large 3D geometries can be prohibitive.

2. Global or Bulk models: These models use bulk properties such as dissolution rate (DR) to propagate resist front as a function of time. Most of the existing dissolution models, e.g., SAMPLE-3D [8], fall in this category. A key difference among the various "bulk" dissolution models is the *front-propagation* technique used to propagate the developer-resist interface as a function of time, and the success of the model hinges on the suitability of the propagation algorithm for arbitrarily complex geometries.

We have not found an existing implementation that fully meet our specification for a dissolution model; specifically, the existing model implementations fail the "robustness" criteria when the process design rule is reduced to $\leq 130nm$. Many of the observed problems stem from numerical errors in handling various topological degeneracies that occur when propagating the developer-resist interface as a function of time.

MATHEMATICAL MODEL AND IMPLEMENTATION

To model the resist dissolution process, we first separate the model space into two disjoint sets to create the "initial front": resist and developer; once the two regions are formed, and then the dissolution model tracks the "developer-resist interface" as a function of time, where the speed of the front propagation at each grid point is a function of the *dose*, *depth* and *envelope feature size* at that grid point. We then employ the *Fast Marching Level Set* technique, developed by Sethian [3], to track the interface. In this paper, we provide just an overview of the numerical technique; for detailed discussion of this technique, see [3]–[6], [9].

Equations of Motion

Consider a boundary, separating one region from another, which moves in normal direction with speed $\mathcal{F} = \mathcal{F}(x, y, z)$. Also suppose we know that the boundary is a monotonically advancing front such at $\mathcal{F} > 0$ (eg., the precondition that resist can never be "undeveloped"). Sethian [3] shows that this advancement problem can then be transformed into a **stationary** problem where time is no longer an independent variable. In essence, instead of solving for the front position at each time step, we solve, at each grid point, the time when the front *crossed* that point.



Figure 1: Virtual resist development tool

Following the discussion in [3], let T(x, y, z) be the time at which the boundary crosses the grid point (x, y, z). The boundary T(x, y, z) then satisfies the equation:

$$|\nabla T(x, y, z)|R(x, y, z) = 1 \tag{1}$$

This is the well known *Eikonal equation* from geometrical optics. The position of the front, Γ at a time t is given by the level set (contour) of value t of the function T(x, y, z), that is

$$\Gamma(t) = \{(x, y, z) | T(x, y, z) = t\}$$
(2)

To find the front at time t, simply take the level set (contour) of the function at time t. To solve

$$|\nabla T(x, y, z)| = \frac{1}{R(x, y, z)} \tag{3}$$

we use a finite difference scheme with the following gradient operator (for an one-dimensional case) [5]:

$$|T_x| \approx [(max(D_i^{+x}T, 0)^2 + min(D_i^{-x}T, 0)^2)]^{1/2}$$
 (4)

where we use the standard finite difference notation for 1-dimensional T_x :

$$D_i^{0x}T = \frac{T_{i+1} - T_i - 1}{2h}$$
$$D_i^{-x}T = \frac{T_i - T_i - 1}{h}$$
$$D_i^{+x}T = \frac{T_{i+1} - T_i}{h}$$

 T_i is the value of T at point *ih* with grid spacing h.

Once we obtain the parameters needed to solve Equations 3 and 4, we follow the "Narrow Band" algorithm outlined by Sethian [3] to solve for T(x, y, z) on a Cartesian grid. Once we compute T(x, y, z), we can then animate the dissolution process by simply "contouring" the volume at specific time-steps using the virtual development tool shown in Figure 1.

Table 1: Materials used in simulation studies

Process	Mask absorber	\mathbf{Resist}
Submicron	0.35μ Au	0.5μ APEX-E
LIGA	1.50μ Au	10.0μ PMMA

Implementation

The implementation consists of a series of software tools: "pre-processors" that convert the output of the exposure model [2], either absorbed dose or the rate of deprotection to a dissolution rate matrix; the dissolution model itself, a finite difference solver that computes the front "crossing-times" and produces a 3D volume; and, a GUI that animates of the development process. The numerical code is written in C++ and integrated in EXCON [10] to enable complex simulation studies; the GUI is written in a combination of C++, Tcl and Tk, and uses The Visualization Toolkit [11] for 3D rendering.

Simulation Results

To benchmark the dissolution model, we selected a wide range of applications that show its usability from sub-micron ($\leq 70nm$) to MEMS devices ($\geq 10\mu$), and we present those results here. Table 1 shows the various materials used for the study.

The first example, shown in Figure 2, involves a simple 2D 1:2 70nm periodic line and space pattern, with 0.35μ Au absorber and 0.5μ APEX-E resist. Figure 2(a) shows the developed profile when we used only the "bulk" dissolution rate measured by a DRM, and effects such as depth dependence on the dissolution rate were ignored. Figure 2(b) shows the developed profile when we did include depth dependence in the dissolution rate, and we see the familiar "T-tops" in the APEX-E resist profile.

Figure 3(a) shows the mask pattern and Figure 3(b) shows the resulting resist profile after development. The final developed profile clearly retains some of the diffraction effects due to exposure. Real masks, however, tend to have "rounded" edges, which result in some smoothing of the final developed profile.

A much more interesting example is the case where the resist was applied on pre-existing topography as shown in Figures 4 and 5. The ability to model dissolution over arbitrary existing topography greatly challenges the numerical implementation as well as the overall design of the software.

The next test case shows development of resist exposed by a point source based x-ray lithography process, where the resist was exposed with oblique illumination (2 deg). Figures 6(a) and 6(b) show the mask used and the final developed profile.

Figure 7 shows the application of this model to very high aspect ratio structures typical of LIGA processes used for MEMS devices.

SUMMARY

We have implemented a new resist dissolution model that is numerically stable under arbitrarily complex geometries and shows extendibility across multiple lithographic technologies and across application domains from very small features used in DRAMs ($\leq 70nm$) to very large patterns ($\geq 10\mu$) used in MEMS devices. It is however necessary to have good characterization of the resist dissolution process to be able to accurately predict the final profile. Future work will focus on better characterization of chemically amplified resist dissolution process, and to parameterize the dissolution rate as a function of depth and feature size in addition to the absorbed dose.

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(a) Not using depth dependence



(b) Using depth dependence

Figure 2: Effect of surface inhibition on 70nm lines and spaces



(a) Mask pattern

(b) Developed profile





(a) SEM micrograph (K. Deguchi, NTT)

(b) Developed profile

Figure 4: Resist dissolution over pre-existing topography I







(b) Developed profile

Figure 5: Resist dissolution over pre-existing topography II



(a) Mask pattern



(b) Developed resist profile





(a) SEM Micrograph (Z. Chen, CXrL)



(b) Developed profile

