Process-specific tuning of lithography simulation tools

Mark E. Mason, Robert A. Soper, R. Mark Terry, and Chris A. Mack[†]

Semiconductor Process and Device Center, Texas Instruments, Dallas, Texas
[†]FINLE Technologies, Austin, Texas

ABSTRACT

Clearly, all lithography simulation tools comprise models that depend on certain measures of the lithography process as input. In fact, it can be said that these models are only as good as their input. Therefore, the tuning of these models to fit the particular conditions of a certain process is a subject worthy of investigation. In this work, we extend previous efforts[1] to generate "tuned" parameters for the lithography process models within PROLITH/2[2] by including the evaluation of resist cross-sections under a variety of conditions in our analysis, and by more closely examining the sources of factory-specific tuning problems. Specifically, we identify and quantify error sources related to film thickness measurements, utilize the so-called "Poor-Man's DRM" technique to tune PROLITH's resist and development parameters, and compare the resulting simulations to both swing curves and resist cross-sections of various sizes on multiple substrates. The merit of this tuning approach is evaluated based on these comparisons. We conclude that optimization of simulator parameters is critical for accurate resist profile prediction and that, once optimized, the model provides quantitatively predictive results over a wide range of experimental conditions.

Keywords: optical lithography, simulation, PROLITH/2

1. INTRODUCTION

As a result of ever-increasing market pressures, semiconductor lithographers are constantly forced to push their tools to deliver smaller linewidths with tighter tolerances, which requires finely tuned and highly optimized lithographic processes. These same market pressures demand that lithography tools be used to produce sellable material at the maximum possible rate; this manufacturing requirement leaves little time available for lithographers to run the experiments necessary to tune and optimize their processes. The costly nature of large numbers of lithography experiments and the associated metrology time further compound this problem. In order to satisfy these conflicting requirements, lithographers have looked to off-line simulation tools to provide a way in which to experiment with new process conditions. Unfortunately, process simulators, as delivered from their authors, do not generally provide predictive capabilities that are accurate for any one particular wafer processing facility's unique combination of tools, recipes, and chemicals. Only through careful process characterization can simulators be tuned to successfully predict process outputs under specific real-life conditions.

Of course, simulation always begins by supplying information about the materials and the processing conditions to the simulator. Where photoresist is concerned, most simulation packages, including DEPICT[3], PROLITH/2, Solid-C[4], SAMPLE[5], and others, allow the specification of resist Dill parameters[6]. Some packages have more advanced resist or develop models that allow the specification of the Cauchy coefficients for the resist or dissolution rate information for the develop process. As a particular example of the limitations of the "out-of-the-box" performance, consider the following example of PROLITH/2 simulating a dose-to-clear swing curve for a commonly available high-performance novolac-based i-line resist, JSR PFR-IX790. Figure 1 shows three cases of swing curve data: data using the generic positive resist model with Dill and develop parameters provided by JSR, data using the built-in settings for JSR PFR-IX790 that ship with PROLITH/2, and actual data observed in the laboratory. Note that the simulated curves are different from the observed curve in both phase and amplitude. These differences have been attributed to many causes, including (but not limited to) errors in resist thickness measurements, stepper dose calibration errors, machine setup and recipe differences, etc. Unfortunately, a factory with many machines running high-volume production may be unwilling (or unable) to identify and correct these

problems, possibly disturbing well-characterized processes, just to make the simulator work.
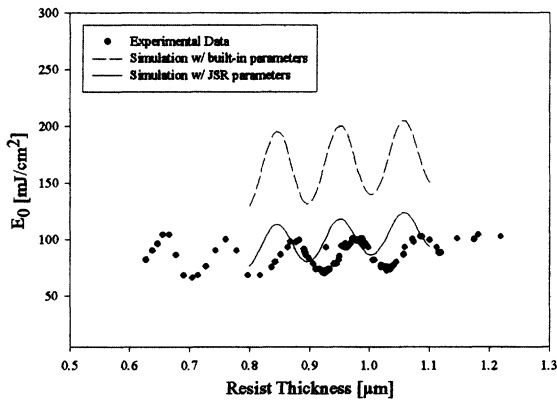
Figure 1: Performance of PROLITH/2 "out of the box" for resist swing curves

The real impact of this type of miscalibration can be seen in Figure 2, where it is clear that the accurate prediction of resist cross sections for any particular process is almost impossible for a simulator "out of the box."
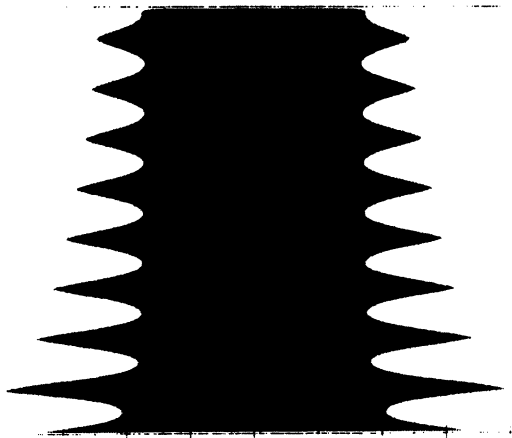
Figure 2: Performance of PROLITH/2 "out of the box" for resist cross sections.

2. SIMULATOR CALIBRATION

Given this line of reasoning, the question becomes "How can the simulator be made to predict the results in a particular factory or laboratory?" The answer is that the simulator must be tuned. In this section, examples of common exposure and development model error sources are presented. Section 3 discussed methods for overcoming

these errors and making PROLITH/2 accurately represent process behavior.

2.1 Swing curve matching errors

Errors in resist thickness measurements are often identified as potential causes of simulation errors, particularly in the case of dose-to-clear simulations[1]. Oftentimes, these errors are the result of miscalibration of the measurement tool, or the use of generic values for the resist film coefficients.

#### 2.1.1 Measurement tool calibration error

Consider the two cases shown in Figure 3. In the first case, a baseline thickness error of 50 Å is introduced into the data. An error such as this could be due to a tool offset of some sort, or possibly due to an uncharacterized substrate condition like the presence of a native oxide In the second case, a calibration curve error of 1.0 percent is added to the thickness data. The resulting change in the "phase" of the swing curve results in significant and variable dose-to-clear errors, as can be seen in Figure 4. In fact, errors of these magnitudes can account for as much as 10% of the total clearing dose. This type of error can also be introduced on perfectly well calibrated reflectance-based thickness measurement tools that are given an index of refraction for a particular resist that is off by as little as 1%.
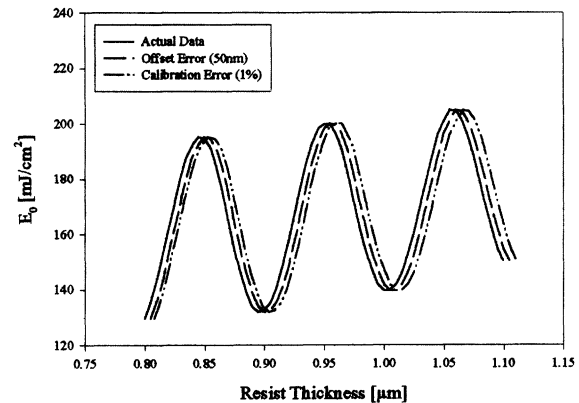
Figure 3: Swing curve "phase" error in dose-to-clear simulation introduced by a constant offset error in the resist thickness measurement compared to a constant 1.0% tool calibration curve error.

2.1.2 Stepper dose calibration error

Dose-to-clear data can also be affected by errors in the stepper dose calibration[1]. It is well know that stepper dose meters can vary widely within the same facility; vendor-to-
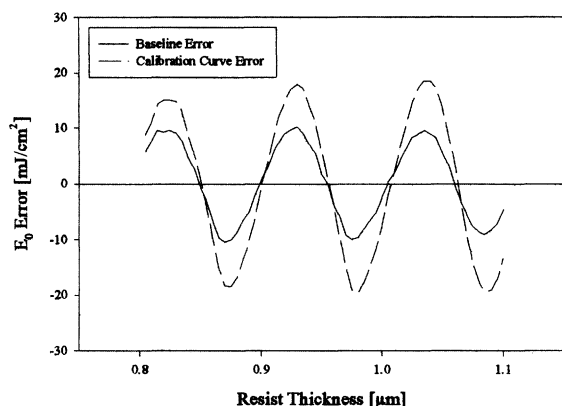
Figure 4: Dose-to-clear measurement error observed due to thickness measurement error at various resist thicknesses. Note that the E_0 error can be as much a 10% for a 1% resist thickness measurement error.

vendor variations compound this problem. Placement within the stepper field and precise sensor angle are also known to contribute to errors between measurements.

Figure 5 illustrates the type of errors that can be obtained when a single dose meter is used to match the dose setting on seven nominally identical steppers. In this figure, observed CD values are plotted against E_0 on one axis and dose meter energy on the other. E_0 is defined as the minimum exposure energy required to clear a particular thickness of resist from bare silicon, commonly referred to as the clearing dose.
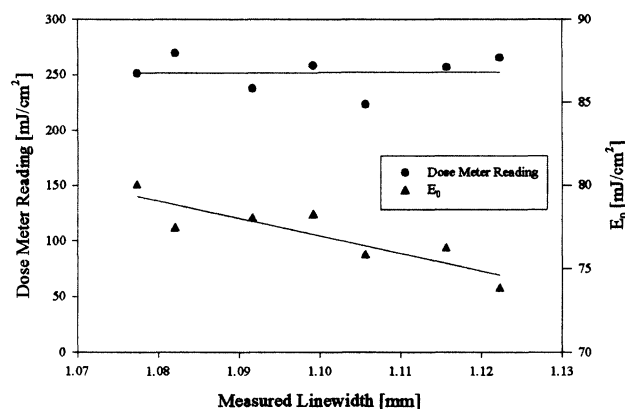

Figure 5: Steppers that have been matched with meters can still show differences in the clearing dose and CD.

It is clear that even after precise matching of the seven steppers with a UV dose meter, differences in the clearing dose (and subsequently the CD values produced by those

machines for identical settings) did exist. These differences, missed by the dose meter, are captured by the clearing dose tests on those machines, and the resulting data correlated nicely to the observed CD values. Of course, the point is that if one meter in one factory can have this sort of reproducibility problem, then it is not reasonable to expect that the stepper at another fab (and in particular at a resist vendor) is well calibrated to the meter used in any other fab.

2.1.3 Clear reticles vs. Open frames

Another thing to consider when analyzing dose-to-clear data is exactly how the stepper measures the dose. PROLITH/2, for example, requires an input of the dose, defined as the actual dose striking the wafer in a large clear area. However, many steppers measure dose (for the purpose of dose control) in the illuminator (before the reticle in the optical path). Thus, anything that might change the dose at the wafer plane relative to the dose before the reticle plane would cause a systematic error in what is meant by "dose." The simplest example is the presence or absence of a blank glass reticle during dose to clear measurements. The E_0, defined based on an actual dose striking the wafer, would of course be independent of such a detail. In practice, however, the dose value used in the stepper may be different from our intuitive definition of dose. Figure 6 shows the clearing dose for the same stepper under the conditions of no reticle (plotted on the y-axis), and a blank reticle (plotted on the x-axis). While it is common for lithographers to measure E_0 with no reticle (a so-called "open frame"), for consistent comparison to PROLITH/2 simulations, the use of a blank reticle would be needed for E_0 measurements on this stepper.
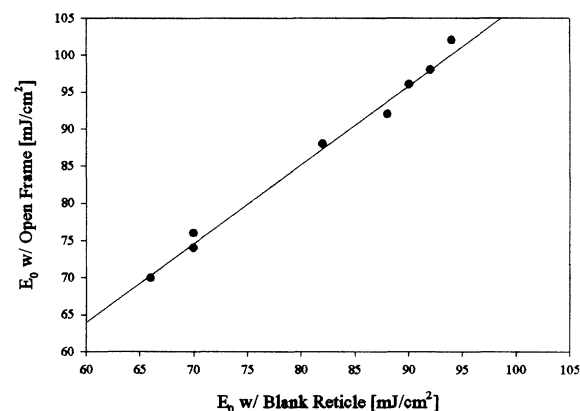
Figure 6: Dose-to-clear test for "open frame" and "blank reticle" cases. Note that the open frame case clears at a dose that is almost 7% lower on average than the blank reticle case.

2.2 Develop model errors

The biggest challenge with develop model parameters is that they are typically unknown. Even if they are reported for a particular resist, odds are that the develop conditions at the resist manufacturer (or wherever the parameters were measured) differ at least subtly (and often significantly) from the factory conditions. In fact, most development parameters are determined using data taken under tank development conditions, while most high resolution lithography is accomplished with puddle develop; this inconsistency can complicate many comparisons.

For the purposes of this study, several wafers were coated identically, blanket exposed with different doses, and developed on a track equipped with an in-situ dissolution rate monitor (DRM). The measured resist thickness versus time traces were compared to the output of the DRM simulator in PROLITH/2 using development parameters provided by the resist manufacturer; the results can be seen in Figure 7. Note that, while reasonable agreement is obtained at higher exposure energies, there is considerable error at low dose. This error in prediction near the resist exposure threshold is consistent with, and easily attributable to, errors in the develop model parameters that also show up in the swing curve. As in the swing curve in Figure 1, the JSR-supplied parameters overestimate the exposure dose required to clear the resist.
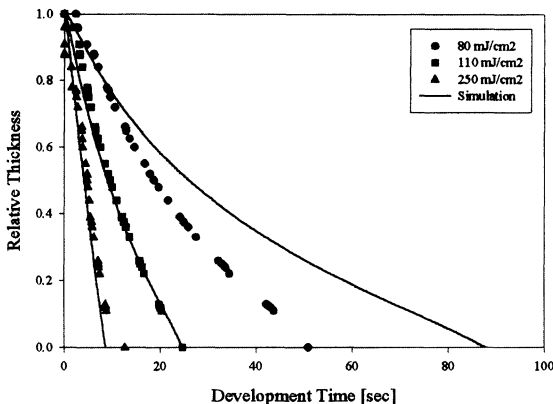

Figure 7: DRM data from puddle develop vs. PROLITH/2 simulation using JSR-supplied parameters for PFR-IX790.

3. TUNING THE SIMULATOR

Once error sources have been identified, the work of tuning the simulator can begin.

3.1 Resist thickness measurement errors

First, it is necessary to correct the phase error in the swing curve shown in Figure 1. In this particular case, a tool calibration error was detected that was contributing to (but did not completely explain) this error. Thickness data from the measurement tool in question (a Therma-Wave Opti-Probe) are shown in Figure 8 plotted against those from a spectroscopic ellipsometer, which, for the purposes of this investigation, is assumed to be accurate. These data indicate a thickness error with both a base offset and a calibration curve error of the form Therma-Wave Thickness (Å) = 1.0273 * (SE Thickness) – 121.61Å.
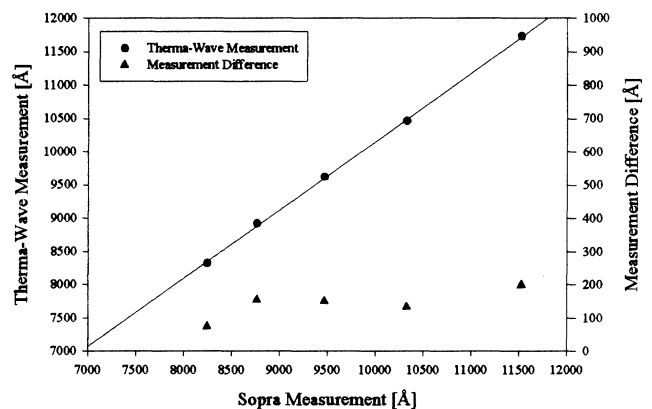

Figure 8: Calibration error observed as a function of thickness.
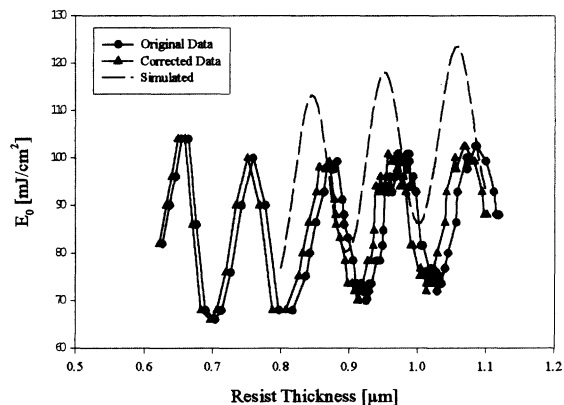

Figure 9: Correction of the resist thickness error reduces the phase error in the resist swing curve.

When the measured data are corrected for this miscalibration, the phase is partially (but not completely) corrected, as can be seen in Figure 9. Note that the corrected data is shifted "to the left," resolving some of the phase error between the measured and simulated data.

In order to remove the remaining residual phase error, the index of the resist reported to the simulator can be adjusted. In this case, changing the value of the refractive index from 1.71 to 1.695 was required to match the phases of the simulated and corrected measurements. As before, the High NA scalar image calculation model from PROLITH/2 was used, which includes the non-vertical propagation of light due to NA and sigma considerations.

3.2 Determination of development parameters

Once the swing curve has been matched by adjusting the refractive index, it is necessary to find optimum values for the development model parameters used in PROLITH/2. Finding these values requires collecting resist thickness data as a function of both exposure dose and development time. This data is typically collected using a development rate monitor, or DRM.

3.2.1 The Poor-Man's DRM

Since most production wafer facilities do not have access to a track-mounted DRM, we began our determination of develop rate parameters utilizing the Poor-Man's DRM (PMDRM) technique, first described in 1996[7]. While a normal dissolution rate monitor measures resist thickness as a function of develop time for a given exposure dose, the PMDRM measures thickness as a function of exposure dose for fixed puddle times.
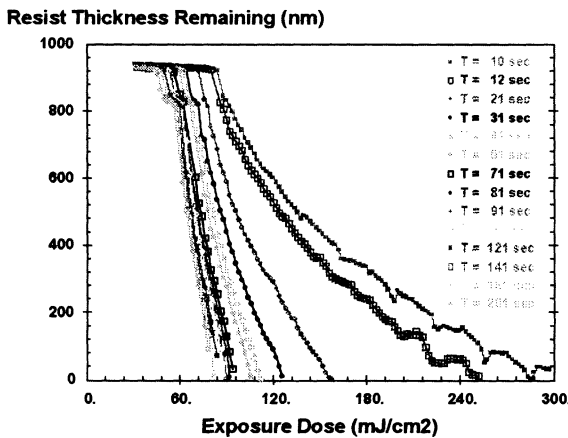
Resist Thickness Remaining (nm)

Figure 10: Example of Thickness vs. dose data taken for various develop times.

For this experiment, three PMDRM trials were run: one at a resist thickness ($0.97\mu m$) corresponding to a peak in the E_0 swing curve, and two at resist thicknesses ($1.03\mu m$ and $0.91\mu m$) corresponding to valleys in the swing curve. These thicknesses are referred to as E_{max} and E_{min}, respectively. The data collected at E_{max} are shown in Figure

10. Once collected, the data are transformed to development rate versus relative PAC concentration and fit to the Mack model using the commercially available ProDRM software[8].

The Mack development model defines four develop parameters, including R_{min} (minimum dissolution rate), R_{max} (maximum dissolution rate), M_{th} (threshold PAC concentration), and n (reaction order). Once the data are collected, the Mack model can be fit to obtain the parameter values of interest. The measured development rate data and resulting model fit for the E_{max} data set in Figure 10 can be seen in Figure 11.
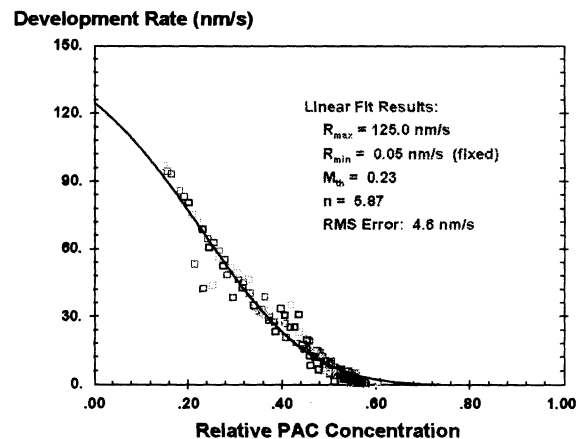
Development Rate (nm/s)

Figure 11: Result of fit of the PMDRM data at E_{max} to the Mack develop model.

After analyzing the E_{max} and E_{min} data separately, the two data sets were combined and the Mack model was again fit with only slight changes in the parameter values. The results from all three cases (using vendor-supplied resist parameters A = 0.698, B = 0.042, C = 0.0128) are shown in Table 1. Note that no tuning of C is necessary if the Poor-Man's DRM technique is used.

Table 1: Fit results for various PMDRM runs

| Parm	E_{min} 1.03µm	E_{max} .97µm	E_{min} .91 µm	All data
R_{max} (nm/s)	190	125	114	143.2
R_{min} (nm/s)	0.05	0.05	0.05	0.05
M_{th}	-1.4	0.23	0.20	0.1
n	4.98	5.87	5.60	5.40
RMS error (nm/s)	7.8	4.6	4.9	6.8

3.2.2 Finding R_{min}

One of the challenges of using the PMDRM technique is in the determination of R_{min}. Since most exposure tools are unable to deliver very low doses, it is not possible to collect meaningful data for calculating R_{min} using only the PMDRM technique. As a result, it is often advisable to fix R_{min} to a reasonable value or to use some independent means of determining it. In this study, $R_{min} = 0.05$ was chosen; to verify this value, pre- and post-development resist thickness measurements were made on unexposed wafers developed for periods ranging from 60 seconds to 107 minutes. The data are presented in Table 2. Based on these data, it is clear that $R_{min} = 0.05$ is a good choice for this resist, although further work to understand this behavior is required.

Table 2: Develop rates for determination of Rmin

| Puddle Time (min)	Pre (nm)	Post (nm)	Average Rate (nm/s)
107	928	899	0.005
45	928	898	0.01
30	929	901	0.02
15	928	897	0.03
8	926	891	0.07
5	929	899	0.10
4	926	890	0.15
2	926	893	0.28
1	926	893	0.55

3.2.3 PMDRM measurements.

It is worth noting that it is sometimes difficult to accurately measure partially exposed resist thickness after develop as required by this technique. At some combinations of under-exposure and under-develop, remaining resist can be seen to have a very rough appearance, even to the naked eye at 1x. As can be seen in Figure 12, a surface plot of partially developed resist for a particular exposure, surface roughness can be extreme in these cases. In fact, Figure 12 represents the worst case observed. To combat this phenomenon in general, resist thickness was measured over large areas and averaged for each site, in an effort to capture the mean thickness for a set of conditions.
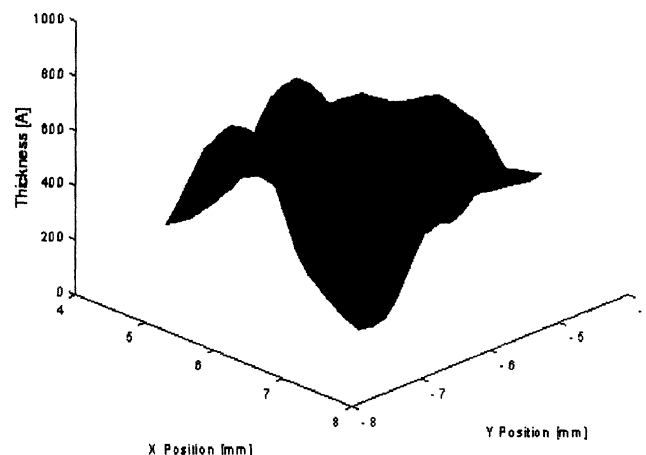

Figure 12: Surface roughness of partially developed resist.

4. VERIFICATION OF CALIBRATION

To evaluate thr effectiveness of the matching, we examine the resulting swing curves on silicon and silicon nitride. Figure 13 shows an excellent match between simulation and experiment, as does Figure 14. Small differences in the exposure dose to clear in Figure 14 can be easily attributed to the fact that PROLITH's built in nitride parameters were used. To get an exact match to simulations, factory specific nitride parameters should be used.
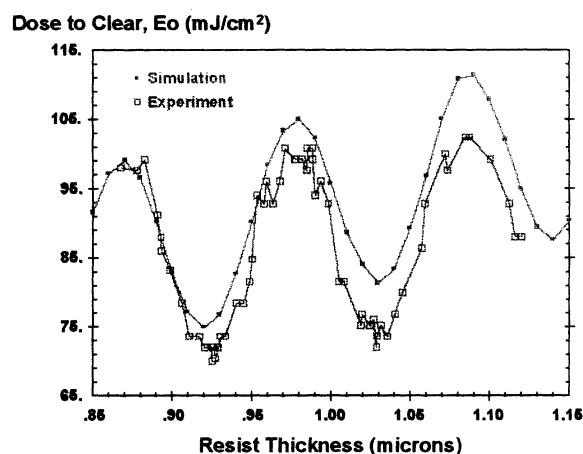

Figure 13: Simulated vs. Experimental swing curves for IX790 after model tuning.
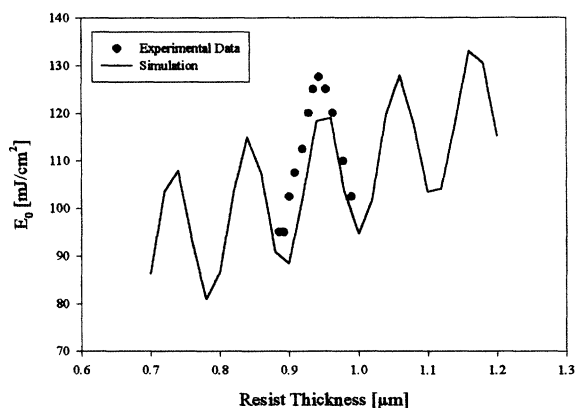
Figure 14: Simulated vs. Experimental swing curve for resist on Silicon Nitride substrate.

In Figures 15 and 16, the ultimate benefit of matching becomes clear. Comparison of the predicted resist profile in Figure 15 to the actual resist cross sections in Figure 16 shows excellent agreement. Most notable is the retrograde resist profile near the resist-silicon interface that is accurately predicted by the simulation. Figure 17 shows good agreement through focus.
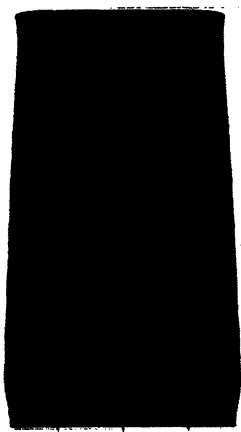
**Figure 15: Tuning improves resist cross-section prediction capabilities.**

5. CONCLUSIONS

In this work, we have extended previous techniques and generated "tuned" parameters for the lithography process models within PROLITH/2 by including the evaluation of resist cross-sections under a variety of conditions in our analysis, and by more closely examining the sources of factory-specific tuning problems. Specifically, we have identified and quantified error sources related to film thickness measurements, utilized the so-called "Poor-Man's DRM" technique to tune PROLITH's resist and

development parameters, and compare the resulting simulations to both swing curves and resist cross-sections. The merit of this tuning approach is shown evaluated based on these comparisons.

Figure 16: Actual resist cross section of 0.34 μm dense lines.
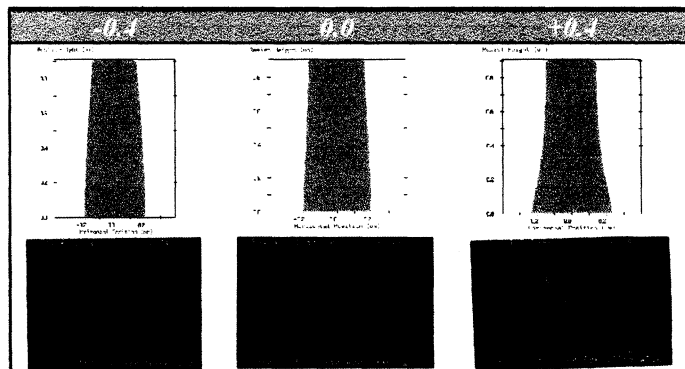
Figure 17: Cross sections through focus.

ACKNOWLEDGMENTS

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