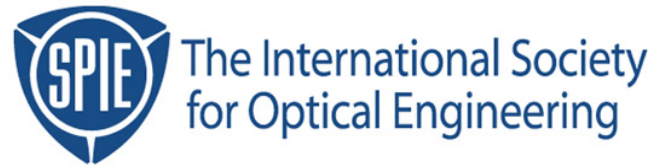


Copyright 1999 by the Society of Photo-Optical Instrumentation Engineers.



This paper was published in the proceedings of  
Optical Microlithography XII, SPIE Vol. 3679, pp. 183-192.  
It is made available as an electronic reprint with permission of SPIE.

One print or electronic copy may be made for personal use only. Systematic or multiple reproduction, distribution to multiple locations via electronic or other means, duplication of any material in this paper for a fee or for commercial purposes, or modification of the content of the paper are prohibited.

# Matching Simulation and Experiment for Chemically Amplified Resists

Chris A. Mack<sup>1</sup>, Monique Ercken<sup>2</sup>, Myriam Moelants<sup>2</sup>

<sup>1</sup>FINLE Technologies Inc., P.O. Box 162712, Austin TX, 78716, [chris\\_mack@finle.com](mailto:chris_mack@finle.com)

<sup>2</sup>IMEC, Kapeldreef 75, Leuven B-3001, Belgium

## Abstract

In this paper, the method for tuning a lithography simulator to match simulation to experiment, proposed by Thornton and Mack, was extended to a chemically amplified deep-UV resist process. After performing the Thornton-Mack tuning, the post-exposure bake (PEB) parameters of the resist were adjusted in the simulator to match experimental results. In particular, measurements of  $E_0$  versus time and temperature of the PEB were used to “calibrate” the actual PEB hotplate to the simulated hotplate and to estimate the amount of base quencher in the resist. Once tuned, the simulator was used to predict CD performance and compared to experimental results.

**Keywords:** Optical Lithography, Lithography Simulation, Model Tuning, Chemically Amplified Resist, PROLITH

## I. Introduction

For many applications, lithography simulation has proven extremely effective at predicting or explaining important lithographic trends, providing insight and direction for problem solving, and extrapolating lithographic technology into the future [1]. For some applications, however, the usefulness of lithography simulation depends on its ability to match experimental results for a specific process. When simulation and experiment do not match, there are three possible reasons. First, the experimental results could be wrong due to setup, process, and/or measurement errors. Second, the models used in the simulator may not adequately describe the physical realities present in the experiment. And third, the input parameters used for the simulation may not adequately describe the experimental conditions. Of these three, incorrect input parameters is by far the most common source of simulation to experiment mismatch in optical lithography modeling.

Recently, a systematic approach to matching simulation to experiment for a given process, called “tuning” the model, was proposed [2]. A simple  $E_0$  (dose-to-clear) swing curve experiment was used to remove uncertainties in experimental measurements of resist thickness and exposure dose for an i-line resist process. Further work allowed simple *in-situ* measurement of development rate parameters. The use of such tuning techniques resulted in extremely close matching of experimental swing curve results to simulation on a variety of substrates. Further work on tuning by Mason et al. [3] extended the tuning concept and showed good agreement between simulated and experimental resist cross-sections.

In this paper, the tuning method proposed by Thornton and Mack [2] was extended to a chemically amplified deep-UV resist process using a technique similar to that shown by Byers et al. [4]. After performing the Thornton-Mack tuning, the post-exposure bake (PEB) parameters of the resist were adjusted in the simulator to match experimental results. In particular, measurements of  $E_0$  versus time and temperature of the PEB were used to “calibrate” the actual PEB hotplate to the simulated hotplate and to estimate the amount of base quencher in the resist. Once tuned, the simulator was used to predict CD performance and compared to experimental results.

## II. Experimental

All exposures were done on the ASM-L PAS5500/300 Deep-UV stepper, which is equipped with a projection lens with a continuously variable numerical aperture (NA) between 0.4 and 0.57 at the full 22×22 mm field size. The coherence factor ( $\sigma$ ) can be varied between 0.3 and 0.8 without a significant intensity loss at the wafer level. The stepper is interfaced with a TEL Mark8 coat and develop track. Track and stepper are chemically filtered to prevent airborne contamination. Top-down CD metrology was performed on a Hitachi 8820S in-line SEM (measurement method used was the linear approximation), and cross-section pictures were taken with a Philips SEM XL30. The 4× binary test reticle for line/space exposures, manufactured by IMEC, was characterized on the KLA8100ER SEM.

Dose repeatability and accuracy of the stepper were determined in the region 1-10 mJ/cm<sup>2</sup>. For each energy, the standard deviation over 100 laser pulses was not higher than 0.1mJ/cm<sup>2</sup>. The ability to read  $E_0$  from the wafers was estimated to have an error of  $\pm 0.1$ mJ/cm<sup>2</sup>, giving an overall measurement uncertainty of  $\pm 0.15$ mJ/cm<sup>2</sup> one sigma.

Shipley's UV5 photoresist was used for the experimental work. Standard post-apply bake (PAB) conditions were 90s, 135°C. Development conditions were 60s single puddle using a standard normality developer (OPD262). For the dose-to-clear ( $E_0$ ) experiments, post-exposure bake (PEB) conditions were varied: baking time from 30 to 120s and baking temperature from 110 to 140°C. For the determination of the swing curve, a 90s, 125°C PEB was applied using NA = 0.57 and  $\sigma = 0.6$ .  $E_0$  experiments were performed without using a reticle (resulting in approximately 7% difference in dose compared to the use of a blank reticle [3]). To exclude differences in baking temperatures from hotplate to hotplate, always the same hotplates were used for PAB and PEB. Resist coating was performed manually. For the line/space exposures, AR2 was used as a BARC. The AR2 was baked for 60s at 190°C to get a thickness of about 80nm. Here, the PEB time was fixed at 90s.

## III. Tuning Results

The first step in the Thornton-Mack tuning procedure is to adjust the resist index of refraction to match the systematic differences in measuring resist thickness from fab to fab. Figure 1 shows the results of comparing simulated to experimental  $E_0$  swing curves before tuning. For the simulation, default UV5 resist parameters shipped with PROLITH/2 v6.0.4 were used. Two obvious problems are observed. First, the phase of the two swing curves do not match. This phase error is due to a miscalibration between the resist thickness used in the simulation and the resist thickness measured in the fab. The measured  $E_0$  swing curve can be used to calibrate the PROLITH/2 resist thickness to match the experimental resist thickness by adjusting the resist index of refraction in the simulation until the phases of the two swing curves match. When this was accomplished, the UV5 refractive index went from its default value of 1.7693 to its "tuned" value of 1.782.

Another problem apparent from the  $E_0$  swing curve comparison in Figure 1 is the mismatch in dose values. For *i*-line resists, Thornton and Mack attributed such mismatches to dose calibration errors [2] and tuned the simulation dose values by adjusting the resist exposure rate constant  $C$ . For chemically amplified resists, there are two sources of "dose"; exposure dose and thermal dose during PEB. Thus, the tuning for chemically amplified resists can either adjust  $C$  to compensate for exposure dose calibration errors or adjust the resist amplification rate constant to adjust for hotplate thermal calibration errors. From a simulation perspective, either adjustment gives comparable results. As will be clear later in this section, most of the tuning work for chemically amplified resists involves calibrating the hotplate in the fab to the simulator's "virtual" hotplate. Thus, it will be most convenient to simply fix the value of

$C$  ( $0.05\text{cm}^2/\text{mJ}$  is this case) and use the amplification reaction rate constant to tune the dose-to-clear values of the simulated swing curve. Details of the amplification rate constant tuning will be given below, however the results are seen in Figure 2.

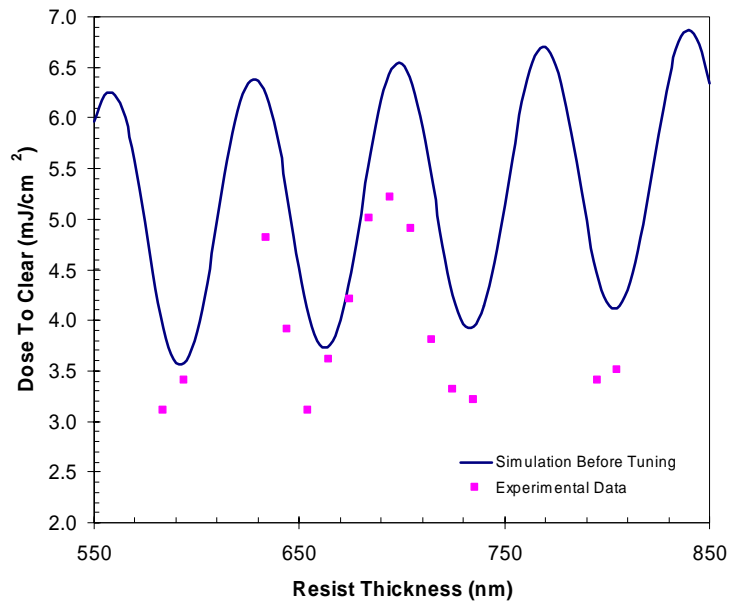


Figure 1. Comparison of simulated and experimental swing curves before tuning shows the classic problems: phase and dose mismatch.

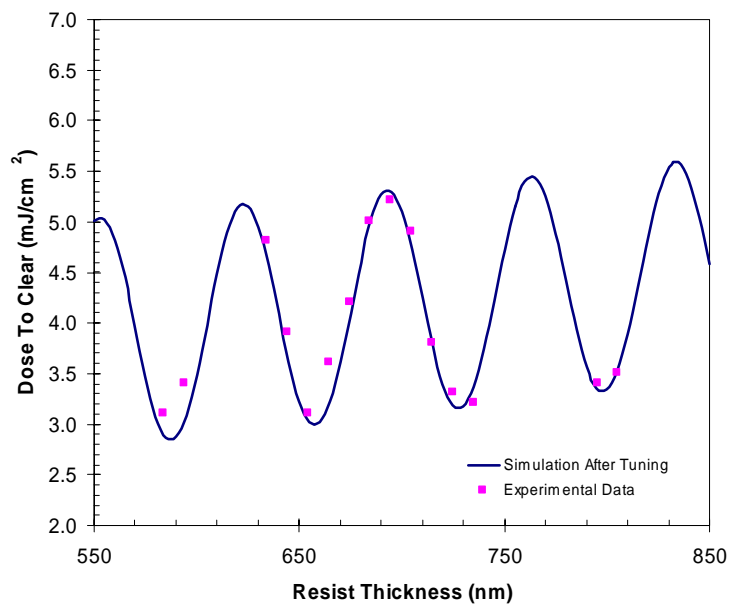


Figure 2. Comparison of simulated and experimental swing curves after tuning the resist index of refraction and the PEB amplification reaction rate constant.

The great sensitivity of chemically amplified resists to PEB conditions means that even small variations in the wafer thermal cycle (wafer temperature as a function of time during the PEB/chill process) can produce different resist responses. Experimentally, great care must be taken to calibrate multiple hotplates in a fab in order to match their thermal cycles to produce consistent lithographic results. The same is true when matching simulation's "virtual" hotplate to a specific fab hotplate. However, rather than changing the temperature used in the simulation, we will tune the simulator's hotplate by tuning the PEB reaction rate constants.

Table I shows the simulation starting point for tuning in this work. The parameters in this table represent the simplest model for a chemically amplified resist. All acid loss mechanisms, such as acid evaporation or airborne base contamination, have been turned off. The influence of diffusion on the reaction rate has been disabled (by making the diffusion-controlled reaction rate constant very large). The diffusivity has been assumed to be constant (at a given temperature), the amplification reaction order fixed at 1.0, and no base quencher was assumed.

Table I. Initial simplified PEB modeling parameters for UV5 tuning.

<b>Parameter</b>	<b>Value</b>
Room Temperature Diffusion Length (nm)	0.0
Amplification Reaction Order	1.0
Base Quencher Concentration	0.0
Diffusivity Variation Type	Constant
PEB Diffusivity Activation Energy (Kcal/mol)	45.0
PEB Diffusivity ln(Arrhenius Coefficient) (nm <sup>2</sup> /s)	61.0
Amplification Reaction Activation Energy (Kcal/mol)	35.0
Amplification Reaction ln(Arrhenius Coefficient) (1/s)	42.0
Diffusion-Controlled Reaction Rate Constant (1/s)	100,000
Bulk Acid Loss Rate Constant (1/s)	0.0
Acid Evaporation Rate Constant	0.0
Airborne Base Contaminant Concentration	0.0

Again, the dose-to-clear has been used as a monitor of the process. Dose-to-clear was measured as a function of time and temperature of the post-exposure bake. Then simulation was performed to match to this data. Besides the PEB parameters given in Table I, other modeling parameters are shown in Table II. The initial results are shown in Figure 3. Obviously, there is a large discrepancy between simulation and experiment. The first and most interesting observation is the behavior of  $E_0$  for high temperature, long time bakes. The experimental data levels off at an  $E_0$  value of 2.5 - 2.6 mJ/cm<sup>2</sup>, while the simulation goes to zero at the extreme bake conditions. It is apparent that the experimental data exhibits a minimum exposure dose, below which no amount of thermal dose can result in sufficient reaction to cause the resist to clear. Such behavior is characteristic of the presence of a base quencher.

Table II. Initial non-PEB modeling parameters for UV5 tuning.

Parameter	Value
Bleachable Absorption Coefficient A (1/μm)	0.0
Non-Bleachable Absorption Coefficient B (1/μm)	0.52
Exposure Rate Constant C (cm <sup>2</sup> /mJ)	0.05
Refractive Index	1.782
Development Rmax (nm/s)	1000
Development Rmin (nm/s)	0.3
Development Mth	0.65
Development Selectivity n	12
Relative Surface Development Rate	1.0
Resist Thickness (nm)	660
Development Time (sec)	60.0

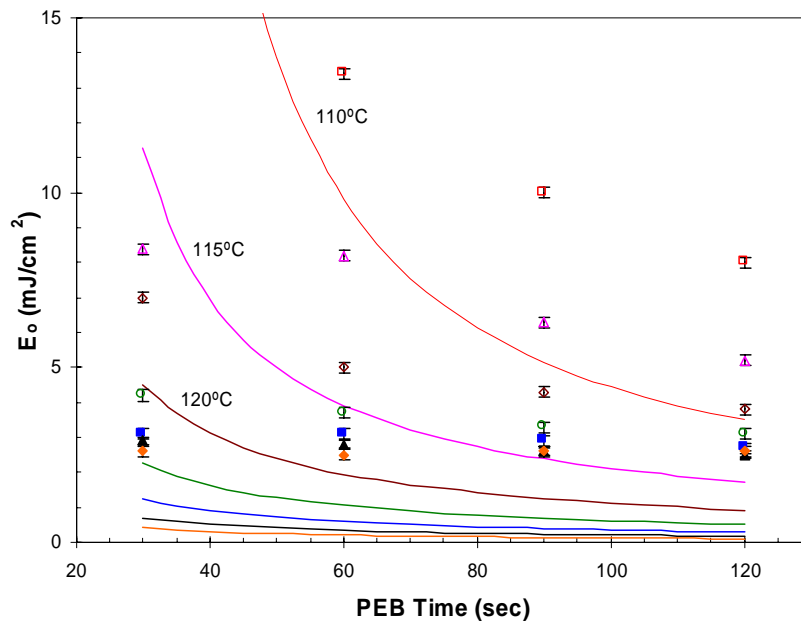


Figure 3. Initial results comparing simulation to experimental  $E_0$  values before tuning.

Figure 4 shows simulated  $E_0$  versus PEB time (at 125°C) for various amounts of base quencher (base quencher expressed as a concentration relative to the initial PAG concentration). As expected, increasing amounts of base quencher produces an increasing “turn-on” dose before amplification will begin. Thus, by tuning the base quencher concentration, the best match to the experimental  $E_0$  data can be obtained. A relative quencher concentration of 0.155 was required to match the behavior of the experimental  $E_0$  data as a function of PEB conditions. By also adjusting the amplification reaction rate

constant Arrhenius coefficient and activation energy, the match of simulation to experiment shown in Figure 5 was obtained. [As it turned out, the initial guess of the amplification reaction rate constant activation energy was close enough that no adjustments were needed. In general, however, it is expected that some adjustment to match the through temperature data would be required.] The natural logarithm of the amplification reaction Arrhenius coefficient was adjusted from 42.0 to 41.5 in order to best match the data.

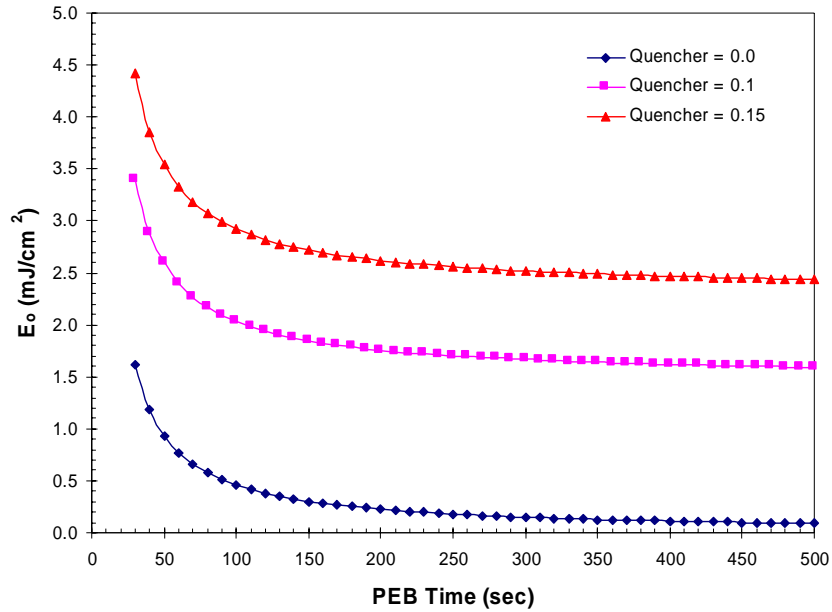


Figure 4. Example of the impact of base quencher on the  $E_0$  versus PEB time curves.

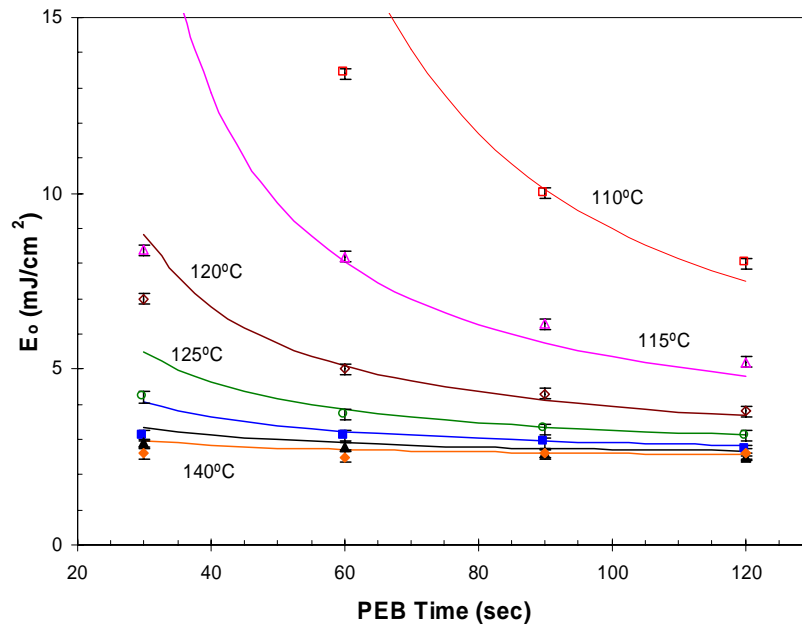


Figure 5. Final results of tuning the base quencher and amplification reaction Arrhenius coefficient to best match the experimental data.

Note that the simulated versus experimental  $E_0$  values match quite well over a very wide range of temperatures except at the shortest PEB time, the 30 second bake. At this bake time, the experimental  $E_0$  values are much lower than expected.

#### IV. Simulation Results vs. Experiment

Using the modeling parameters tuned only with the  $E_0$  data presented above, experiment and simulations of mask linearity and focus-exposure response were used to test the tuned model. There is one complication that must be addressed when comparing  $E_0$  and dose-to-size data. As Mason et al. pointed out [3], most steppers control exposure dose using a sensor in the illumination system located before the reticle plane. Thus, the dose that is controlled is the dose incident on the reticle, not the dose incident on the wafer. When an exposure dose is used in a lithography simulator such as PROLITH/2, this dose is defined as the energy incident on the wafer after passing through a large clear area of the mask. However, for the  $E_0$  measurements carried out here and described above, the reticle plane was left empty rather than using a blank quartz mask. The result is about a 7% error in the dose actually reaching the wafer for the  $E_0$  measurements versus the lithography measurements which employed a reticle [3]. This was corrected for in the subsequent simulations by lowering the value of  $C$  by 7%, to  $0.0465\text{cm}^2/\text{mJ}$ .

Figure 6 shows the simulated and measured linearity response of this resist at two PEB temperatures,  $125^\circ\text{C}$  and  $130^\circ\text{C}$ . As can be seen, the simulated and experimental data match very well except the sub 200nm features at  $130^\circ\text{C}$ . Excluding these two data points, the RMS error between simulation and experiment is 1.0nm.

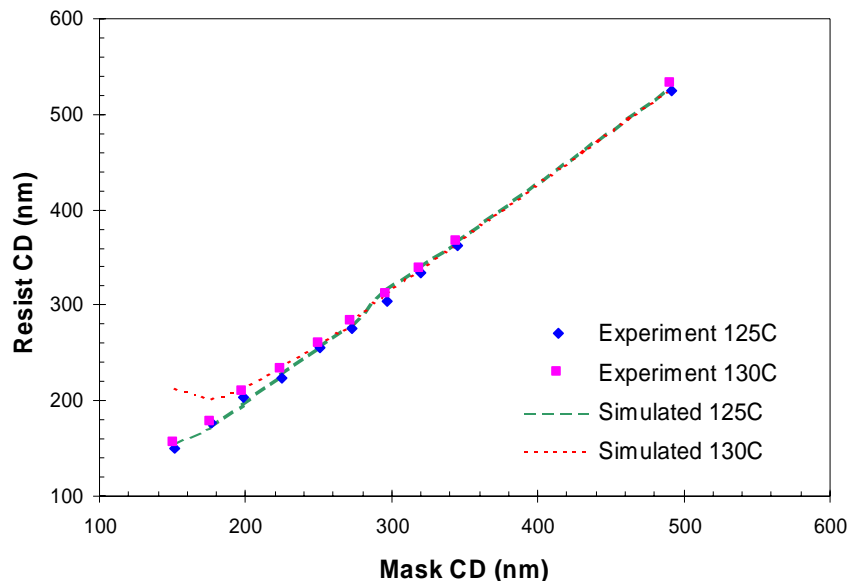


Figure 6. Comparison of simulated and experimental linearity curves at two different PEB temperatures using the tuned model.

Next, the focus-exposure response of the data was compared to simulation for the standard  $125^\circ\text{C}$ , 90sec PEB using a 250nm line/350nm space repeating pattern. Figure 7 shows that the basic



dose-to-size, focus latitude, and exposure latitude all match quite well between experiment and simulation. However, it is apparent that the simulation is not predicting the correct isofocal bias (the CD value at which the change in CD through focus is a minimum). This simulation is predicting an isofocal CD of about 245nm whereas the data shows an isofocal CD of about 270nm.

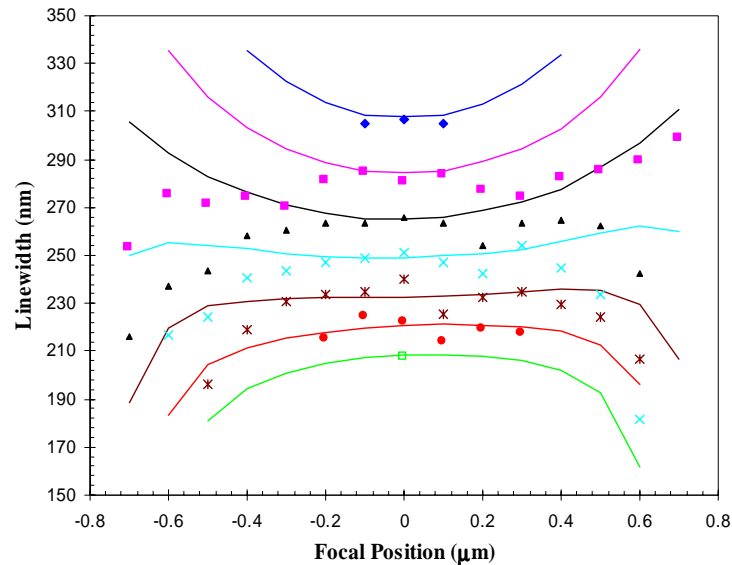


Figure 7. Comparison of simulated (lines) and experimental (points) focus-exposure behavior at a 125°C, 90 sec bake. Exposure doses ranged from 11 to 17 mJ/cm<sup>2</sup>.

Finally, the behavior of the resist cross-section through focus was studied. Using the base-line 125°C, 90sec PEB for the 250nm line/350nm space mask pattern, simulated versus experimental cross-sections are shown in Figure 8.

## V. Discussion of Results

Using nothing more than the simple  $E_0$  tuning of the Thornton-Mack method extended to include PEB conditions, the effective base quencher concentration and the temperature dependence of the amplification rate constant were measured. The use of these “tuned” modeling parameters allowed a much closer prediction of the lithographic response of a specific process than the generic parameters would allow. However, it is also obvious that these two PEB modeling parameters (quencher concentration and amplification rate constant) are not sufficient to completely define the lithographic properties of this chemically amplified resist. By comparing simulation to experiment, several discrepancies were observed.

First, the original tuning data,  $E_0$  versus PEB time and temperature, showed anomalous behavior at the shortest bake time of 30 seconds. This discrepancy might be expected due to the warm-up time of a wafer baked in proximity mode. It is expected that about 20 -30 seconds is required for the wafer to reach within 5°C of the wafer temperature at 90 seconds [5]. The simulation, however, assumes that the wafer temperature has reached the set point instantly as the bake begins. The use of the actual time-temperature thermal history of the wafer during the PEB (including the chill cycle) could significantly

improve the accuracy of short bake time simulations. Room temperature amplification (before the beginning of the PEB) could also be a factor, although UV5 is a high activation energy resist so that this possibility seems remote.

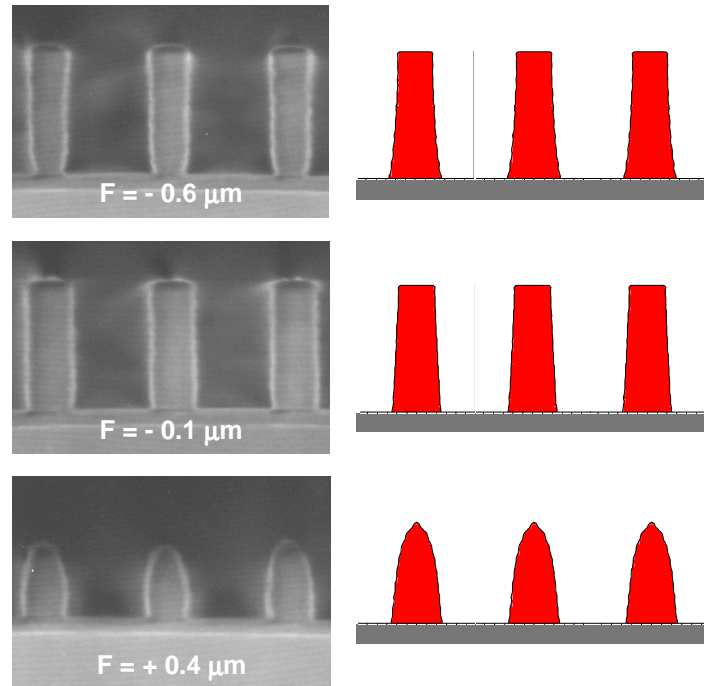


Figure 8. Comparison of simulated and experimental resist cross-sections through focus for a 125°C, 90 sec post-exposure bake.

Second, the simulation failed to predict the experimentally observed iso-focal CD response (Figure 7). There are two likely culprits here that need further investigation. The metrology assumed in the simulation measured the resist profile at the bottom. It is not clear how these simulated CD values relate to the top-down CD measurement algorithm employed when the resist profile changes significantly through focus. As can be seen in Figure 8, the behavior of the experimental resist cross-sections is quite different at each side of focus. Measuring the resulting linewidth near the top of the resist profile would result in very different behavior compared to measurements at the middle or at the bottom. Also, the acid diffusion behavior can impact the iso-focal response of a given mask pattern. No attempt was made to investigate the impact of diffusion in this study.

Finally, the simulated versus actual resist profiles through focus shown in Figure 8 indicate a discrepancy at negative focus (focus above the top of the resist). There is a small undercut at the bottom of the resist profile, probably due to an insufficient bake of the AR2 bottom coating. But more importantly, the bulk resist profile is becoming slightly negative (bottom smaller than the top) at this negative focus, whereas the simulation shows the opposite behavior. This problem is most likely due to variations in development rate through the thickness of the resist. While the simulation assumed, for simplicity, no surface inhibition, most modern resists have well engineered solvent gradients that provide a gradually increasing development rate through the resist. This solvent-induced depth dependence to the

development rate counteracts the impact of optical absorption to provide steeper sidewalls. It also has the tendency to cause negative profiles when the focal plane is shifted above the top of the resist.

## VI. Conclusions

Using a simple extension of the Thornton-Mack tuning technique, measurement of resist dose-to-clear ( $E_0$ ) as a function of post-exposure bake time and temperature was used to calibrate the thermal model of amplification for a chemically amplified resist and to measure the effective amount of base quencher present in the resist film. Using only these straightforward measurements, good, though not perfect, match of simulation to experiment was obtained for resist linearity, focus-exposure CD response, and resist cross-sections. Further work will identify other experiments to elucidate the diffusion behavior, perhaps by measuring the iso-dense print bias as a function of PEB conditions. Either through accurate solvent diffusion modeling [6] or empirical surface inhibition functions, better match of resist profiles can be obtained by describing the depth dependence of the development rate. And finally, metrology matching will eliminate the uncertainty in the interpretation of top-down linewidth measurements in the presence of changing resist profile shape.

## References

1. C. A. Mack, Inside PROLITH: A Comprehensive Guide to Optical Lithography Simulation, FINLE Technologies (Austin, TX: 1997).
2. S. H. Thornton and C. A. Mack, "Lithography Model Tuning: Matching Simulation to Experiment," *Optical Microlithography IX, Proc.*, SPIE Vol. 2726 (1996) pp. 223-235.
3. M. E. Mason, R. A. Soper, R. M. Terry, and C. A. Mack, "Process-specific Tuning of Lithography Simulation Tools," *Optical Microlithography X, Proc.*, SPIE Vol. 3051 (1997) pp. 491-498.
4. J. Byers, J. Petersen, and J. Sturtevant, "Calibration of Chemically Amplified Resist Models," *Advances in Resist Technology and Processing XIII, Proc.*, SPIE Vol. 2724 (1996) pp. 156-162.
5. D. P. DeWitt, T. C. Niemoeller, C. A. Mack, and G. Yetter, "Thermal Design Methodology of Hot and Chill Plates for Photolithography," *Integrated Circuit Metrology, Inspection, and Process Control VIII, Proc.*, SPIE Vol. 2196 (1994) pp. 432-448.
6. C. A. Mack, K. E. Mueller, A. B. Gardiner, J. P. Sagan, R. R. Dammel, and C. G. Willson "Modeling Solvent Diffusion in Photoresist," *Jour. Vac. Sci. Tech.*, Vol. B16, No. 6, (Nov., 1998) pp. 3779-3783.