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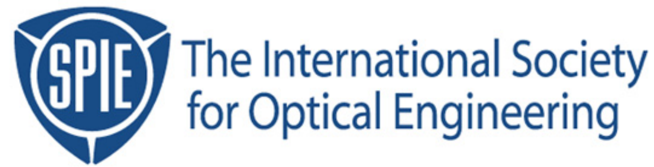

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Lithography Model Tuning: Matching Simulation to Experiment

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ABSTRACT

A method is presented for adjusting the input parameters of a lithography simulator to more accurately match a given set of experimental conditions. Using a dose-to-clear swing curve on bare silicon, the index of refraction of the photoresist is adjusted to account for relative resist thickness measurements made in the fab. The resist exposure rate constant *C* can be adjusted to account for dose calibration differences, or these differences could be included in the development parameters. The develop parameters can be tuned using the exposure margin, or a measurement technique called the Poor Man's DRM could be used to measure a new set of development parameters. Results of these tuning procedures are presented and the tuned set of parameters is shown to give good quantitative agreement of simulation to experiment.

I. Introduction

Process simulation is a valuable tool that enables process engineers to save time and money when characterizing a process. However, to get the most benefit from this tool, certain elements of the models must be fine tuned to match a given process. This paper will show why tuning is necessary and provide a methodology for doing so. When a lithographer in today's high volume fab uses a modeling tool, in this case PROLITH/2 from FINLE Technologies, to aid in defining or characterizing a photolithography process, he/she typically finds that experimental results don't always match up with the software model. There are several reasons for this phenomenon. First, the resist thickness value that the typical lithographer measures is usually not an absolute measure of resist thickness. This is due to the fact that most fabs set up their measurement tools to use the default settings for the tool. Because of this, the tool does not use the true index of refraction of the resist that is being measured. In fact, fab measurements of resist thickness do not need to be absolute -- a relative resist thickness is all that is necessary. In the case of the swing curve, this inaccurate measurement results in a shift in the phase of experimental swing curve data relative to the simulation. The model's phase can be shifted to account for the measurement method by adjusting the resist's index of refraction setting in the model.

Another reason that experimental results don't match up with the model is due to inaccurate dose calibration. Like the resist thickness measurement tool, dose meters don't usually yield absolute measurements and are really only needed to provide relative measurements (dose matching among steppers, etc.). In fact, dose meters can vary as much as 20% from meter to meter. Therefore, the meter used to dose check the stepper used in the experiment typically does not match the meter used when the resist company measured their Dill ABC parameters. Because of this, in the case of the swing curve, the model does not match the experiment in the y-axis, which represents E_o. The model can be adjusted in the y-axis to match the experiment by changing the *C* parameter (representing the exposure rate constant) of the Dill ABC parameters to match the lithographer's process and account for the difference in dose calibration.

Development parameters are another source of potential mismatch between simulation and experiment. Develop model parameters are often measured by the resist manufacturer for their recommended process. However, the process used in the fab is often different, sometimes in subtle ways like a different temperature, other times in obvious ways like the use of a different developer. Tuning the development parameters can account for these differences. Other parameters can also be adjusted for fine tuning of the model such as lens aberrations and the CD metrology method.

This paper will seek to define a process whereby a lithographer can use this fine tuning method to tune the models to the photolithography process on bare silicon. Then, using the same adjustments, one can accurately model the rest of the photolithography processes on differing substrates and under other conditions, thereby saving time, money, and utilizing the full potential of the modeling tool.

II. Tuning Resist Thickness Measurements

The first step in tuning a lithography model to a given process is to fine tune the model to the resist measurement tool by using the swing curve. This must be done due to several reasons. First, most fabs don't completely adjust their measurement tool to the correct parameters for each resist that they may be using. Second, adjusting the measurement tool to all the correct parameters for a resist doesn't guarantee absolute resist thickness measurements (there are no resist thickness calibration standards). In fact, absolute resist thickness measurements are not necessary in the fab. For the purposes of simulation, relative ones will suffice if one fine tunes the process model to account for these relative measurements.

To accomplish this tuning, PROLITH/2 was used to simulate the experimental process conditions using the resist parameters that came with the software (see the "before tuning" parameters in Table I). Next, bare silicon wafers were coated with Shipley 3813 photoresist at thicknesses varying from 1.0 to 1.3 microns, exposed with a boustrophedonic exposure pattern in which exposure energy was incrementally increased with each exposure, and developed with a standard PEB and 75 sec dip develop using AMD's in house Contrast 2000 MIF developer. Table II gives a complete set of experimental conditions. The dose to clear, E_o, was determined for each resist thickness and plotted with PROLITH/2 to yield an experimentally determined swing curve. This experimentally determined swing curve was plotted against the simulated swing curve from the model. As can be seen in Figure 1, the experimental data was somewhat out of phase with the simulated data.

This shift in phase is due to inaccurate resist thickness measurements in the experimentally determined data set and/or an inaccurate value of the index of refraction used in PROLITH/2. This shift can be corrected by making an adjustment to the resist's index of refraction parameter in the model. The amount of adjustment can be determined by using PROLITH/2's file management option to plot both data sets. Then, by placing the mouse pointer on a data point of the simulated data and clicking the right button, an (x,y) coordinate is displayed. Performing the same operation on a comparable data point (one on the same hump or valley) of the experimental data will yield that data point's (x,y) coordinate. By comparing the displayed x coordinates of each curve, one can calculate the percentage of the resist thickness offset required and adjust the index of refraction by the same percentage. This results in a phase shift of the simulated data which matches it to the experimental data.

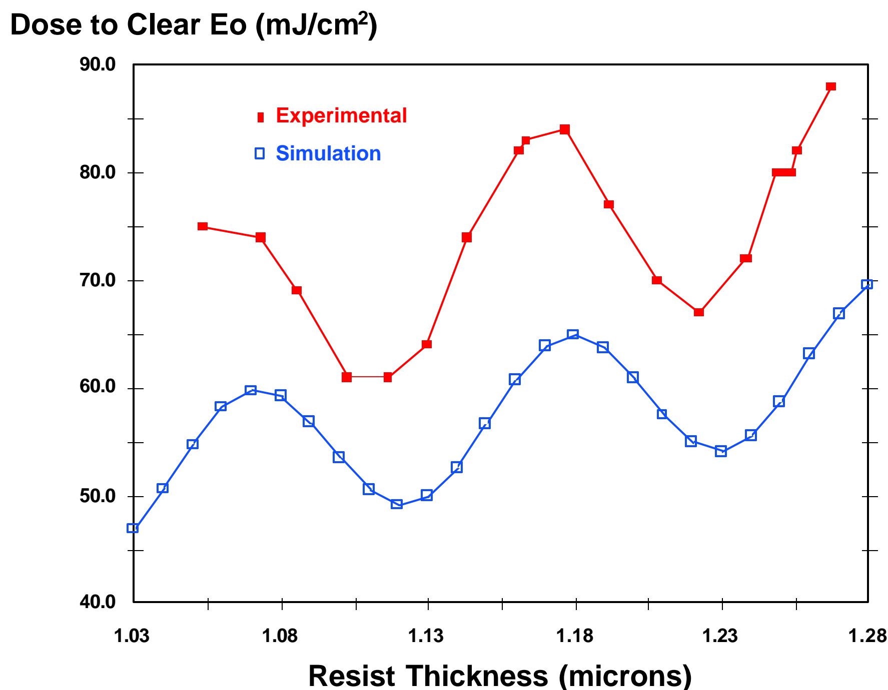

Figure 1. Comparison of initial (untuned) simulation to actual experimental data using an E_o swing curve to make the comparison.

The initial index of refraction for Shipley 3813 photoresist used in the simulation was 1.700. After comparison of simulated and experimental data, the index of refraction in the simulation was increased by 8.8% to 1.715. The result, shown in Figure 2, is a perfect match of the phase of the simulated and experimental swing curves. With this adjustment, the model is matched to the resist thickness measurement tool for this resist.

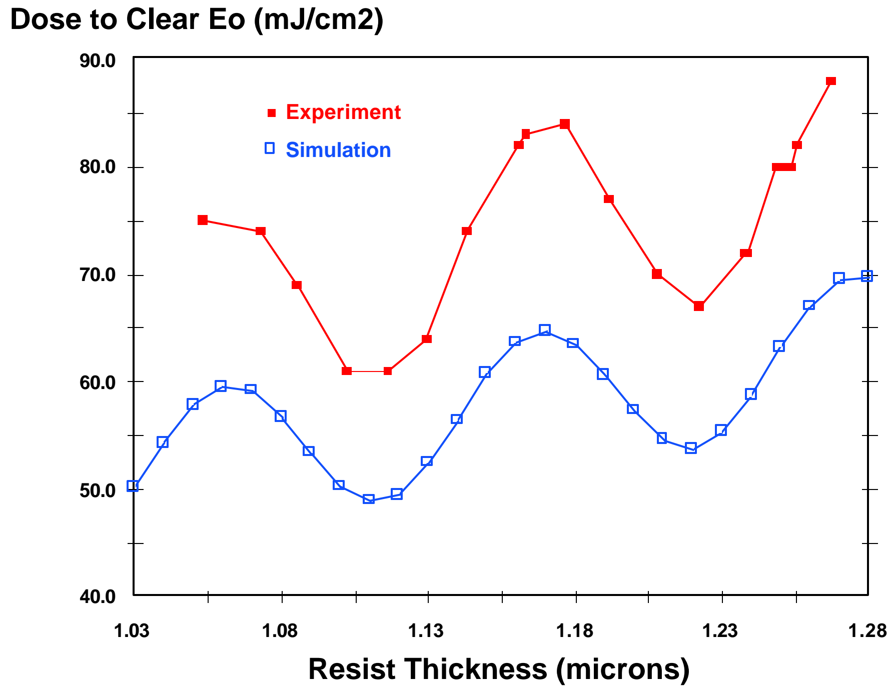

Figure 2. Adjustment of the index of refraction of the photoresist used by the simulation matches the resist thickness to the experiment and results in a perfect match of the phase of the two swing curves.

Table I. Simulation Parameters Before and After Tuning

Parameter	Before Tuning	After Tuning
A (µm^{-1})	1.165	1.165
B (µm^{-1})	0.133	0.133
C (cm^2/mJ)	0.0304	0.0240
refractive index	1.700	1.715
R_{max} (nm/sec)	159	100.3
R_{min} (nm/sec)	0.01	0.10
m_{th}	-10.	0.06
n	4.5	4.74

Table II. Experimental Conditions

Coat/Develop Process:	TEL Mark V track
HMDS vapor prime:	60 sec. vapor prime @ 190ºC
Resist:	Shipley 3813
Coat cycle:	1000 rpm dispense for 3 sec., 5 ml of resist, 23ºC 20 sec. spin at variable spin speed
Softbake:	60 sec. hard contact bake @ 105ºC.
Thickness measurement:	Prometrix SM 300/e, 49 sites.
Exposure:	ASML PAS2500/40 stepper, i-line, NA = 0.4
PEB:	60 sec. hard contact bake @ 115ºC.
Development:	AMD Contrast 2000 developer (0.255 N TMAH) 75 sec. dip develop, 20 sec. rinse

III. Tuning Exposure Dose

To further match the software model to the experimental data, the model can be adjusted in terms of exposure dose. Exposure dose meters can vary greatly from meter to meter. In addition, the probes used with the meters can vary and will attenuate with time. Because of this variation and attenuation, the meters and probes used in a typical fab, even though they are calibrated periodically, will not always yield absolute exposure energy measurements. Again, absolute measurements are not always necessary if a lithographer has adjusted the process models to match the experimental data.

With the phases of the curves matched, the next step in tuning the model to the process is to match the simulation to the experiment in the y-axis of the swing curve plot. This can be accomplished in much the same way as described in the previous section. Again, the experimentally determined swing curve was plotted against the simulated swing curve from the model. As can be seen in Figure 2, the experimental data does not match the simulated data in the y-axis. Although this shift may be due to errors in the development parameters as described below, it may also be due to a mismatch in the resist sensitivity. The meter used to dose check the stepper in the fab typically does not match the meter used when the resist company measured their Dill ABC parameters. This mismatch in dose calibration can be adjusted in the model by making an adjustment to

the resist's *C* parameter, the exposure rate constant. In Figure 2, the simulation predicts dose-to-clear values that are about 20% too low. By adjusting the resist *C* parameter in the simulation by this same percentage, the simulated data will move up to match the experimental data.

The initial *C* parameter for Shipley 3813 photoresist used in the simulation was 0.0304 cm^2/mJ. After comparison of simulated and experimental data using PROLITH/2, the *C* parameter in the simulation was reduced by 21% to 0.0240 cm^2/mJ. This resulted in a match to the experimental data as can be seen in Figure 3. This adjustment matches the model to the stepper's dose calibration. With both adjustments implemented, the swing curves of the simulated and experimental data are matched and further swing curves on different substrates can now be accurately modeled. Note that no adjustment was made to change the amplitude of the simulated swing curve.

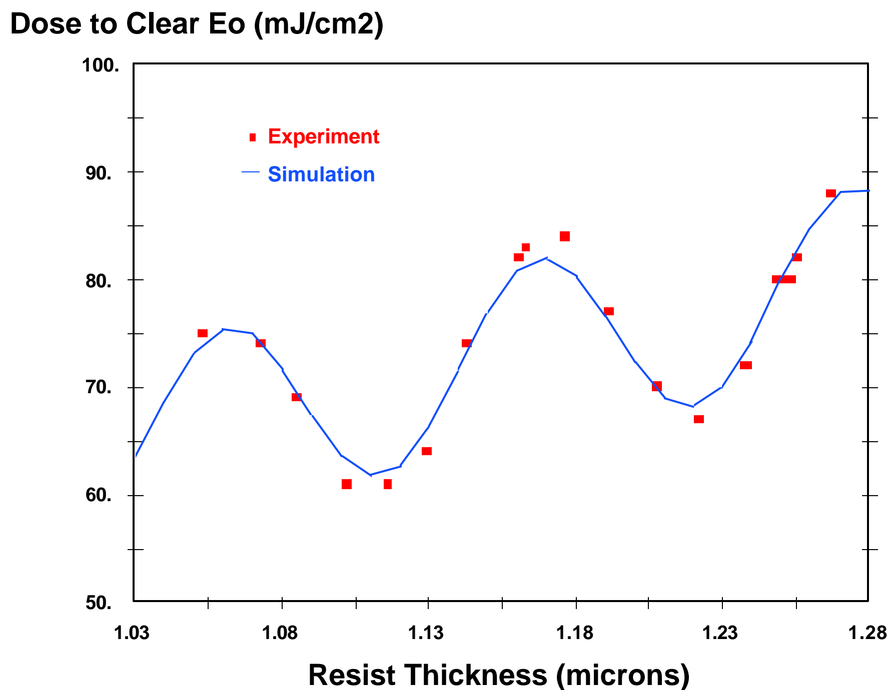

Figure 3. Tuning of the resist *C* parameter shifts the dose of the simulation to match the experiment.

Although the example above used the resist *C* parameter to shift the dose to clear of the simulation, development parameters can also have the same effect. In fact, in most circumstances it is more likely that the development parameters need adjustment more than the *C* parameter. If, however, the development parameters are either known to be reliable or the user has no interest in adjusting them, the *C* parameter is a convenient tuning parameter. In the sections below, a thorough description of tuning the development parameters is given.

IV. Tuning Develop Parameters

Parameters for development models are not only very important in obtaining quantitative agreement with experimental results, they are often very difficult to obtain. In general, development model parameters for a given resist/develop process are obtained by making special real-time measurements of resist thickness during development using a development rate monitor (DRM) [1]. The resist thickness versus develop time curves are measured at many different incident exposure doses. Taking the derivative of this data gives development rate (R) as a function of incident dose (E) and depth into the resist (z). By modeling the exposure process, a given exposure dose turns into a distribution of photoactive compound concentration (m) after exposure as a function of depth. Combining the measured $R(E,z)$ with the simulated $m(E,z)$ produces a resultant $R(m,z)$ data set. This data is then fit with a development model [2,3] and parameters for the model are extracted.

The above method of determining development parameters can be both accurate and convenient, given the proper hardware [1]. However, for many environments (such as a manufacturing line) use of a specialized tool such as a DRM is not practical. How, then, can one model lithographic results without these development parameters? Often, a base-line set of develop parameters can be found for the photoresist in use, usually from the vendor of the resist material. However, the measurement conditions for these parameters (spray vs. puddle, developer temperature, resist bake conditions, etc.) may differ considerably from the conditions to be modeled. This is another situation where tuning a given set of parameters is appropriate.

A. Simple Tuning

The most common model of development rate is the Mack model [2]:

$$R = R_{\max}\frac{(a+1)(1-m)^n}{a+(1-m)^n}+R_{\min} \tag{1}$$

where

$$a = \frac{(n+1)}{(n-1)}\left(1-m_{TH}\right)^n$$

and R_{max} is the maximum development rate (corresponding to fully exposed resist where $m = 0$), R_{min} is the minimum development rate (corresponding to unexposed resist where $m = 1$), m_{TH} is the value of m at the inflection point of the data, called the threshold PAC concentration, and n is the dissolution selectivity parameter which controls the contrast of the photoresist. If a baseline set of values for these four parameters exists, they can be tuned to give a better match to given process.

The two parameters R_{max} and R_{min} are the easiest to interpret and the easiest to tune. Two simple experiments allow reasonably accurate measurement of these two parameters. To measure the maximum development rate, simply expose a large clear area of the resist (an open frame exposure on a stepper) with a very high dose (say, 1 J/cm^2 for a typical resist). Run the standard develop process but use the shortest

develop time possible (this will vary from track to track due to hardware and software constraints). Since automated tracks are not geared towards very short develop times, it is a good idea to time the actual develop cycle with a stop watch rather than trusting the programmed develop time. If the resist does not clear in the allotted short develop time, measure the resist thickness remaining in the exposed area. The maximum develop rate will be the resist removed divided by the develop time. If the resist is completely removed in the allotted time, then a visual measure of the resist clearing time (using a stop watch) can give an approximate value for R_{max}. Likewise, R_{min} can be estimated by developing an unexposed wafer for a very long time (say, 10 minutes) and measuring the amount of resist removed. For resists with very low unexposed development rates, this measurement may also be difficult.

The dissolution selectivity parameter n is the most important parameter for modeling purposes. A high value of n corresponds to a high contrast resist process, giving larger exposure latitude and depth of focus. A good method of tuning this parameter is using the exposure margin. Exposure margin is defined as the dose to size divided by the dose to clear. As Hansen has noted [4], the exposure margin is directly proportional to the photoresist contrast and thus to the dissolution selectivity n. Figure 4 shows the results of a simulation of exposure margin versus n. Since exposure margin is easily measurable in the fab, a graph like Figure 4 can be generated for the current set of process simulation parameters and the correct dissolution selectivity chosen to give the requisite value of exposure margin.

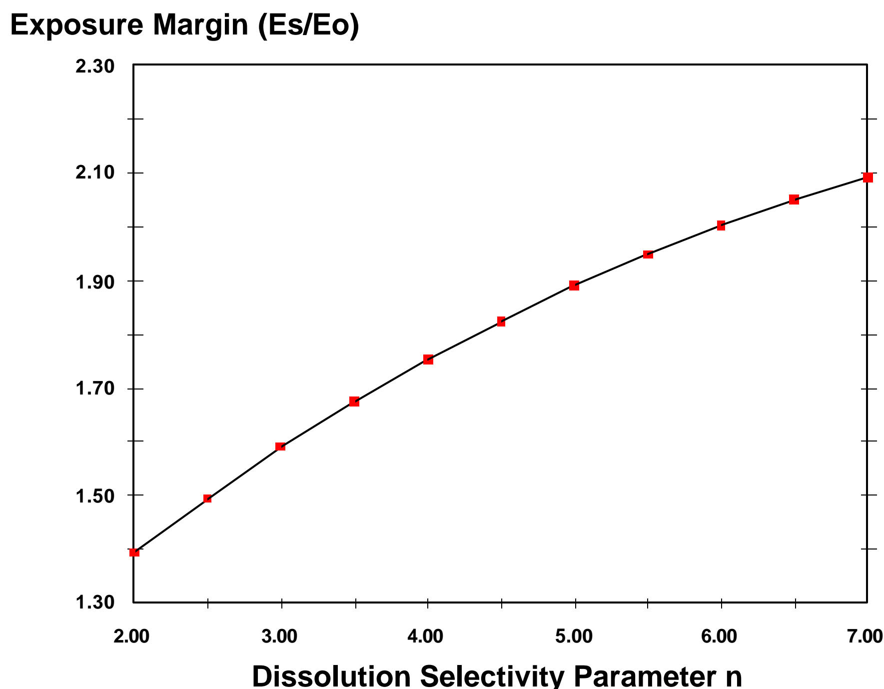

Figure 4. Adjustment of the dissolution selectivity parameter n can be used to match the simulated exposure margin to experiment.

The maximum development rate can be used to tune for exposure dose calibration differences rather than the exposure rate constant *C* if only small adjustments are needed. Since a stop watch measurement of R_{max} can give considerable error for large values of R_{max}, making some adjustments to match the E_o axis of the swing curve is justified.

B. The Poor Man's DRM

The above tuning procedure gives reasonable values of development parameters in most cases. However, in some circumstances a more accurate set of parameters is needed. In our case, the development parameters initially used were measured for Shipley 3813 resist but with a completely different developer. It was unknown whether the developer actually being used (an AMD home-brew called Contrast 2000) would have similar parameters. Although the ultimate method for obtaining new parameters is the use of a DRM, there is still another alternate, which we shall call the Poor Man's DRM. The Poor Man's DRM involves the measurement of multiple contrast curves -- resist thickness remaining as a function of exposure dose for open frame exposures -- at different development times. The equipment needed is readily available in any wafer fab and involves running on the order of 15 to 20 wafers. Until recently, the most difficult aspect of this approach was the data analysis.

To demonstrate the application of the Poor Man's DRM, 14 wafers were coated and exposed with a standard open frame exposure pattern using the processing conditions given in Table II. The range of exposures was varied depending on the development time to be used. Each wafer was then developed at different times ranging from 9 seconds to 201 seconds (in our case, 9 seconds was the shortest development time that could be used on the develop track). Each wafer was then measured on a Prometrix SM/300 film thickness measurement tool. The resulting data is shown in Figure 5.

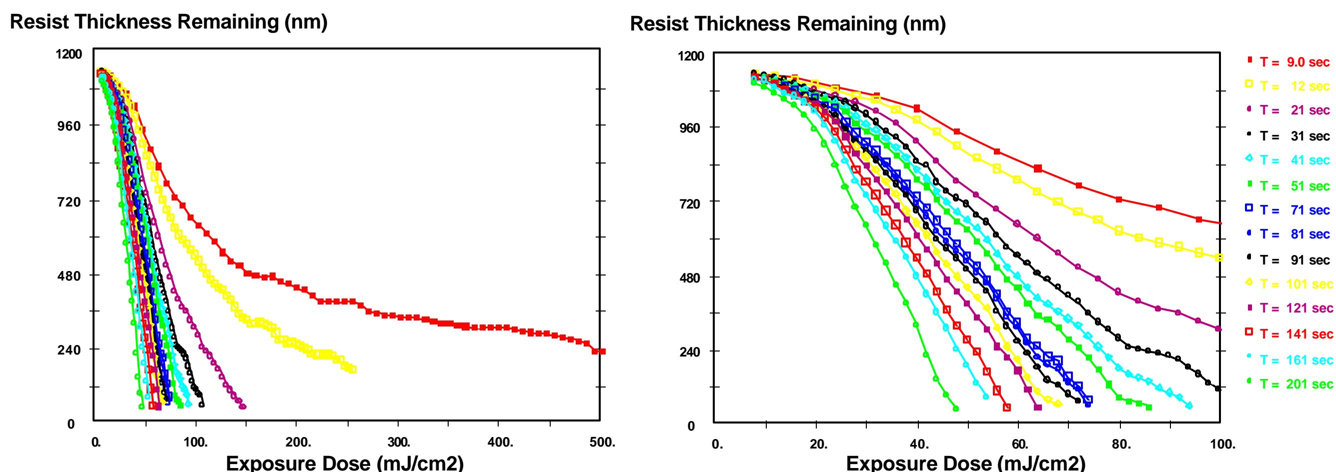

Figure 5. Measured contrast curves at many different development times (shown here over two different exposure scales).

Analyzing the information in Figure 5 to obtain development rate, and eventually development parameters, is not trivial. The thickness as a function of dose and development time is first converted to rate as a function of dose and depth into the resist, $R(E,z)$. From here, analysis is the same as for conventional DRM data. To make this effort practical, the analysis was automated with a software package called ProDRM [5]. This software uses a simple difference method to take the derivative of the contrast curve data and generate the $R(E,z)$ function. As expected, this function has a fair amount of noise in the data. However, no smoothing was attempted. Instead, each data point was kept and "smoothing" was accomplished during the fitting process at the end. ProDRM then uses a built-in exposure model to predict $m(E,z)$ for the experimental conditions of the data. Combining the $R(E,z)$ data with the modeled $m(E,z)$ results in a data set of $R(m,z)$.

The $R(m,z)$ data for this experiment showed no appreciable z dependence (indicating a lack of any significant surface inhibition). Figure 6 shows the full set of data. Using a Levenson-Marquat non-linear least squares fit algorithm, the data was fit to equation (1) and the best fit is shown as the solid line in Figure 6. Even though taking the derivative of the experimental data gives appreciable noise, a reasonable fit of the data is still obtained. The resulting development parameters were then used as the new "tuned" parameters.

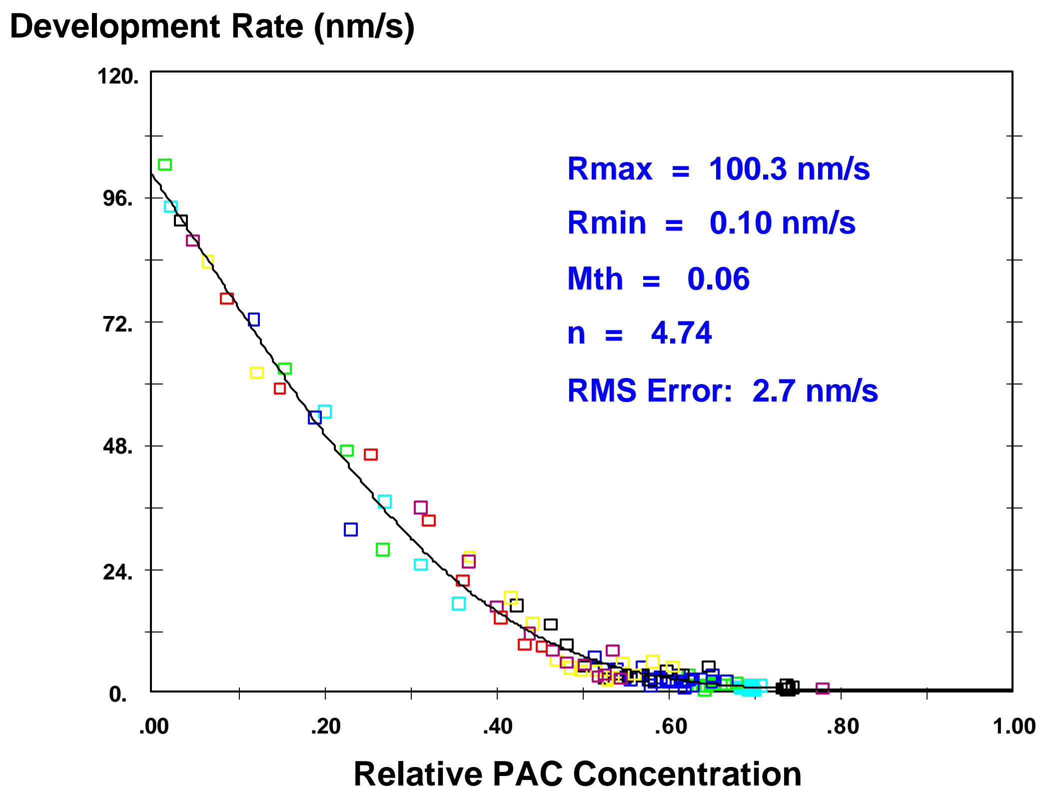

Figure 6. Analysis of the contrast curves by the ProDRM software generates an $R(m)$ data set, which is then fit to the Mack development model (best fit is shown as the solid line).

V. Comparison of Simulation to Experiment

The test of this tuning procedure is to determine whether the lithography simulator, together with the "tuned" set of parameters, can accurately predict new lithographic behavior (i.e., results which were not used in the tuning process). For example, the index of refraction and develop parameters were tuned to match the swing curve on bare silicon wafers. If the tuned parameters are correct, the simulator should also give accurate swing curve results on other film stacks. Figure 7 shows two swing curves for different substrates: 130nm polysilicon and a film stack of 95nm nitride on 40nm oxide. In both cases, the simulation with the parameters that were tuned on bare silicon give good agreement with the experiment data. (As an aside, the original untuned parameters gave very poor agreement with this data, just as in Figure 1.)

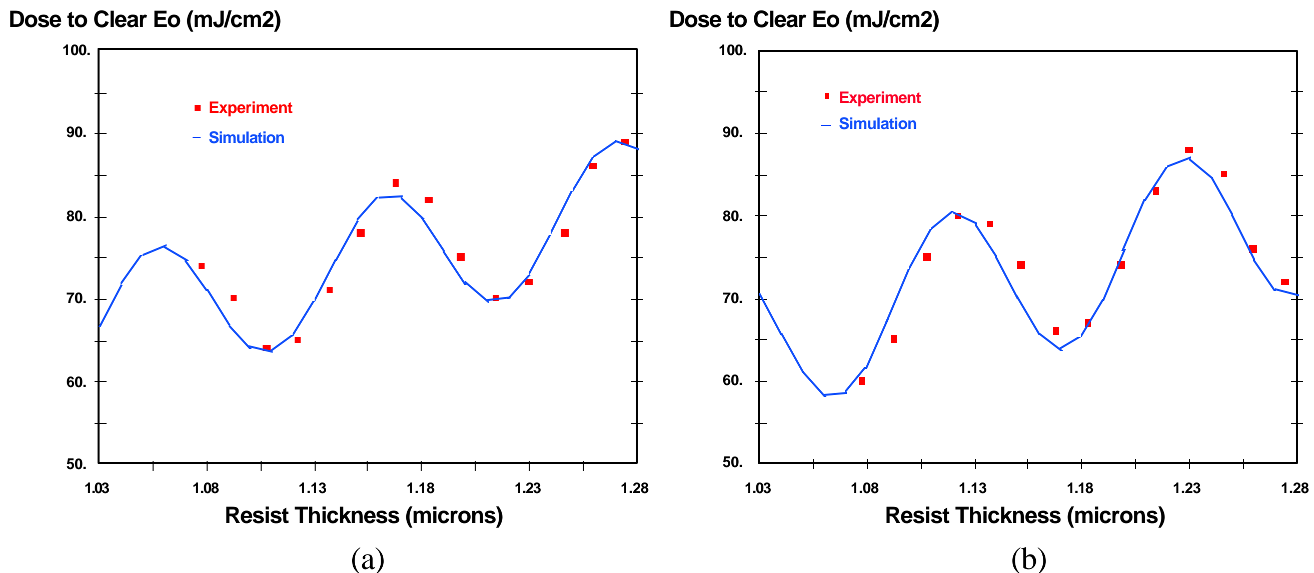

Figure 7. Comparison of simulation to new experimental data without further tuning of the resist parameters: (a) swing curve on 130nm of polysilicon, and (b) swing curve on a film stack of 95nm nitride on 40nm oxide.

Although the agreement between model and experiment shown in Figure 7 is quite good, there is a slight but noticeable phase shift shown in both plots. If a better match is desired, more careful characterization of the films used is required. The polysilicon used in the experiment was doped and partially annealed, but the simulation used standard amorphous polysilicon optical parameters. The nitride/oxide film stack was nominally 95nm and 40nm thick, respectively, but the oxide thickness was not verified.

VI. Conclusions

Lithography simulation has proven to be an extremely effective tool for process design, characterization, and trouble shooting. In many cases, only qualitative results are needed from the simulation. However, in some cases quantitative predictive ability is desired. For such cases, a good set of accurate input parameters is a requirement. Commercial lithography simulators such as PROLITH/2 are shipped with an extensive database of resist and material parameters. Most of these parameters were either measured and published in the literature or provided by the resist suppliers. As with any measured quantity, the validity of the parameter is a function of the experimental conditions of the measurement. If the parameters were measured under one set of experimental conditions, their accuracy decreases as the experimental conditions of the application deviate from the conditions of the measurement.

If the user of lithography simulation wants quantitative agreement of the model to a specific set of experimental results (i.e., for a specific existing process), the parameters that came "right out of the box" with the simulation program may be less than perfect. Of course, the user could generate all of the parameters needed through measurements made using the specific process in question. This experimentally intensive approach is not always feasible, however. If the current set of parameters is close to correct, a simple tuning process can be used to adjust the parameters using readily available or easily measured data.

In this paper, a simple swing curve was used as the vehicle for tuning the lithography simulator PROLITH/2. First, the index of refraction of the resist was tuned to account for the relative nature of resist thickness measurements made in the fab. Then, the resist exposure rate constant C was adjusted to account for differences in dose calibration of the stepper compared to the exposure tool used to measure the ABC parameters. Alternatively, the dose calibration issues could be imbedded in the development rate parameters and taken into account by tuning these parameters. Two methods were presented for obtaining development rate parameters. First, the parameters could be tuned (adjusted slightly) using the exposure margin as a metric for the development parameter n and R_{max} as a way to calibrate dose. If all new parameters must be obtained, the Poor Man's DRM of resist contrast curves for different development times can be used. This relatively simple data collection combined with the ProDRM software analysis resulted in an entirely new set of development parameters for a new developer that was being used.

The result of the tuning process was a set of parameters that gave quantitative agreement of simulation to experiment.

There is more work on this topic that can be done. Simulation and experimental verification of focus-exposure matrix data can be used to evaluate the image quality of a given lens. Simulation including aberrations can be matched to actual data to understand the possible aberrations in an actual lens. Tuning of the resist metrology used in the simulation to the metrology used in the fab will allow quantitative comparison of simulated to actual linewidths. Work in these areas is on-going.

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