Advanced topics in lithography modeling

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ABSTRACT

The model PROLITH is used to simulate advanced topics in lithography such as multi-level resists, contrast enhancement lithography, linewidth variations over topography, anti-reflective coatings, post-exposure bakes, and dyed photoresists. The applicability and usefulness of this model for these topics is discussed. Other areas in which the model PROLITH may be applied are suggested.

INTRODUCTION

In recent years the theory and practice of optical lithography modeling have advanced to the point of making computer simulation of the lithography process a viable research tool. Models such as PROLITH [1] and SAMPLE [2] have been found to accurately predict the exposure and development of positive photoresists given appropriate input parameters. Current research efforts, however, are concentrating on more advanced techniques for fine-line lithography. Therefore, there is a need for an optical lithography model capable of modeling such advanced topics as multi-level resists, contrast enhancement lithography (CEL), exposure over topography, and the many techniques used to reduce the standing wave effect.

This paper discusses the use of PROLITH (the Positive Resist Optical Lithography model), v1.02, to model the advanced lithography techniques mentioned above. The use of a multi-level resist is easily modeled with the use of the analytical standing wave expression found in PROLITH [1]. The multi-layer capability of this expression is also employed when modeling a contrast enhancement layer. A bleaching model and a description of the developmental surface inhibition effect are also used when modeling CEL. The application of a planar model to non-planar substrates can be accomplished under certain conditions. The accuracy of this method is discussed. Finally, three methods to reduce the standing wave effect (anti-reflective coatings, post-exposure bakes, and dyed photoresists) are modeled.

The result of this work is an optical lithography model that can be used to simulate not only standard processes, but also the advanced processes often used in the research environment.

MULTI-LEVEL RESISTS

Multi-level resists (MLR's) can, in most cases, be modeled in a straightforward manner. For example, 0.6 μm of AZ1350 photoresist on 0.1 μm of silicon nitride on 2.0 μm of a planarizing layer can be directly modeled by PROLITH. The only additional fact which must be known is the complex index of refraction of the planarizing material. One possible modeling study would be to examine the effects of adding an absorbing dye to the bottom layer of this multi-level resist [3]. If Hunt 204 positive resist, baked at 160°C for 30 minutes, is used as the planarizing material, the index of refraction would be $1.68\text{-}i0.007$ [3]. If a 0.8 μm space is projection printed with a typical g-line stepper ($NA = 0.28$, $\sigma = 0.7$, no defocus) on the above MLR on an aluminum substrate, PROLITH would predict a resist profile as shown in Figure 1. If, however, the bottom layer is dyed with 3% Coumarin 314, the index of refraction of the dyed Hunt 204 will be $1.68\text{-}i0.036$ (see section on dyed resists). Using this slightly modified MLR, the resultant resist profile can be seen in Figure 2. Obviously, the addition of a dye into the bottom layer of a MLR can drastically reduce the standing waves in the top layer.

One of the major goals of a MLR is to reduce the effects of topography on the lithography process. The hope is that the bottom layer planarizes the surface allowing the top layer of resist to be flat. Even if this is the case, topography will effect the process in the form of thickness variations of the bottom layer. This situation can be easily modeled by changing the thickness of the bottom layer (and possibly substrate type) and looking at the effect on the resist profile, in particular the predicted linewidth.

The portable conformable mask (PCM) technique can also be modeled by PROLITH, but in a less straightforward way. This technique forms an image in the top layer of a bilevel resist structure and then uses this image as a mask for the deep-UV exposure of the bottom layer, typically dyed PMMA. Modeling the image formation in the top layer is done as described above for the conventional MLR process. Image formation in the bottom layer can be modeled as a contact printing process with the top layer as the mask [4]. PROLITH uses a rigorous form of Kirchoff's diffraction theory [1] and thus provides a fairly accurate method of predicting the intensity within the bottom layer. A reasonable value for the mask to wafer distance (nominally between zero and the thickness of the top layer) must be determined by comparison of the predicted and experimental data. Further, if the bottom resist can be modeled as a conventional positive photoresist, a developed resist profile can be predicted.

Other multi-level resist schemes can be modeled in similar ways, assuming the pertinent properties of the various layers are known.

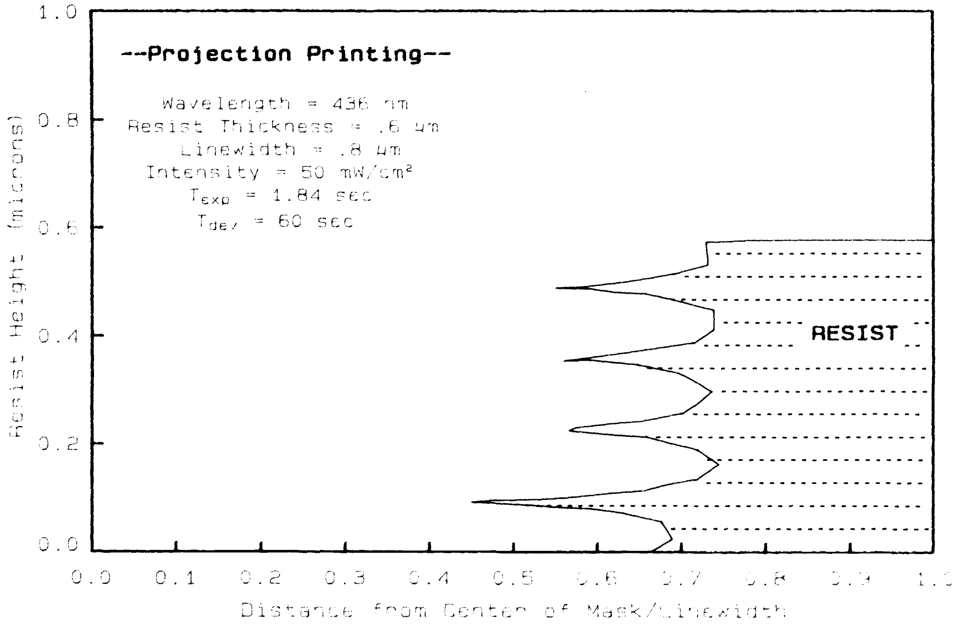

Figure 1 : Photoresist profile in the top layer of a trilevel resist process (no dye in the bottom layer).

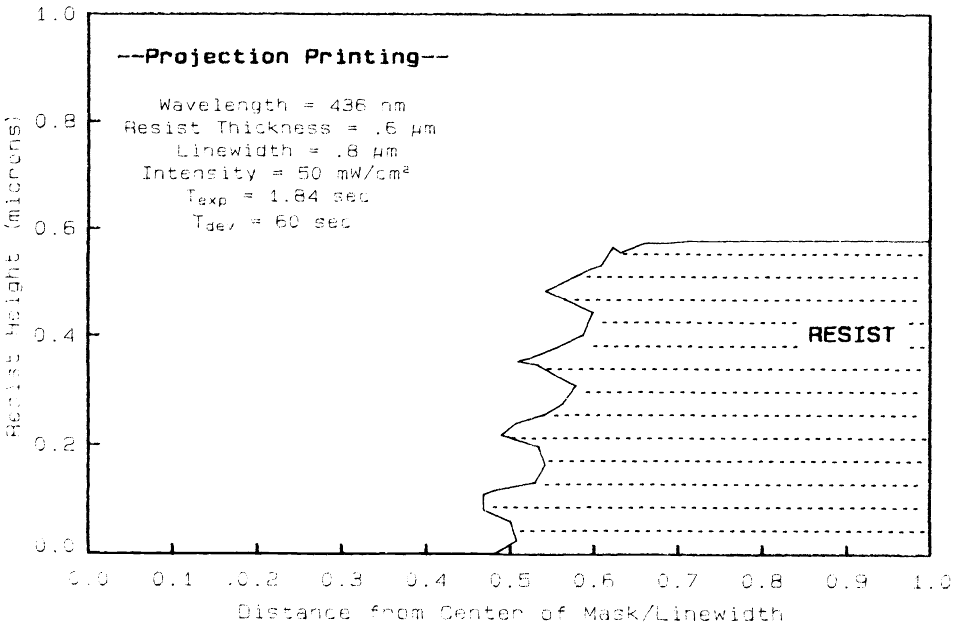

Figure 2 : Photoresist profile in the top layer of a trilevel resist process (3% dye in the bottom layer).

CONTRAST ENHANCEMENT LITHOGRAPHY

Unlike multi-level resist lithography, contrast enhancement lithography (CEL) can not be modeled by a simple extension of a single layer resist model. Thus, PROLITH, v1.02, contains a CEL model which can be used in conjunction with the conventional model. The details of this model will be published elsewhere, this section will deal only with its use. As with any model, in order to use it one must know the appropriate parameters. There are six parameters which must be known in order to characterize the effects of a CEL process. The first three are the well known ABC parameters used to describe conventional positive photoresists. The forth is the index of refraction of the contrast enhancement material. The last two parameters are used to describe the surface induction effect commonly observed during the development step of a CEL process. For the purposes of this study, the development process was assumed to have no surface induction, and thus these two parameters will not be specified. Values for the ABC parameters for CEM-388 (manufactured by General Electric) are given in Table I.

Table I

Modeling parameters for CEM-388

Wavelength	A (μm^{-1})	B (μm^{-1})	C (cm^2/mJ)	Reference
436 nm	4.07	0.069	0.029	5
405 nm	11.99	0.178	0.0786	5
365 nm	9.86	0.696	0.0637	5
405 nm	11.5	0.3	0.79 [sic]	6
436 nm	5.4	0.08	0.06	*
405 nm	12.0	0.10	0.093	*
365 nm	12.9	1.0	-	*

*measured by author

For the purposes of this study, a nominal process is defined by the parameters given in Table II. These values are used in all modeling runs except where noted. A matched substrate was used in order to eliminate the effects of standing waves and simplify the measurement of sidewall angle. In all cases (except the ΔCD curves), the exposure energy was adjusted to give the nominal linewidth at the bottom of the resist pattern. With these guidelines in mind, a series of modeling studies were undertaken to better understand the behavior of contrast enhancement lithography.

Table II

Nominal parameters used with PROLITH for CEL modeling studies

Projection System:	Wavelength = 405 nm $NA_0 = 0.28$ $\sigma = 0.7$ Linewidth = 0.8 μm Pattern = space	Resist Parameters:	A = 0.6 μm^{-1} B = 0.1 μm^{-1} C = 0.020 cm^2/mJ Refractive index = 1.65 Thickness = 0.8 μm
CEL Parameters:	A = 12.0 μm^{-1} B = 0.10 μm^{-1} C = 0.10 cm^2/mJ Refractive index = 1.70	Developer Conditions:	Develop time = 60 sec R_{max} = 200 nm/sec R_{min} = 1 nm/sec $m_{TH} = 0.5$ n = 5
Exposure Energy:	variable		

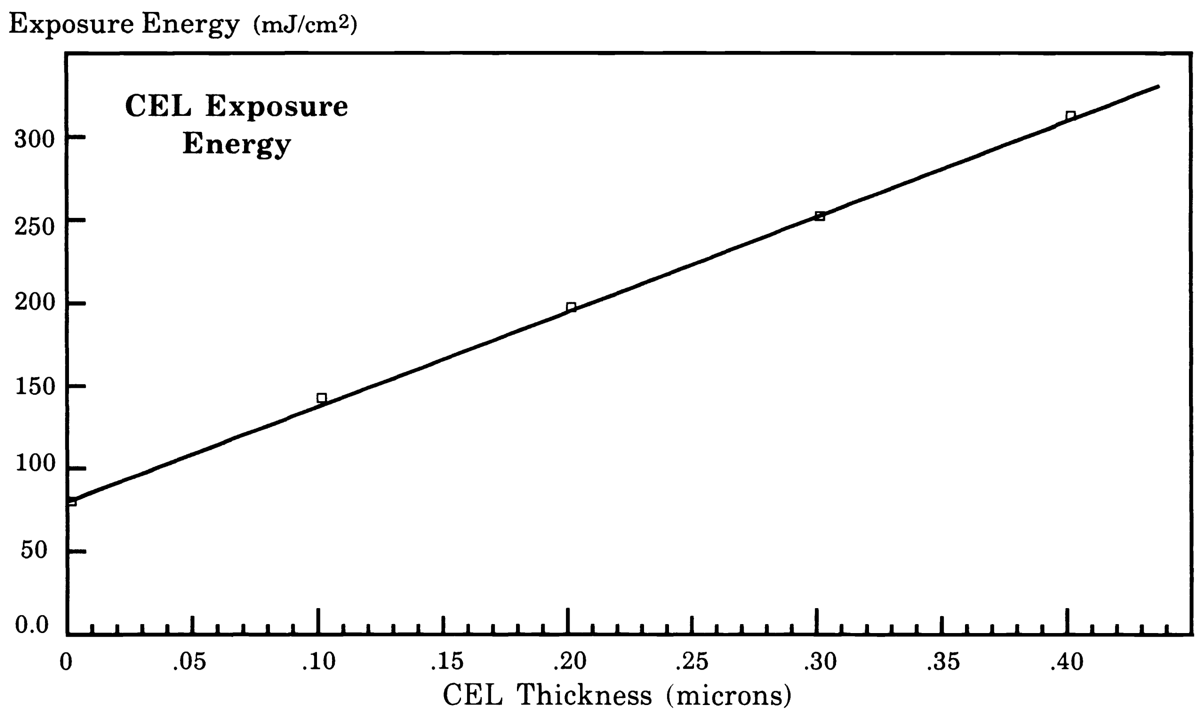

Figure 3: Exposure energy required for various CEL thicknesses.

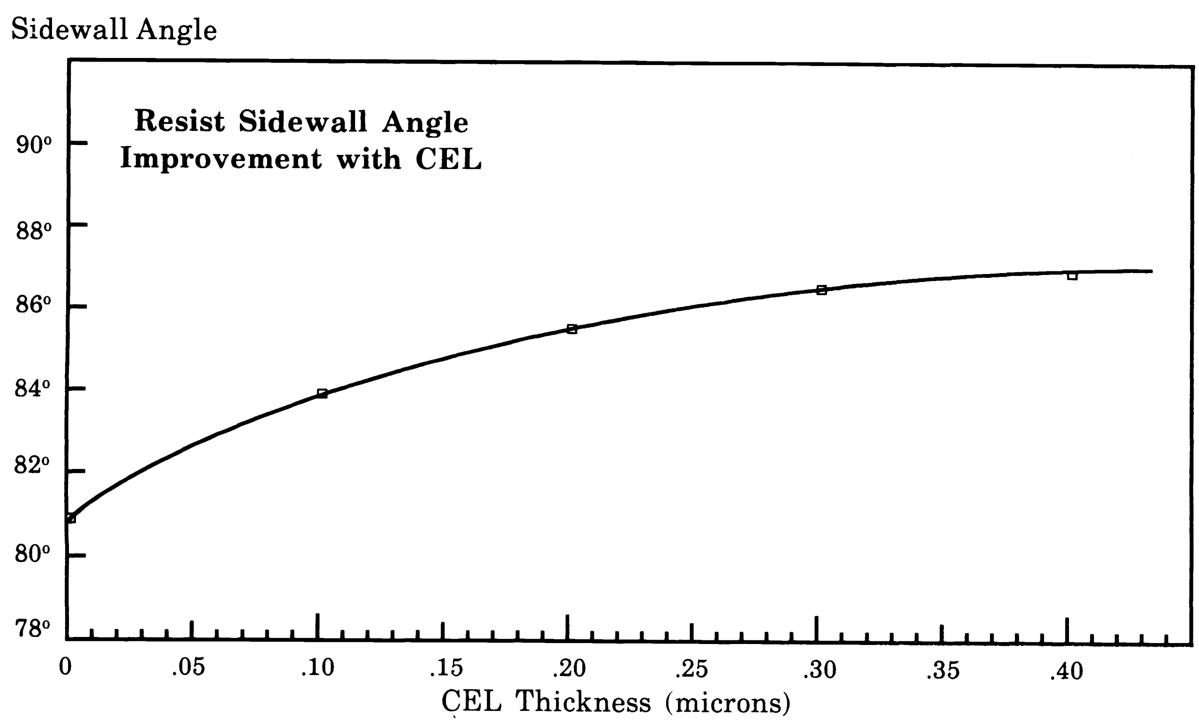

Figure 4: Resulting resist sidewall angle for various CEL thicknesses.

The first modeling study examines the effects of contrast enhancement material thickness on exposure energy required and resulting resist sidewall angle. The outcome of this study is well known: resist sidewall angle is improved at the expense of increased exposure energy (Figures 3 and 4). It was also observed that the CEL exposure penalty varies linearly with CEL thickness. Thus, once the exposure penalty is known for one thickness of CEL, one can predict the energy required by any other CEL thickness. This study was repeated for different numerical apertures (thus changing the "contrast" of the image) and the sidewall angle plotted versus CEL thickness in Figure 5. If, for example, a sidewall angle of 80° is desired, there are various numerical aperture-CEL thickness combinations which give this result. Keep in mind that all simulations were performed assuming a matched substrate, so that the conditions represented in these studies are idealistic. It is the trends, however, not the absolute numbers that are the subject of this study.

A very interesting question arises when the properties of contrast enhancement lithography are examined. For a given CEL material, is there an optimum resist material to be used with this CEL? To look into this question, the resist parameter C (the bleaching rate constant) was varied in order to determine its effect on sidewall angle. The results, for various CEL thicknesses, are shown in Figure 6. There is quite definitely an optimum range of values for C. For the hypothetical CEL material used in this study, the optimum value of C is about 2-3 time greater than that of most commercial positive photoresists. In a similar fashion it is possible, through a series of simulations, to find the optimum CEL parameters for a given resist material. This could be a very important tool in the development of future CEL systems. This type of study is easily accomplished via an appropriate model, but is virtually impossible to perform experimentally.

There has been some question as to whether contrast enhancement lithography has better exposure latitude than a single layer photoresist process. To help answer this question, the linewidth of a nominal 0.8μm space was simulated for various exposure energies. This was then repeated for different CEL thickness. The resulting curves are plotted on a scale so that the energy required to give the nominal dimension is normalized to 1. The result, given in Figure 7, shows that there is no difference in exposure latitude among the different cases. Upon closer inspection of the data, there is a very slight improvement in exposure latitude as thicker contrast enhancement layers are used, but the difference is too small to be seen in Figure 7.

There has been some concern that the CEL process is so sensitive to changes in CEL thickness as to make it impractical. The fact that CEL processes are currently being used successfully indicates otherwise. For this reason, a study was performed to investigate the linewidth change due to CEL thickness changes. The results are shown in Figure 8. The exposure energy was fixed so as to give the nominal linewidth when 200 nm of the contrast enhancement material was used. The result is very similar to an exposure latitude curve in mirror image. This is to be expected since an increase in CEL thickness by a set amount is equivalent to a decrease in exposure energy by a set amount.

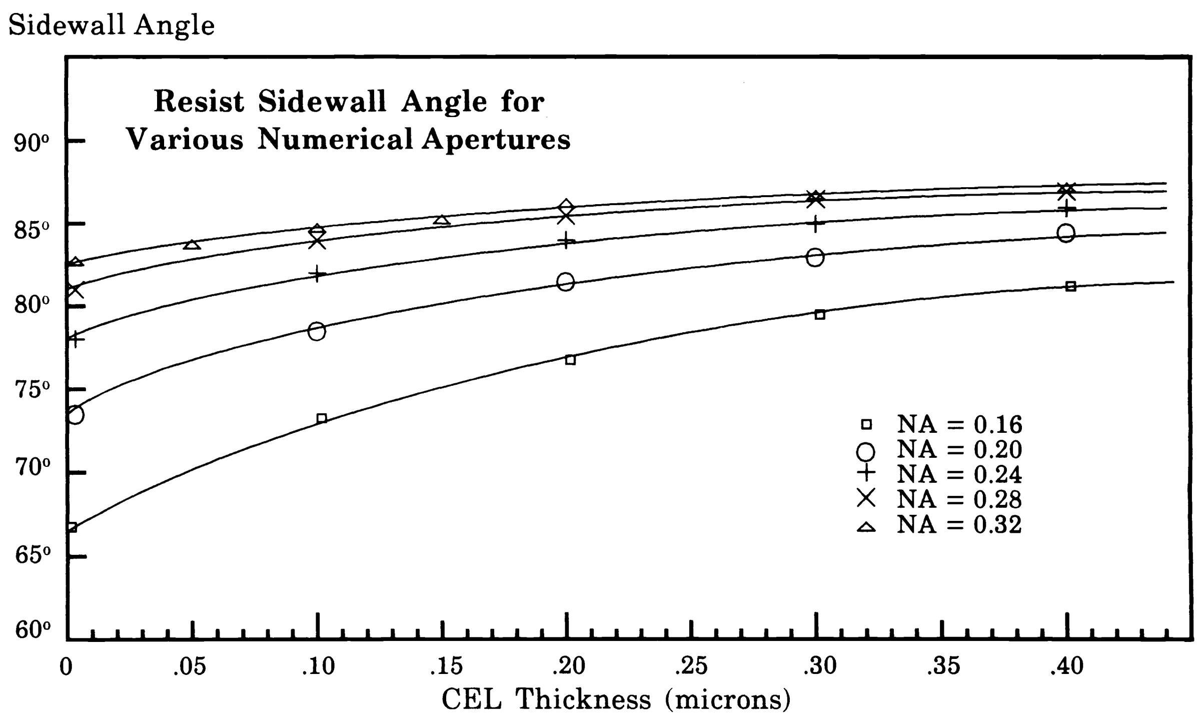

Figure 5: Resulting resist sidewall angle for various CEL thicknesses and numerical apertures.

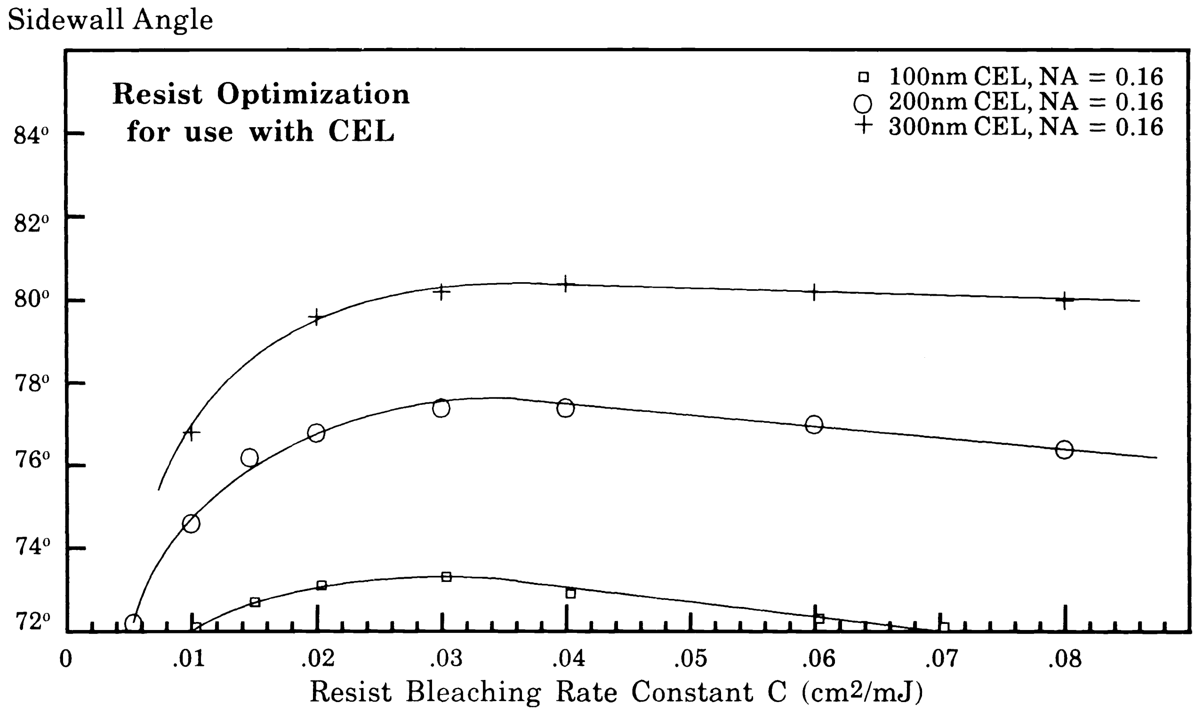

Figure 6: Optimization of the resist bleaching rate constant C in terms of sidewall angle for use with a CEL.

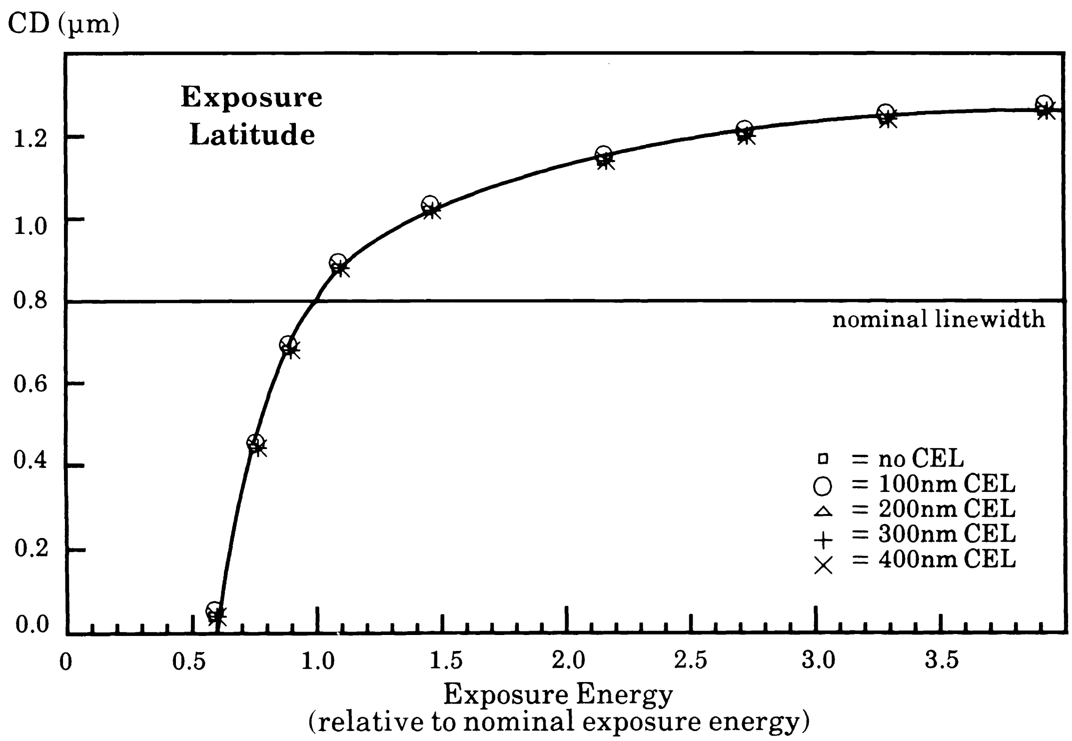

Figure 7: CD variation with exposure energy.

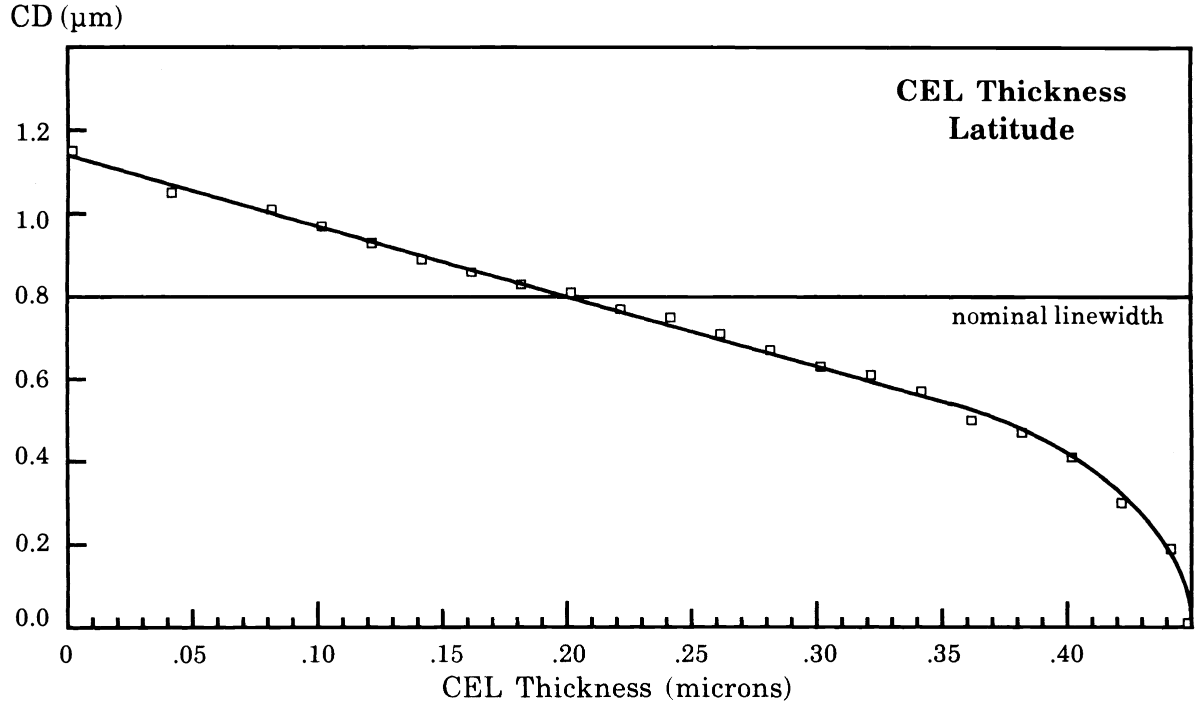

Figure 8: CD variation with CEL thickness.

TOPOGRAPHY

Most, if not all lithography simulation programs in use today are based on exposure of photoresist on a planar substrate. There is a need, however, to model the effects of exposure over non-planar substrates (e.g., steps). Thus, there have been attempts to use a planar model for non-planar cases [7]. Unfortunately, these attempts have not been accompanied by an explanation of the error introduced in using a model which assumes no topography. In essence, the planar models assume that light, impinging vertically on all surfaces, will be reflected vertically. If, however, there are non-horizontal surfaces to reflect the light (such as the sidewall of a reflecting step), this assumption fails (Figure 9). Thus, if light reflected from a step is considered to be significant, a planar model can not be applied successfully. If, however, the step is of a material which does not reflect light, a planar model can be used. The criterion for applicability, then, is for the index of refraction of the step to be close to that of the resist. Thus, steps of oxide or nitride can be modeled with fair accuracy, but metals or silicon can not.

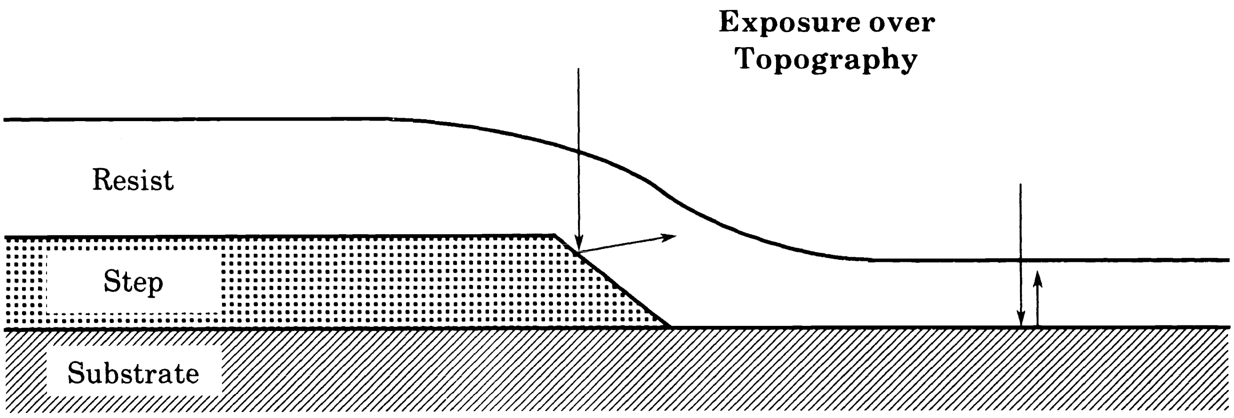

Figure 9 : Reflections from a step are not accounted for in a planar resist exposure model.

As an example, a 200 nm oxide step over silicon is covered with 800 nm of AZ1350. To accurately model a real situation, the best approach is to examine a SEM cross section of the resist covered step and obtain values of resist and oxide thickness as a function of position relative to the position of the step. For this example, a 1.2 µm line is printed over the step shown in Figure 9. Before the results can be presented, a definition of linewidth must be given. There are several ways of measuring linewidth, both experimentally and with a model. Usually, linewidth is measured at the top of the resist or at the bottom. However, when standing waves are present it is difficult to identify a width even if a position for measurement is specified. Optical linewidth measurement tools tend to "average-out" the standing waves, giving a relative number that is difficult to relate to an absolute position on the resist. A similar, though more defined approach was taken in reference [8] and is essentially used for this study. With this in mind, the modeled linewidth variation over the oxide step is shown in Figure 10.

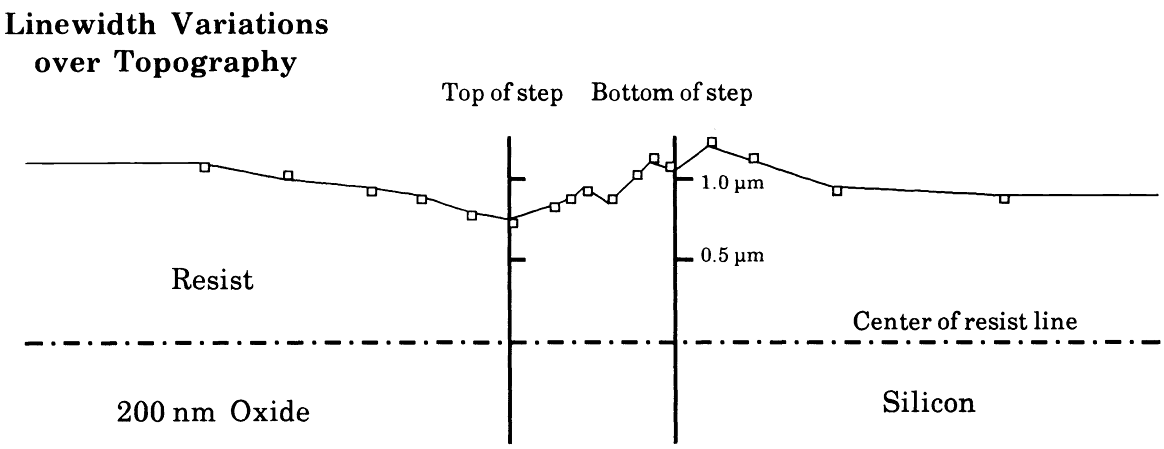

Figure 10 : Predicted linewidth variations over a 200 nm oxide step.

STANDING WAVE REDUCTION

A considerable amount of work is being done to reduce the effects of standing waves during photoresist exposure. There are several proven ways to reduce these ridges in the resist profile, each with its own advantages and disadvantages. In this section, three of the most common techniques for reducing the standing wave problem will be modeled. With this modeling capability, one can better evaluate the overall usefulness of each method in relationship to its added process complexity.

The first approach to the standing wave problem is the most obvious, to reduce the reflections from the substrate with an anti-reflective coating (ARC). There are several commercially available ARC's, typically dyed polyimides. PROLITH can easily model an ARC once the complex index of refraction of the material is known. For Bewer's ARCL2, the indices of refraction are [9]: 1.78 - i0.44 at 436nm, 1.78-i0.38 at 405nm, and 1.78-i0.26 at 365 nm. Modeling studies can be performed to determine the appropriate thickness of the ARC, as well as to compare different ARC materials.

The post-exposure bake (PEB) has been known to reduce the standing wave effect for over 10 years [10]. The bake, which takes place after exposure but before development, is thought to cause diffusion of the photoactive compound within the resist, thus smoothing out the standing wave ridges. Standard diffusion theory can be used to model the PEB, with the result given in equation (1).

$$m^*(x,z) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \int_{-\infty}^{+\infty} m(x-x_o,z-z_o)\, exp(-r^2/2\sigma^2)\, dx_o dz_o \qquad (1)$$

where m = the relative photoactive compound (PAC) concentration before diffusion

m* = the relative photoactive compound concentration after diffusion

$r^2 = x_0{}^2 + z_0{}^2$

$\sigma^2 = 2Dt$ (σ is called the diffusion length)

D = diffusion coefficient of the PAC in resist at temperature T

t = time at which the resist was baked at temperature T.

Thus, in order to model a post-exposure bake one must know the diffusion coefficient as a function of bake temperature for the resist of interest. Unfortunately, there is a void of experimental data in this area making accurate simulations impossible. However, one can still use a PEB model to evaluate trends.

Finally, there has been much discussion recently about the use of dyed photoresists to reduce the standing wave effect. Although the ability of dye additives to reduce reflections, and thus standing waves, is in doubt [11], PROLITH can be used nonetheless to model dyed photoresists. Based on the original model by Dill [12], the absorption coefficient, α, is given by

$$\alpha = Am + B \tag{2}$$

where $A = (a_M - a_P)M_0$

$B = a_P M_0 + a_R R + a_S S$

M, P, R, S = the concentration of photoactive compound, exposure product, resin and solvent, respectively

a_M, a_P, a_R, a_S = the molar absorption coefficients of the respective components

$m = M/M_0$ (the relative PAC concentration)

M_0 = the PAC concentration before exposure.

Equation (2) does not change with the addition of a dye, D, but the constant B takes a new form.

$$B = a_P M_o + a_R R + a_S S + a_D D \tag{3}$$

Thus, the effect of adding dye to the photoresist is an increase in the value of B by the amount $a_D D$.

For this study, the photoresist OFPR-800 with approximately 30% solids was used. The dye Coumarin 314 (manufactured by Kodak) was added to the photoresist in concentrations of 0, 2, and 3% by weight based on the weight of solids in the photoresist. The resist was spin coated on a 4 inch borosilicate glass wafer at 5000 rpm for 30 seconds to a thickness of about 1.0 µm. The sample was then convection oven prebaked at 95°C for 30 minutes. The parameters A, B, and C were measured at the g, h, and i lines of the mercury spectrum. The results are shown in Table III. The index of refraction was not know at each wavelength and the values in Table III are assumed. From the measured values of B, the molar absorption coefficient of the dye, a_D, can be determined. For convenience, units of $\mu m^{-1}/\%$ dye are used. These values (as a function of wavelength) are also listed in Table III. Note that this particular dye is very effective in absorbing light at 436 nm (high a_D), is not very effective at 405 nm (low a_D), and is transparent at 365 nm ($a_D = 0$).

Table III
Measured OFPR-800 parameters for
various dye concnetrations

Wavelength	365 nm	405 nm	436 nm
A (μm^{-1})	0.78	0.85	0.40
C (cm^2/mJ)	0.015	0.020	0.014
B (μm^{-1}) - no dye	0.30	0.10	0.085
B (μm^{-1}) - 2% dye	0.30	0.23	0.67
B (μm^{-1}) - 3% dye	0.30	0.30	0.90
index of refraction	1.65	1.65	1.65
a_D ($\mu m^{-1}/\%$)	0.0	0.07	0.28

With the values given in Table III, one can model the effects of the dye on exposure energy and resist profile. However, the dye also has an effect on the development of the photoresist. This effect must be measured and taken into account before a complete model can be used.

CONCLUSIONS

Research efforts in optical lithography are taking many directions to solve the problems of submicron resolution. If lithography modeling is to aid in these efforts, it must be capable of modeling the advanced topics currently under investigation. PROLITH, v1.02 is an attempt to keep pace with recent developments in optical lithography research, as well as provide for the simulation of standard production processes.

ACKNOWLEDGEMENTS

The author wishes to thank Arthur Adams for helping to measure the CEL parameters, John Covington of Texas Instruments for providing samples of the dyed photoresist, and Paul West and Ken Polasko of General Electric for providing CEM-388 samples.

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