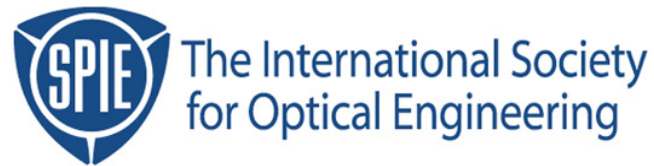


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A Comparison between the Process Windows calculated with Full and Simplified Resist Models

Mark D. Smith^{*}, Jeffrey D. Byers, Chris A. Mack
KLA-Tencor Corp.

ABSTRACT

While numerical simulation is generally regarded as indispensable for wavefront engineering tasks such as OPC decoration and phase-shift mask design, full resist models are rarely used for this purpose. By “full resist models”, we mean models derived from a physical, mechanistic description of the chemical response of the photoresist to exposure and the subsequent PEB and develop processes. More often, simplified models such as an aerial image threshold model or the Lumped Parameter Model (LPM) are used because these models are much faster and make optimization of optical extension technology more tractable. Simplified resist models represent a compromise between computational speed and simulation accuracy. The purpose of this study is to quantify the differences between the process windows calculated with simplified and full resist models.

Our approach is first to fit the parameters in the simplified models to match results obtained with a full resist model, and then to compare the predictions of the simplified resist models with those obtained with the full model. We take two approaches to model tuning: mathematical derivation of relationships between the models, and least-squares fitting of FE matrix data for isolated and dense lines.

Keywords: Photoresist modeling, aerial image threshold model, Lumped Parameter Model, LPM, lithography simulation, PROLITH

1. INTRODUCTION

As feature sizes continue to shrink, lithography processes are being pushed to their limits. Technologies that were once considered exotic, such as off axis illumination, phase-shifted reticles, and double exposure processes, are now moving into the mainstream. All of these efforts to implement low k_1 lithography are very engineering intensive, and as a result, numerical simulation is an indispensable tool for wavefront engineering. However, even though many of these techniques concentrate on manipulation of the image projected onto the wafer, the evolution of the modern photoresist has led to similar gains in resolution as our advances in the optical systems [1], so a complete model for the lithographic process requires both a model for the optical system and a model for the resist.

There are many different photoresist models that have been proposed, and these models range in complexity from very detailed, molecular-level descriptions of the resist to very fast, semi-empirical representations. It is useful to examine a few examples of each of the different types of photoresist models commonly used by lithographers today. Molecular-scale models of the photoresist include dynamic Monte-Carlo [2], molecular dynamics [3,4], and ab initio quantum calculations [5-7]. These models are useful for developing a deeper understanding of resist chemistry and physics from a molecular standpoint, and these models can be used to examine new resist formulations. While we will not study these models further, it is interesting to note that the results from molecular-scale models can be used to calibrate the parameters in continuum models for photoresist. For example, the ab initio quantum calculations in [7] were used to calculate the absorbance of various candidate polymer resins for 157nm resist formulations, and these absorbance values could serve as input to other types of lithography models.

Process capability and process optimization studies are usually performed with a model based on a continuum approach, and the examination of various continuum models will be the focus of this paper. We

^{*} mark.d.smith@kla-tencor.com; phone 1-512-381-2318; 8834 North Capital of Texas Highway, Suite 301, Austin, TX 78759

divide continuum models into two broad groups of models: “Simplified” models and “Full Physical” models. The “Simplified” group of models predicts the response of the photoresist directly from the aerial image. These models include the aerial image threshold resist model, the variable threshold resist model [8], and the Lumped Parameter Model [9-12]. The basic philosophy behind the Simplified models is that the model should describe the resist with a minimal number of parameters, and calculations with the model should be very fast. While the model may be physically motivated, the model is not intended to be a mechanistic description of resist response. Simplified models are commonly used for model-based OPC decoration of mask designs, and can provide reasonably accurate results in a short amount of time – full-chip simulations are commonly performed with aerial image threshold models in less than a day. One of the disadvantages of the Simplified models is that the model parameters do not have a physical meaning, so a change in the lithography process will usually require that the model be recalibrated.

An example of a “Full Physical” model is type of model found in PROLITH [13], which is built from continuum, mechanistic models for each step in the lithography process. The philosophy behind these models is that excellent agreement between simulation and experiment can be obtained if each step in the lithography process is described by detailed, mechanistic model. These models are useful for process optimization. For example, film stack optimization is a very common use case for Full Physical models, because the thin-film interference effects in the stack are modeled in detail. By contrast, a change in the film stack would require that most Simplified models be re-tuned so that they again match experimental results. However, the level of detail and the flexibility of the Full Physical models usually lead to a model with a large number of input parameters, and some of these parameters may be difficult to measure experimentally.

With such a wide variety of models available, each with advantages and disadvantages, one might ask, “Which model is the ‘best’ model for a photoresist?” The obvious response is given by the famous quote by Albert Einstein: “Things should be as simple as possible, but no simpler.” However, the fact that there are so many different models for photoresist demonstrates that “as simple as possible” depends entirely on the task at hand. To compound the issue further, today’s task may be different from yesterday’s task, warranting a change to a different type of model. For this reason, the goal of the current study is not to determine which model is best, but to develop relationships between different types of models, so that an investigation performed with one type of model will lead to conclusions that are consistent with a different model, which might be more (or less) complex. By developing relationships between the most common types of photoresist models, the lithographer can move seamlessly between different models.

We will investigate three models in this study. The first model is an aerial image threshold (AIT) model, and the second model is the Lumped Parameter Model (LPM). Both the AIT model and the LPM will be compared with predictions from the Full Physical models in PROLITH. The outline of this paper is as follows. In Section 2, the AIT model and LPM are described in detail. A brief overview of the Full Physical model in PROLITH will be given as well. The governing equations outlined in this section will be the starting point for deriving relationships between the Simplified models and the Full Resist model, in Section 3. In Section 4, we will use the AutoTune module from the Klarity ProDATA software to perform a least-squares fit between the LPM and the Full Physical model for FE matrix data for isolated and dense features. The purpose of this fitting exercise is to determine if any discrepancies between the LPM and the Full Physical model are due to a poor choice of the parameters chosen in Section 3, or due to a shortcoming of the LPM. In Section 6, we will offer our conclusions.

2. GOVERNING EQUATIONS FOR SIMPLIFIED AND FULL RESIST MODELS

Both the aerial image threshold (AIT) model and the lumped parameter model (LPM) can be defined in terms of a the develop rate equation. For the AIT model, the develop rate for the photoresist is assumed to depend only on the relative intensity of the aerial image at the top of the resist. In addition, the develop rate is a step function of the intensity: if the relative intensity exceeds some threshold value, all of the resist washes away; otherwise, the resist remains on the wafer. Mathematically, the develop rate is described by

$$R(x, y) = \begin{cases} 0, & \text{if } I(x, y) < I_{threshold} \\ \infty, & \text{if } I(x, y) \geq I_{threshold} \end{cases} \quad (1)$$

where $I(x, y)$ is the aerial image relative intensity at the top of the resist, and $I_{threshold}$ is the aerial image threshold value for conversion of the resist from an insoluble to a soluble film. Optically, the resist is assumed to have the properties of air; that is, an index of refraction of 1.0, and an absorbance of zero.

For the LPM, the develop rate is assumed to have a power-law dependence on the dose received at each point in the resist. In addition, the image in resist is calculated with a two-step procedure that accounts for physics not included in the AIT model. First, the image in resist is assumed to have the form

$$I(x, y, z) = \{I_0(x, y) + I_1(x, y) \cdot z + I_2(x, y) \cdot z^2\} \cdot \exp(-\alpha_{eff} z) \quad (2)$$

where the first term (in braces) allows the model to account for defocus within the resist film and the second term (the exponential) accounts for absorbance within the film. The parameter α_{eff} is the “effective absorbance”, and the photoresist film is assumed to have an “effective thickness”, D . Both α_{eff} and D can be used to account for effects not explicitly represented in the model, such as substrate reflectivity and surface inhibition during develop.

The second step in the LPM is to “diffuse” the image in resist with a diffusion length L . Diffusion of the image intensity can be used to account for vibrations during the exposure process, diffusion of photoactive compound during post-exposure bake (PEB), and other effects that decrease image quality [11].

After the image in resist has been calculated, the resist is assumed to dissolve with a develop rate given by

$$R(x, y, z, E) = R_0 \left(\frac{E \cdot I(x, y, z)}{E_0} \right)^\gamma + R_{min} \quad (3)$$

where E is the exposure dose, E_0 is the dose-to-clear, γ is the resist contrast, and R_{min} is the minimum develop rate. The parameter R_0 is not an input parameter, but rather is calculated from α , D , and the other parameters in equation (3).

For chemically amplified resists, the solubility change of the resist is modeled in the Full Physical resist models as a two step process. First, a photoacid is generated during the exposure process. The photochemical reaction is assumed to be first order in intensity (density of photons) and first order in the relative concentration of the photoacid generator molecule, m :

$$\frac{dm}{dt} = -CI(x, y, z)m \quad (4)$$

where C is the Dill parameter related to the photospeed, and the intensity within the resist film accounts for the optical properties of the resist and the underlying film stack. The absorbance of the resist is described by the Dill parameters A and B ,

$$\alpha = Am + B \quad (5)$$

The relative concentration of photoacid, H , after exposure is related to the unreacted photoacid generator by the equation

$$H = 1 - m \quad (6)$$

Next, the acid deblocks the polymer resin during PEB. This is described by a reaction-diffusion model, given by

$$\frac{\partial H}{\partial t} = \nabla \cdot (D_H \nabla H) - k_{loss} H - k_{quench} H Q \quad (7)$$

$$\frac{\partial Q}{\partial t} = \nabla \cdot (D_Q \nabla Q) - k_{quench} H Q \quad (8)$$

$$\frac{dW}{dt} = -k_{amp} H W \quad (9)$$

where D_H is the diffusivity of the acid, k_{loss} is the acid loss reaction rate constant, k_{quench} is the acid-base quench rate constant, Q is the relative concentration of base quencher, D_Q is the diffusivity of the base quencher, W is the relative concentration of blocked polymer sites, and k_{amp} is the deblocking reaction rate constant. We will also use the notation t_{PEB} to designate the duration of the PEB process.

The develop rate is then calculated from the relative concentration of deblocked polymer, P , which is related to the concentration of blocked polymer by the equation

$$P = 1 - W \quad (10)$$

For the calculations presented here, we will use a bulk develop rate model combined with surface inhibition, given by

$$R(x, y, z) = R_{bulk}(P(x, y, z)) \{1 - (1 - R_0) \exp[-z / \delta]\} \quad (11)$$

where R_{bulk} is the bulk development rate, R_0 is the relative develop rate at the surface of the resist, and δ is the inhibition depth. The bulk development rate is described by the enhanced Mack model [13,14],

$$R_{bulk}(P) = R_{resin} \frac{1 + k_{enh} P^n}{1 + k_{inh} (1 - P)^l} \quad (12)$$

where k_{enh} is the rate constant for the develop rate enhancement mechanism, n is the enhancement reaction order, k_{inh} is the rate constant for the develop rate inhibition mechanism, l is the enhancement reaction order, and R_{resin} is the development rate of the polymer resin. It is also necessary to specify the duration of the develop process, or develop time, t_{dev} . The enhanced Mack model is usually fit to experimental data with the following parameters: R_{max} , R_{min} , R_{resin} , n , and l , where R_{max} and R_{min} are given by

$$R_{min} = \frac{R_{resin}}{1 + k_{inh}} \quad (13)$$

$$R_{max} = (1 + k_{enh}) R_{resin} \quad (14)$$

In the current study, we will compare the AIT model and the LPM with results calculated with the Full Physical model in PROLITH for the 193nm Sumitomo resist PAR 710. The parameters for this model are given in Table 1.

Parameter	Value	Parameter	Value
Dill Parameters		Develop Parameters	
A	0.0	R_{max}	567.0 nm/sec
B	$1.1160 \mu\text{m}^{-1}$	R_{min}	0.05 nm/sec
C	$0.0214 \text{ cm}^2/\text{mJ}$	R_{resin}	567.0 nm/sec
PEB Parameters		n	17.0
D_H	$30.66 \text{ nm}^2/\text{sec}$	l	12.0
k_{loss}	0.0	R_0	0.125
k_{quench}	Instantaneous	δ	220.0 nm
$Initial Q$	0.125	t_{dev}	60 sec
D_Q	0.0	Film Stack	
k_{amp}	0.114 sec^{-1}	$Resist, thickness$	350 nm
t_{PEB}	60 sec	$AR19, thickness$	85 nm
		$AR19, n$	$1.73 + 0.395 i$

Table 1: Parameters for the Full Physical model for the 193nm Sumitomo resist PAR 710 on a Shipley AR19 BARC on silicon.

3. RELATIONSHIPS BETWEEN THE SIMPLIFIED AND FULL RESIST MODELS

In order to derive a relationship between the Simplified models and the Full Physical model, it is necessary to convert the develop rate equations for the Simplified models, which depend directly on the aerial image or exposure dose, to a form which depends on the concentration of deblocked polymer. If we neglect diffusion during PEB, then we can relate the deblocked polymer concentration to the intensity and dose by combining equations (4), (6), (9), and (10):

$$P = 1 - \exp \left[-k_{amp} \frac{1 - \exp[-k_{loss} t_{PEB}]}{k_{loss}} \text{Max}(1 - \exp[-CIE] - Q, 0) \right] \quad (15)$$

Note that the Max function is necessary to approximate the acid-base quenching reaction, because the acid concentration can never be less than zero.

For the AIT model, we assume that the develop rate equation is a step function of the deblocked polymer concentration, so that the develop rate equation is similar to the form given by equation (1):

$$R(x, y, z) = \begin{cases} 0, & \text{if } P(x, y, z) < P_{threshold} \\ \infty, & \text{if } P(x, y, z) \geq P_{threshold} \end{cases} \quad (16)$$

where $P_{threshold}$ is the threshold value of the deblocked polymer concentration. We can combine equations (15) and (16) by setting the deblocked polymer concentration to $P_{threshold}$ and the relative intensity to $I_{threshold}$ in equation (15). This leads to an equation that relates the input parameter in the AIT model ($I_{threshold}$) to the exposure dose and parameters in the Full Physical model:

$$E = \frac{\tilde{E}}{I_{threshold}} \quad (17)$$

where

$$\tilde{E} = -\frac{\ln\left\{\frac{\ln[1-P_{threshold}]}{k_{amp}t_{PEB}} + 1 - Q\right\}}{C} \quad (18)$$

We will use equation (17) to calibrate our comparisons between the predictions of the AIT model and the Full Physical model for PAR 710. The only parameter in equation (18) that is not found in Table 1 is $P_{threshold}$. We choose this parameter as the value of P that gives a develop rate for equation (12) so that the entire resist thickness will clear during the develop time. We will use a resist thickness of 350nm, which leads to $P_{threshold} = 0.328$.

For many of the parameters in the LPM, there is a direct correspondence between LPM parameters and Full Physical model parameters. For example, because the Dill parameter A is zero, we can use the Dill parameter B as the effective absorbance value α_{eff} . The resist thickness and the minimum develop rates in the two models can be equated as well. Another obvious choice is to use the dose-to-clear calculated with the Full Model as input to the LPM. However, it is interesting to note that the dose-to-clear will be different if the film stack changes, and that the effective absorbance will be equal to the absorbance in the Full Physical models only on a perfect BARC. If light is reflected off the substrate, a different effective absorbance will be required [15],

$$\alpha_{eff} = B \left(\frac{1 - |\rho_{23}|^2 \exp[-2BD]}{1 + |\rho_{23}|^2 \exp[-2BD]} \right) \quad (19)$$

where ρ_{23} is the electric field reflection coefficient between the resist and the substrate (the intensity reflectivity is $|\rho_{23}|^2$). We will only examine results on a BARC in the current study, so equation (19) will not be required.

The two remaining parameters in the LPM are the aerial image diffusion length and the resist contrast. We will estimate the aerial image diffusion length from the PEB diffusion length in the Full Physical model. However, we will later use equation (15) to estimate the resist contrast, and in this equation, diffusion of the photoacid during PEB has been neglected. In a previous paper [16], we demonstrated that if the reaction-diffusion model for PEB is decoupled into a diffusion problem followed by a reaction problem, the results can only be made to match if the amount of diffusion during PEB is reduced by an amount that depends on the spatial frequencies present in the latent image in resist at the end of the exposure process. (The maximum spatial frequency in the plane of the resist will depend on the optical properties of the stepper, such as the numerical aperture, NA , and the exposure wavelength, λ .) We use this result here to estimate the aerial image diffusion length:

$$L = \sqrt{\frac{2 \ln \left\{ \frac{1 - \exp\left(-\left(\frac{2\pi NA}{\lambda}\right)^2 \frac{\sigma_{PEB}^2}{2}\right)}{\left(\frac{2\pi NA}{\lambda}\right)^2 \frac{\sigma_{PEB}^2}{2t_{PEB}} \frac{k_{loss}}{1 - \exp[-k_{loss}t_{PEB}]}\right\}}{-\left(\frac{2\pi NA}{\lambda}\right)^2}} \quad (20)$$

where the PEB diffusion length is given by

$$\sigma_{PEB} = \sqrt{2D_H t_{PEB}} \quad (21)$$

For the parameters given in Table 1, the PEB diffusion length for the Full Model is 60.7nm. By contrast, the diffusion length given by equation (20) is only 41.6nm – this is the value we will use for the aerial image diffusion length in the LPM.

The only remaining parameter in the LPM is the resist contrast, γ . In order to obtain a value for γ , we match the develop rate versus exposure dose equation for the LPM given by equation (3), to the response of the Full Physical model. An equation that directly relates the develop rate for the Full Physical model to the exposure dose can be obtained by neglecting develop surface inhibition and substituting the approximate relationship for the deblocked polymer concentration, described by equation (11) into the bulk develop rate model, equation (15). This leads to

$$R(E) = R_{re\ sin} \frac{1 + k_{enh} \left(1 - \exp\left\{-k_{amp} t_{PEB} \text{Max}[1 - \exp(-CIE) - Q, 0]\right\}\right)^n}{1 + k_{inh} \left(\exp\left\{-k_{amp} t_{PEB} \text{Max}[1 - \exp(-CIE) - Q, 0]\right\}\right)^y} \quad (22)$$

Notice that we have written equation (22) with k_{loss} set to zero, which is consistent with the value of k_{loss} in Table 1. Next, we obtain a value for γ by performing a least-squares fit between the develop rate predicted by equations (3) and (22). As shown in Figure 1, it is not possible to obtain a good fit through the entire range of dose values, so we perform the fit for doses up to 10mJ/cm² in order to obtain good agreement near the line edge.

In order to evaluate the quality of the fit between the Full Physical model and the Simplified models, process windows are calculated with the parameters in Tables 1 and 2. 130nm isolated and semi-dense (1:1.5) lines are simulated through dose and focus with an exposure wavelength of 193nm, numerical aperture of 0.6, and a partial coherence of 0.5. Results are shown in Figure 2 and 3. For both sets of calculations, we find that the shape of the process window is qualitatively correct for the LPM, while the AIT model gives a process window for the semi-dense features that appears to be too far from the iso-focal region and looks qualitatively more like an isolated feature. Both the AIT model and the LPM do not predict the correct dose-to-size: the “best dose” for the Simplified models is too large when compared to the process window for the Full Physical model.

The lack of agreement between the Simplified models and the Full Physical model can be attributed to two different sources. First, the matching equations derived in this section could be based on incorrect assumptions. If this is the case, then better agreement would be obtained if better choices were made for the input parameters to the Simplified models.

Another possible cause for the discrepancy between the Simplified and Full Physical models is that there are certain resist responses that cannot be described by the Simplified models. For example, neither the AIT model nor the LPM can predict a CD swing curve on a reflective substrate. This is not, of course, a shortcoming of the Simplified models because they were not designed to explicitly describe the interactions between the resist and the film stack. On the other hand, the widespread use of Simplified models for tasks such as model-based OPC decoration of a mask design is an indication that Simplified models are expected to at least qualitatively describe the shape and position of the process window. If it is determined that the lack of agreement shown in Figures 2 and 3 is due to a shortcoming of the Simplified models themselves, and not so much due to an incorrect choice of parameters, this would call into question the use of such models for process window oriented tasks. In order to determine the root cause of the lack of agreement between the models, we will use a “brute force” approach to determining the best possible input parameters for the Simplified models in the next section.

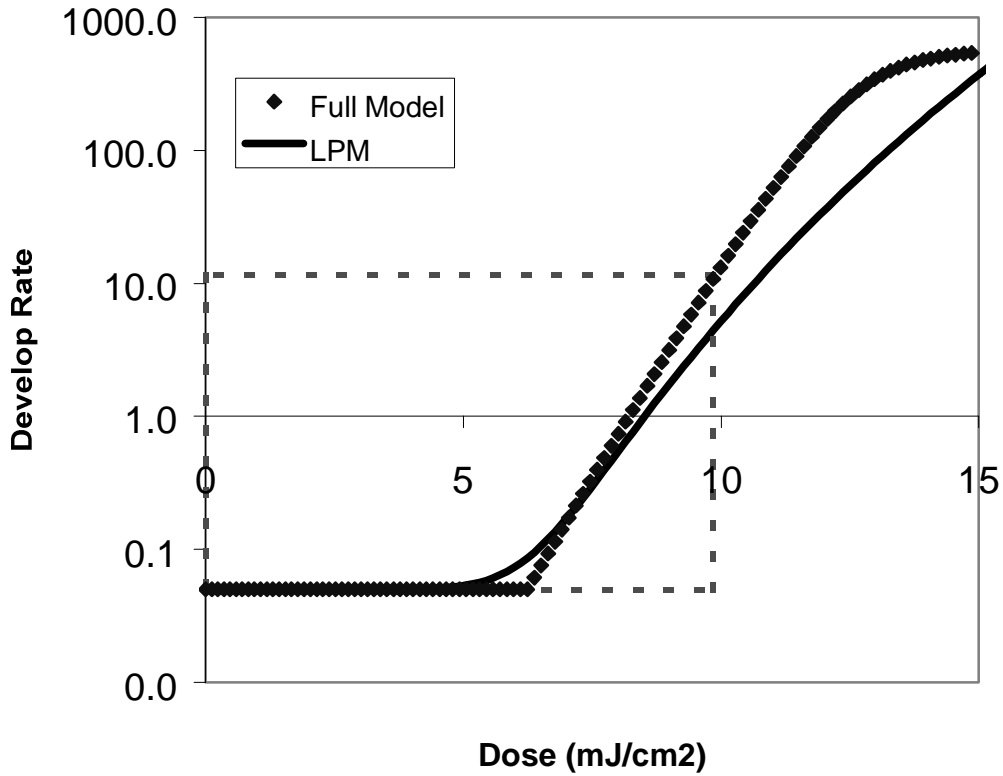


Figure 1: The develop rate as a function of dose for the LPM, given by equation (3), and for the approximate solution to the Full Physical model, given by equation (22). The resist contrast for the LPM is obtained by least-squares fit over the range of dose values shown by the dashed box. From the fit we obtain $\gamma = 9.451$.

Parameter	Matched Value (Section 3)	Least-Squares Fit Value (Section 4)
AIT Model		
\tilde{E}	9.451	7.395
LPM		
Effective Absorbance, α_{eff}	$1.116 \mu\text{m}^{-1}$	$0.739 \mu\text{m}^{-1}$
Thickness, D	350.0 nm	350.0 nm
Aerial Image Diffusion Length, L	41.62 nm	29.65 nm
Dose to Clear, E_0	13.05 mJ/cm^2	13.05 mJ/cm^2
Min. Develop Rate, R_{min}	0.05 nm/sec	0.05 nm/sec
Resist Contrast, γ	10.53	7.163

Table 2: Parameters for the AIT model and the LPM chosen to match the results from the Full Physical model for PAR 710. The values in the second column were obtained by using the equations in Section 3, whereas the values in the third column were obtained by choosing parameter values that led to the best agreement between the Simplified and Full Physical models.

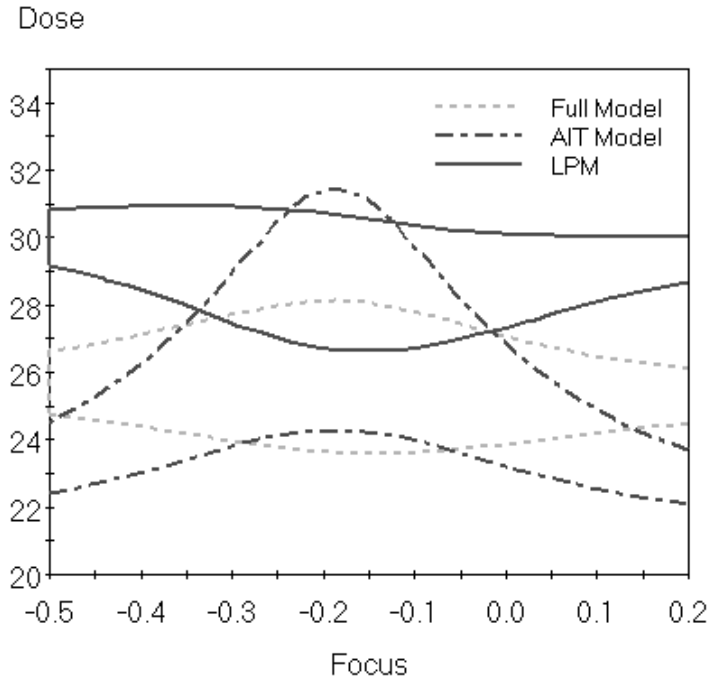


Figure 2: Calculated process windows for semi-dense 130nm lines on a 325nm pitch for the Full Physical model, the AIT model, and the LPM. The parameters for the AIT model and the LPM were obtained by matching to the Full Physical model with the equations in Section 3.

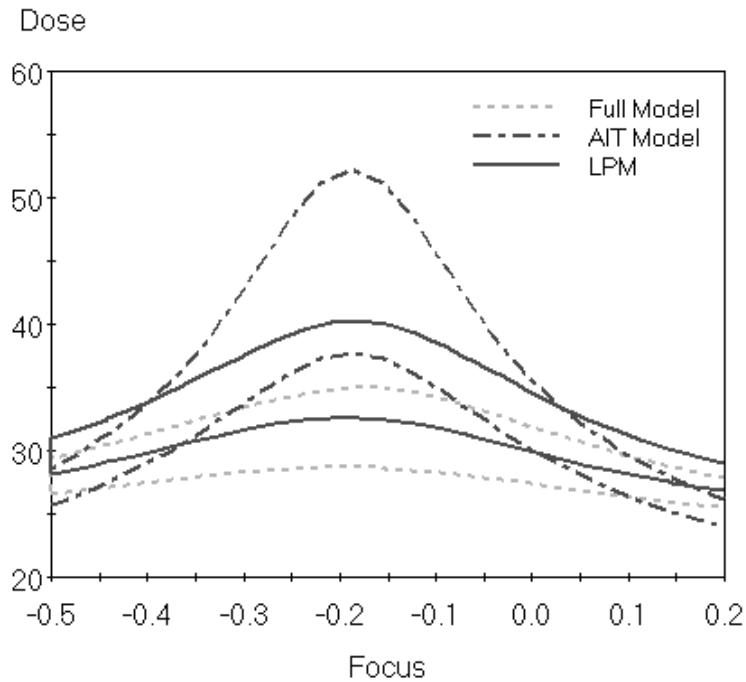


Figure 3: Calculated process windows for isolated 130nm lines for the Full Physical model, the AIT model, and the LPM. The parameters for the AIT model and the LPM were obtained by matching to the Full Physical model with the equations in Section 3.

4. BEST FIT MATCHING BETWEEN SIMPLIFIED AND FULL RESIST MODELS

In order to determine if the Simplified models are capable of describing the process windows predicted by the Full Physical model, in this section we abandon the matching approach in the previous section, and we search for the “best fit” parameters for the Simplified models. For the AIT model, we choose the parameter \tilde{E} so that the dose-to-size is correct for the isolated line at best focus. For the LPM, we use the nonlinear least squares algorithm in the Klarity ProDATA AutoTune™ software package [17,18] to find the effective absorbance, the aerial image diffusion length, and the resist contrast. The new parameters for the AIT model and the LPM are given in Table 2, and the calculated process windows are shown in Figures 4 and 5.

The process windows calculated with the new Simplified model parameters demonstrate better agreement with the results from the Full Physical model. This is especially true for the LPM, where the process windows for the Full Physical model and the LPM almost completely overlap for the semi-dense features. Agreement is also improved for the isolated features. On the other hand, while the results for the AIT model are improved, the shape of the process windows is still qualitatively incorrect compared with the Full Physical model. Other choices for \tilde{E} do not appear to change the qualitative shape of the process window for the AIT model, so this model does not seem capable of predicting the results of the Full Physical model.

5. SUMMARY AND CONCLUSIONS

In this study, we have examined matching Simplified models such as the AIT model and the LPM to results calculated with the Full Physical model in PROLITH. We have developed several relationships between the two Simplified models and the parameters in the Full Physical model, but these relationships appear to only give qualitative agreement between the process windows calculated with the Full Physical model. The comparison between the LPM and the Full Physical model demonstrated that the shape and position of the process windows from the Full Physical model could be predicted with the LPM. However, the matching relationships derived in Section 3 only gave qualitative agreement, whereas a good match was obtained when the LPM parameters were determined from a least-squares fit to the data from the Full Physical model. This indicates that the LPM is capable of predicting the lithographic response calculated with the Full Physical model, and that the matching relationships can be improved. Specifically, the assumption that photoacid (and quencher) diffusion could be neglected should be revisited. Also, the impact of surface inhibition on the develop rate in the Full Physical model should be incorporated into the matching conditions for the LPM as well.

For the AIT model, it appears that it is not possible to choose input parameters so that the AIT model predicts the same process window as the Full Model. This is an indication that the AIT model should not be used for process optimization or to calculate process capability. Instead, either a Full Physical type of model or a different Simplified model should be used, such as the LPM. It is worth noting that the VTRM [8] uses both the aerial image intensity and the slope of the intensity to calculate the feature edge, so this model will likely perform much better than the AIT model. We leave the comparison between the VTRM class of models and the Full Physical model in PROLITH as an interesting direction for future research.

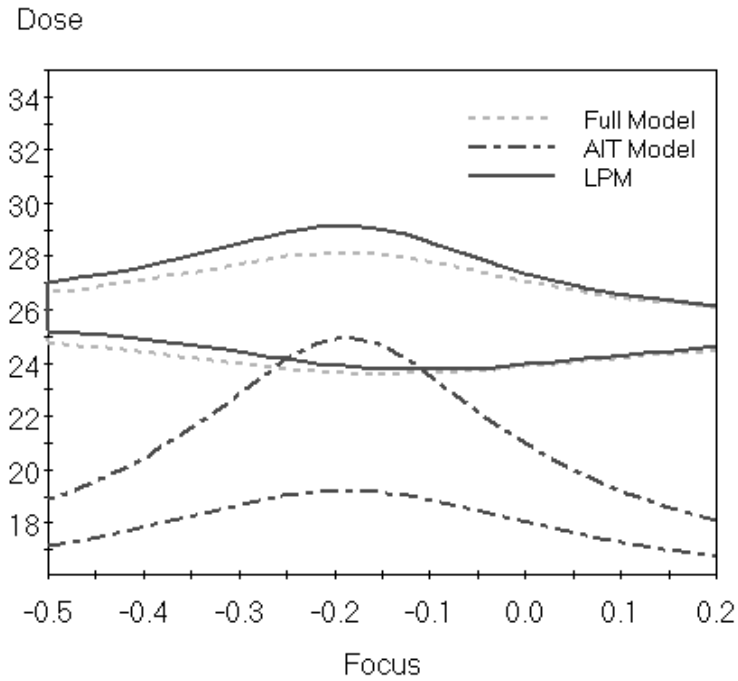


Figure 4: Calculated process windows for semi-dense 130nm lines on a 325nm pitch for the Full Physical model, the AIT model, and the LPM. The parameters for the AIT model and the LPM were obtained from a “best fit” to the Full Physical process window as described in Section 4.

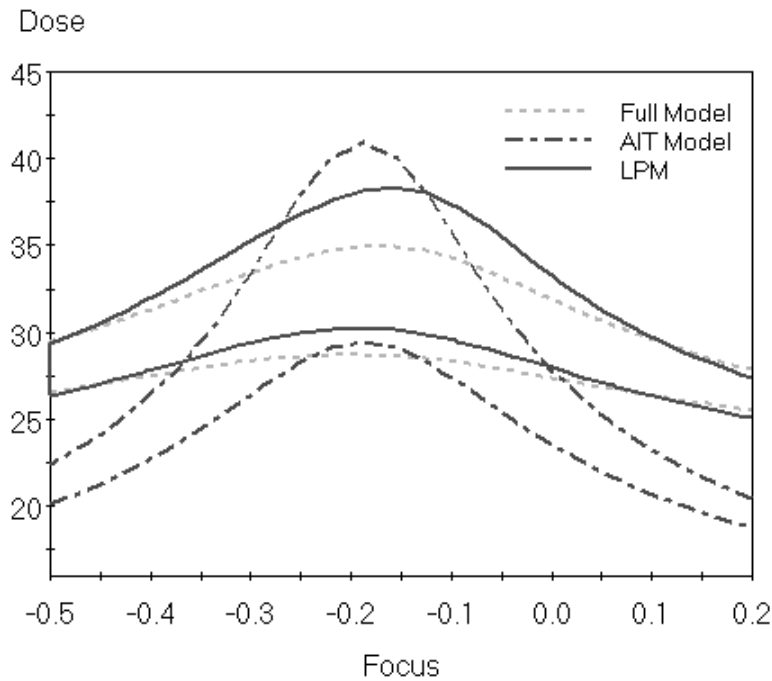


Figure 5: Calculated process windows for isolated 130nm lines for the Full Physical model, the AIT model, and the LPM. The parameters for the AIT model and the LPM were obtained from a “best fit” to the Full Physical process window as described in Section 4.

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