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3D Lumped Parameter Model for Lithographic Simulations

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ABSTRACT

Simplified resist models are desired for fast simulation of resist profiles over large mask areas. The Lumped Parameter Model was originally developed as one such model. However, the LPM model has been limited to 2D resist simulations of 1D aerial image slices with positive tone resists. In this paper we present a modified Lumped Parameter Model applicable to 3D resist simulations of both positive and negative tone resists. In addition several new LPM parameters are introduced that further improve accuracy. The derivation of the 3D LPM model, rationale for including the new parameters, and simulation results using the new model are given.

Keywords: Lumped Parameter Model, Resist Simulation

1. INTRODUCTION

For lithographic simulations of 2D masks a lithographer typically must choose between a fast aerial image model and a slower but more accurate physical model. In the aerial image model the resist feature edge is defined at any point in the image plane where the intensity falls below a threshold value. This threshold intensity can be a single fixed value or adjusted based upon localized mask geometry and as a function of the image gradient[1]. The predictability of this approach is limited and requires extensive imaging experiments to determine the threshold look up function for various imaging conditions. Also the resulting “parameters” for the model have no physical meaning so intuition cannot be used to transfer parameters from one resist process to a slightly modified process. However, given their speed, such aerial image based models are routinely used for optical proximity correction calculations in which many simulations are performed to determine the ideal mask pattern. The more physical models correctly describe the physics of the resist process and are more accurate over a wide range of processing conditions[2]. However, these physical models require 3D resist calculations that quickly become the time limiting step in simulating 2D mask patterns. Also, these physical models require the experimental determination of up to 25 individual resist parameters[2]. The determination of these parameters for a given resist is often more difficult than most lithography simulation users wish to undertake.

The Lumped Parameter Model [3] was originally developed as a compromise solution. It is nearly as fast as an aerial image threshold model yet reasonably represents the physical response of the resist to an arbitrary aerial image. It provides resist sidewall angle and loss as well as resist feature CD. Furthermore, this simple model requires only three resist parameters that are easily fit to a small set of experimental data and used to explore other lithographic conditions. The addition of the diffusion parameter and improved develop path assumptions[4] increased the range of the LPM model’s predictability. However, the LPM model has been limited to 2D resist simulations of positive tone resist and 1D aerial image slices. A 3D LPM model is desirable to enable simulation of 2D mask structures with the speed and utility equal or better than the existing 2D LPM models

Any resist model must convert the 3D image intensity in the resist to a 3D resist profile after development. The full physical resist model simulates the exposure and bake steps to convert the 3D image intensity into a modified chemical composition for each point in the resist. These models then assume a form of the resist develop rate as a function of the chemical composition. The final resist profile is computed by solving the 3D develop problem using this calculated develop rate as a function of position. The 3D develop profile can be written as a line integral is which the time-to-clear every point in the resist is given as

$$\text{Time-to-Clear}(x,y,z) = T(x,y,z) = \int_0^{s_{xyz}} \frac{\sqrt{x'(s)^2 + y'(s)^2 + z'(s)^2}}{R(x(s),y(s),z(s))}\,ds \qquad (1)$$

where the integral is over the path variable s. The functions x(s), y(s), and z(s) describe the path. R(x,y,z) is the modeled resist develop rate as a function of position. The Principal of Least Action defines the correct path functions x(s), y(s), and z(s) as those that yield the fastest develop time for all locations in the resist. After the complete time-to-clear function is solved, the final resist profile is obtained from the locations in space with the time-to-clear equal to the develop time.

The original lumped parameter model was introduced by Hershel and Mack[3] in 1987. They made two assumptions that allowed analytical calculations of the resulting resist feature width from any 1D aerial image. First, the develop rate for the resist was derived from a constant develop contrast assumption.

$$\frac{d\ln(\mathrm{Rate})}{d\ln(\mathrm{Dose})} = \mathrm{contrast} = \gamma \tag{2}$$

This results in the log of the develop rate for any point in space being proportional to the log of the aerial image intensity at that location.

$$\ln(\mathrm{R}(x,y,z)) = \gamma \cdot \ln(\mathrm{I}(x,y,z)\cdot \mathrm{Dose}) + \mathrm{Constant} \tag{3}$$

or

$$\mathrm{R}(x,y,z) = \mathrm{R}_0 \cdot \mathrm{Dose}^{\gamma} \cdot \mathrm{I}(x,y,z)^{\gamma} \tag{4}$$

where the single parameter γ defines the develop rate function and R_0 is derived from the resist thickness and develop time. The second assumption of the original lumped parameter model was to assume a segmented develop path. Initially the resist development is propagated vertically from the nearest maximum of image intensity then the development proceeds horizontally. This is illustrated in Figure 1. Using these two assumptions, the original LPM model yielded a Dose-to-Size for any resist CD and 1D Aerial Images given by

$$\frac{\mathrm{Dose(CD)}}{\mathrm{E}_0} = \left(1 + \frac{1}{\mathrm{thickness}} \int_0^{\mathrm{CD}/2} \left(\frac{\mathrm{I}(x)}{\mathrm{I}(0)}\right)^{\gamma} dx\right)^{1/\gamma} \tag{5}$$

In subsequent work Mack[5] added an absorbance parameter and further assumed that the image-in-resist was separable into the product of the horizontal aerial image and vertical absorbance terms.

$$\mathrm{I}(x,y,z) = \mathrm{I}(x,y)\cdot \mathrm{I}(z) = \mathrm{I}(x,y)\cdot e^{-\alpha z} \tag{6}$$

This assumption coupled with the basic develop rate equation (4) yielded better predictions of resist sidewall angles and showed how resist absorbance affects imaging performance. This improved model was dubbed the Enhanced Lumped Parameter Model.

Brunner and Ferguson introduced two new improvements to the idea of a lumped parameter model in 1996. First, they allowed for the diffusion of the aerial image by including a Fickian diffusion length L.

$$\mathrm{I}(x) = \frac{1}{2\pi \cdot \mathrm{L}^2} \int_{-\infty}^{\infty} \mathrm{I}(x - x')\cdot e^{\frac{-(x-x')^2}{2\mathrm{L}^2}}\, dx' \tag{7}$$

A third segment was also added to the develop path as illustrated in Figure 1. This third develop segment proceeded parallel to the steepest gradient of the aerial image and intersected both the vertical and horizontal components. By introducing these two improvements Brunner and Ferguson were able to improve the ability of the simplified resist model to fit focus exposure matrices for several feature width and pitch values.
There are four distinct problems with the earlier lumped parameter models that this paper will try to fix: The assumption of constant develop contrast through the entire exposure dose range, neglect of refraction effects and defocus of the aerial image through the resist film, lack of support for negative tone resists, and the fixed segment develop path assumption.

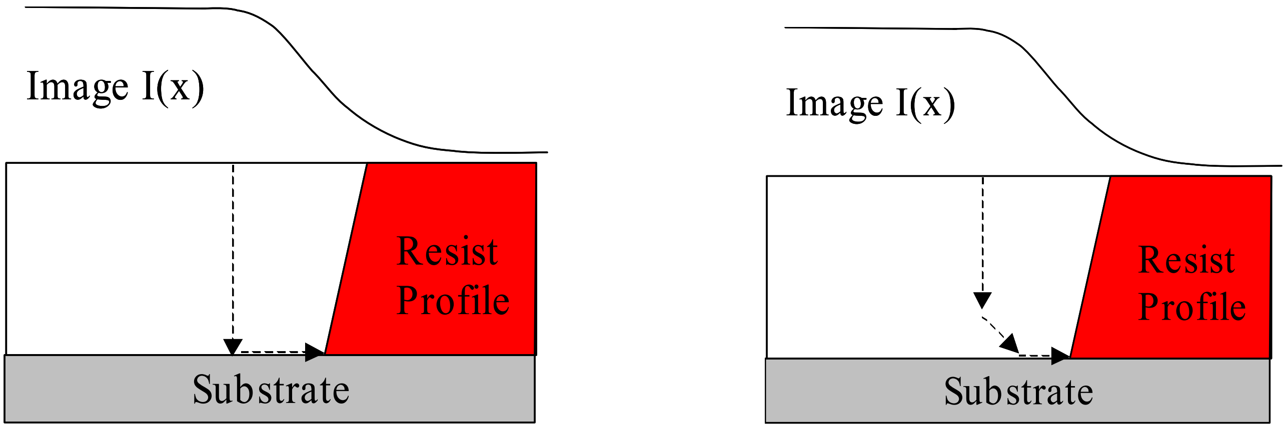


Figure 1: Develop Path assumption for the original lumped parameter model (left) and Brunner/Ferguson lumped parameter model (right) at mask feature edge. For the original lumped parameter model the development path consisted of purely vertical and then horizontal direction. The Brunner/Ferguson lumped Parameter model included a third diagonally segmented develop step.

2. THEORY

Figure 2 shows the resist develop rate as a function of exposure dose for a typical chemically amplified resist. The curve shown was obtained using the full physically based kinetic model available in PROLITH 7.2. Also shown in Figure 2 is a comparable result using the original lumped parameter model with develop contrast of 7.8. Across most of the develop rate range the agreement is fairly good. However significant disagreement occurs in the area of low exposure dose, where the full resist model shows a finite unexposed develop rate or R_{min}. The importance of this disagreement is illustrated by considering the effective develop contrast as a function of the exposure dose. The develop contrast to a large extent controls how well the photoresist can distinguish between exposed and non-exposed regions. The effective develop contrast, as defined by Equation 2, is shown in the right side graph of Figure 2 for the same chemically amplified resist model. For comparison the result for the LPM model with constant γ=7.8 is also shown. When viewed this way the mismatch of the develop models near the mask feature edge (I~ 0.4) is readily apparent.

By a slight modification to Equation 4 the concept of a minimum develop rate can easily be introduced.

$$R(x,y,z) = R_0 \cdot \mathrm{Dose}^{\gamma} \cdot I(x,y,z)^{\gamma} + R_{min} \qquad (8)$$

As with the original lumped parameter model, R_0 can be calculated using the definition that the time-to-clear for a resist of given thickness=d at the dose-to-clear is exactly equal to the develop time, t_{dev}. Inserting Equation 8 into Equation 1 yields

$$t_{dev} = \int_0^d \frac{1.0}{R_0 \cdot I(z)^{\gamma} + R_{min}} dz \qquad (9)$$

$$t_{dev} = \frac{d}{R_{min}} + \frac{1}{\alpha \cdot \gamma \cdot R_{min}} \cdot \ln\left(\frac{R_{min} + R_0 \cdot e^{-\alpha \cdot \gamma \cdot d}}{R_{min} + R_0} \right) \qquad (10)$$

or

$$R_0 = \frac{R_{min}}{\left(e^{\alpha \cdot \gamma \cdot R_{min} \cdot t_{dev}} - 1\right)} \cdot \left(e^{\alpha \cdot \gamma \cdot d} - e^{\alpha \cdot \gamma \cdot R_{min} \cdot t_{dev}}\right) \qquad (11)$$

in the limit of small R_{min} Equation 11 reduces to

$$R_0 = \frac{1}{t_{dev} \cdot \alpha \cdot \gamma} \cdot \left(e^{-\alpha \cdot \gamma \cdot d} - 1\right) \qquad (12)$$

Figure 3 compares the develop rate and contrast with the addition of the R_{min} parameter to the same full resist model used in Figure 2. The agreement near the mask edge is significantly better than obtained without the R_{min} parameter (Figure 2).

The Original Lumped Parameter Model separates the image-in-resist, using Equation 6, as the product of one aerial image term and a z dependent absorbance term. Because of this separability the LPM model requires only one aerial image calculation. This simplification coupled with the analytical CD model, Equation 5, gives the original LPM model its extremely fast computation times. However, this simplification also prevents the LPM model from capturing the refraction of the aerial image at the air/resist interface and the correct defocus of the image through the resist.

A typical image-in-resist is shown in Figure 4 as contours of image intensity. This image was generated using a binary mask and conventional illumination. This is a three beam imaging system in which three diffraction orders combine in the resist to generate the final image. The substrate is assumed to be a perfect ARC so no standing waves are generated. This same image can be represented alternately as line plots either through the horizontal direction or the vertical direction. Both directions are shown in Figure 5. Because of the defocus affects, the image in the “space” decreases with depth into the resist and has negative curvature. However, the image intensity increases with depth into the resist in the “line” and has positive curvature. Near the iso-focal point the image intensity has little variation with depth. The original LPM image assumptions of Equation 6 would show the image decreasing with depth into the resist at all horizontal positions. This non-perfect assumption showed some success since only the aerial images in the space and near the feature edge are important for positive tone images. The line areas never develop so exact representation of these small aerial images is of little importance in the resist model.

A more general representation of the image-in-resist that will properly account for the defocus through the resist can be obtained from three image terms.

$$I(x,y,z) = \left(I_0(x,y) + I_1(x,y) \cdot z + I_2(x,y) \cdot z^2\right) \cdot e^{-\alpha z} \qquad (13)$$

where $I_0(x,y)$ is the image-in-resist at the top of the resist, $I_1(x,y)$ is the linear change of image intensity as a function of depth, $I_2(x,y)$ is the quadratic change of image intensity as a function of depth and α is the absorbance. The image terms $I_0(x,y)$, $I_1(x,y)$, and $I_2(x,y)$ can easily be determined using three calculated images within the resist and the known absorbance. The images at the top, middle and bottom of the resist are the most convenient and effective for this model. We have found that in the absence of standing waves this simple model will effectively represent all image conditions found in lithographic systems. However, because three images are now required, it is expected that the image-in-resist calculation should be three times slower than the simple approximation of the original LPM model, which required just one image term. Since the decomposition of the image into the three image terms ($I_0(x,y)$, $I_1(x,y)$, and $I_2(x,y)$) comes after the calculation of the three images (top, middle, and bottom) this image representation is equally applicable to any image generation model (scalar, full scalar, vector unpolarized, vector polarized, etc…).

Equation 1 is representative of a class of variational calculus problems first proposed by Bernoulli in 1696 as the Brachistichrone ("Least Time") Problem. Analytical solutions are possible for simple functional forms of R(x,y,z) using the Euler-Lagrange method [6,7]. More complex functional forms of the rate function require the use of numerical methods. One can imagine integrating Equation 1 over many proposed paths and keeping only the minimum time-to-clear for every point in space as the final solution. The original LPM model used this procedure with only one proposed development path. In general more rigorous numerical techniques are used to solve the develop time problem in lithography simulation. Equation 1 can be solved using the method of Ritz by expanding the path function x(s) in a basis set of well defined paths and satisfying the Euler condition for the linear combination [6].

$$\frac{d}{dz} F_{x'}(x,z,x') - F_{x}(x,z,x') = 0 \qquad (14)$$

However, the most widely used method for 3D development solves the accompanying partial differential equation form of Equation 1 using the Level-Set procedure. Equation 1 is equivalent to the Eikonal equation 15, which states that the absolute value of the gradient of the time-to-clear function is equal to the develop front velocity at each point in space. Several Level-Set methods for solving Equation 15 have been proposed and implemented [8].

$$\left|\nabla \mathrm{T}(\mathrm{x},\mathrm{z})\right| = \frac{1}{\mathrm{R}(\mathrm{x},\mathrm{z})} \qquad (15)$$

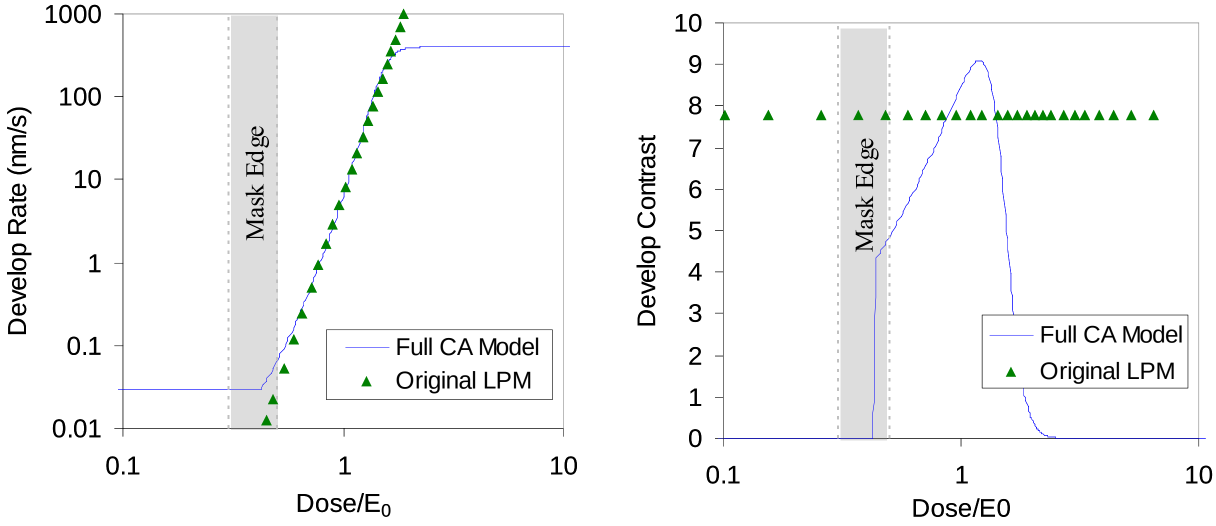


Figure 2: Develop rate (left) and develop contrast (right) for a typical chemically amplified resist model as a function of exposure dose. By comparison the original Lumped Parameter model develop rate and contrast with γ=7.8 is also shown (triangles). The gray region highlights exposure dose values near the printed feature edge.

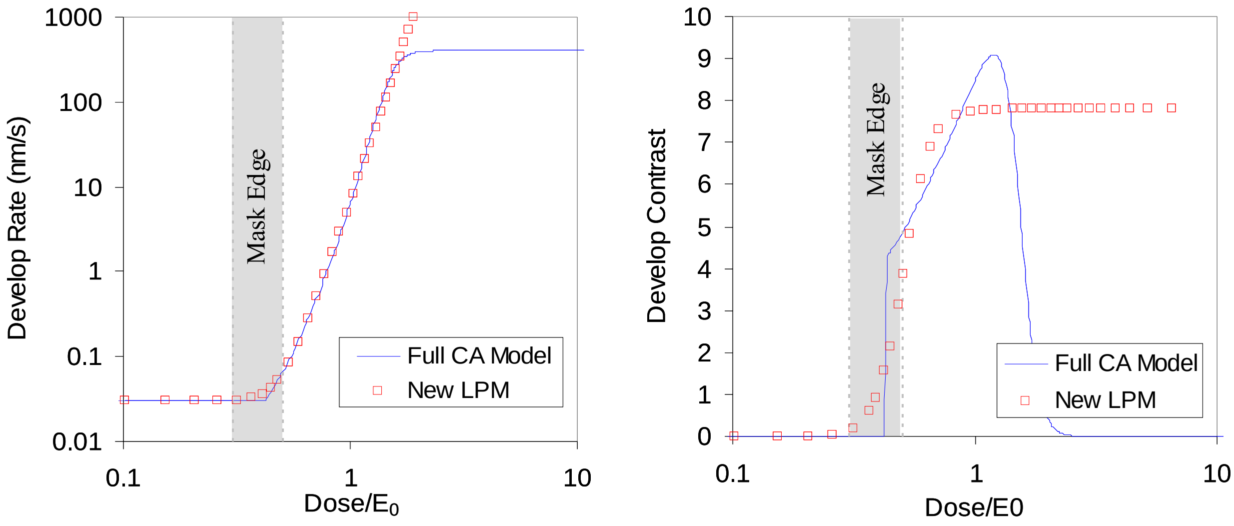


Figure 3: Develop rate (left) and develop contrast (right) for a typical chemically amplified resist model as a function of exposure dose. By comparison the new LPM develop rate and contrast with γ=7.8 and R_{min} = 0.03 is also shown (rectangles). The gray region highlights exposure dose values near the printed feature edge.

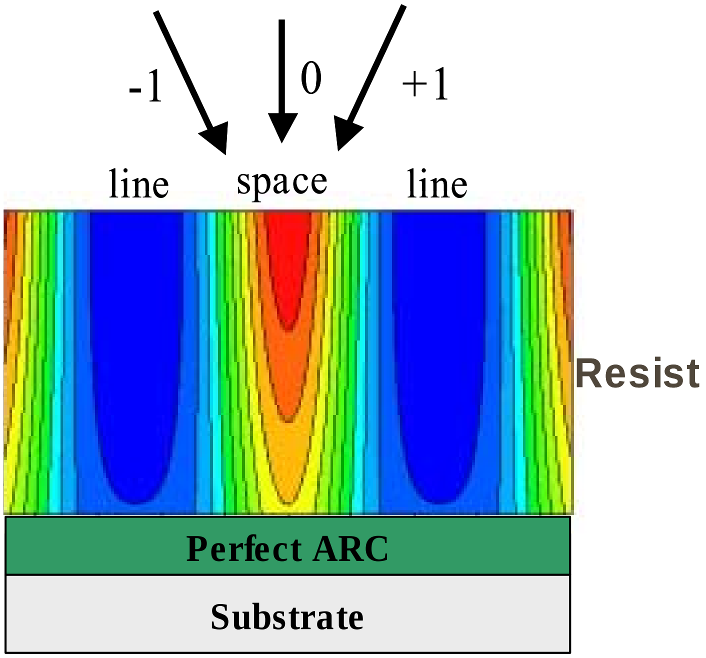


Figure 4: Contours of image intensity in resist for a Line/Space pair generated with 3-Beam imaging conditions (Binary mask, partially coherent illumination, non-reflective substrate).

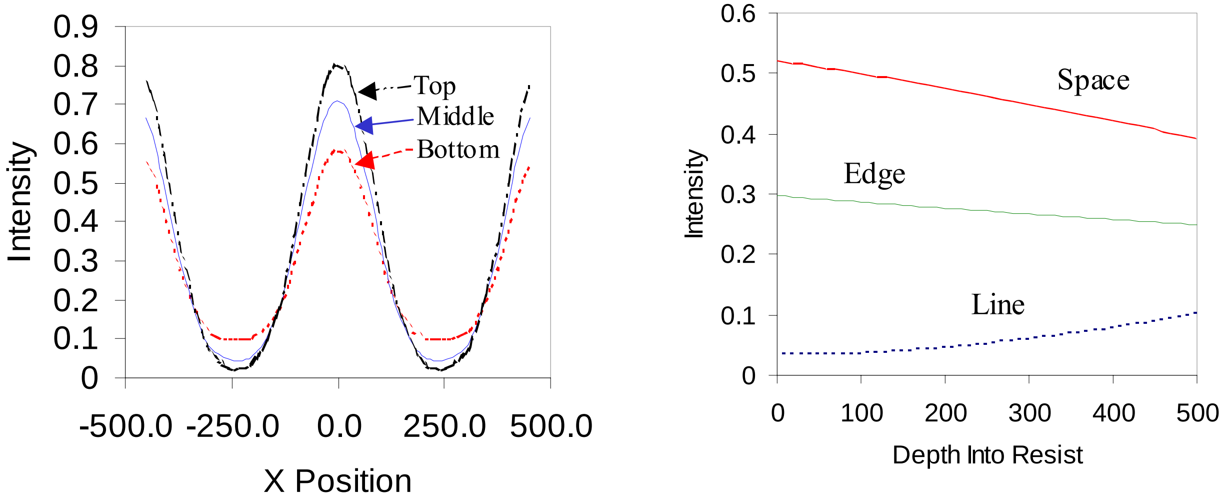


Figure 5: The image-in-resist for a Line/Space pair generated with conventional 3-Beam imaging conditions of Figure 4. Graph on left shows image intensity as a function of horizontal position at three depths into the resist (Top, Middle and Bottom). The Graph on the right shows the same image as a function of depth at three horizontal positions (Center of Space, Mask Edge, and Center of Line).

3. MODEL SUMMARY

The new 3D Lumped Parameter Model is summarized as follows:

Assuming perfect ARC substrate conditions (zero substrate reflection) three image planes are calculated within the resist. The image planes are calculated using any chosen imaging model. For convenience these planes are located at the top, middle and bottom of the resist. The various imaging models available all require the complex refractive index of the resist film, η=n+ik. The imaginary value of the refractive index is determined from the absorbance of the resist material at the exposure wavelength (k=4πα/λ). It has been noticed that the real part of the refractive index for resists at the imaging wavelength varies little from vendor to vendor (less than 2%). It does however depend upon the imaging wavelength. This is a consequence of the basic material platform being dictated by the imagine wavelength (I-line=Novolac, KrF = poly-hydroxystyrene, ArF=aliphatic resin, etc..). For this reason we have chosen to select the real part of the refractive index from the values listed in Table 1.

The three image-in-resist terms (Equation 13) are determined from the three calculated image planes using the following set of equations:

$$I_0(x,y) = I_{Top}(x,y) \tag{16a}$$

$$I_1(x,y) = \frac{4 \cdot e^{\frac{\alpha \cdot d}{2}} \cdot I_{Mid}(x,y) - e^{\alpha \cdot d} I_{Bot}(x,y) - 3 \cdot I_{Top}(x,y)}{d} \tag{16b}$$

$$I_2(x,y) = 2 \cdot \frac{I_{Top}(x,y) + e^{\alpha \cdot d} I_{Bot}(x,y) - 2 \cdot e^{\frac{\alpha \cdot d}{2}} \cdot I_{Mid}(x,y)}{d} \tag{16c}$$

Following Brunner and Ferguson, the 3D image-in-resist is allowed to diffuse using a Fickian type gaussian Kernal function with a characteristic diffusion length L and the appropriate boundary conditions.

$$I(x,y,z)=\frac{1}{2\pi\cdot L^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} I(x-x',y-y',z-z')\cdot e^{-\frac{(x-x')^2+(y-y')^2+(z-z')^2}{2L^2}}\,dx'dy'dz' \qquad (17)$$

The develop rate depends upon the final diffused image-in-resist and the three develop parameters γ, R_{min}, and R_0 through Equation 8. R_{min} and γ are true parameters but R_0 is fixed by Equation 11. By allowing γ to have both positive and negative values this model can simulate both positive and negative tone resists. The final develop profile is the numerical solution of the time-to-clear variational problem described by Equation 1 with the boundary condition $T(x,y,z=0) = 0.0$. The profile edges are those locations within the resist that satisfy the solution condition $T(x,y,z) = t_{dev}$.

Table 1: Average refractive index values found for most commercial resists at common imaging wavelengths.

Wavelength	n
436	1.65
365	1.7
248	1.75
193	1.7
157	1.62

4. RESULTS AND DISCUSSION

The goal of the fast LPM model is to yield the best agreement to a full physically correct resist model for any imaging condition. To this end a methodology for obtaining optimal LPM parameters from a given set of full physical model parameters was introduced by Smith et al [9]. This optimization procedure strives to reduce the deviation between the fast LPM model and the physical model for a set of isolated and dense focus-exposure matrices simultaneously.

For this paper the full resist model for Sumitomo ArF resist PAR710, which is found in the PROLITH 7.2 database, was used. The features imaged were 130nm lines at 310nm and 1300nm pitch. The exposure conditions were 193nm exposure with 0.6NA stepper and 0.7σ conventional illumination. Using the method described by Smith [9], the original LPM model was optimized to yield the results shown in Figure 6. The optimal LPM parameters are shown in Table 2. It was found that one set of LPM parameters does not effectively match the full physical model for both isolated and dense features simultaneously. This is a consequence of both the idealized path model used by the original LPM and the neglect of defocus through the resist. The original LPM parameters can be adjusted to achieve reasonable fits to individual features and compensate for the model approximations. However, the parameter compensation is pitch dependent. This result has been previously reported [4].

Using the new 3D LPM model the same comparison is shown in Figure 7. One set of parameters can effectively match both isolated and dense features. The optimal parameters are shown in Table 2. Even the subtle shift in the center of focus with exposure dose and the asymmetry of CD through focus is reproduced. These asymmetries appear like optical system aberrations but are the result of the resist absorbance. The original LPM model yields both symmetric process windows and a constant best focus through dose. The original LPM model required artificial optical aberrations to model a perfect imaging system and real resist. This deficiency of the original LPM model precluded its use from quantitative description of lens aberration affects on imaging performance.

Typical profiles obtained for through focus simulations are shown in Figure 8 for both positive and negative tone LPM models. The features simulated are 200nm Lines at 600nm pitch using a 0.63NA 248nm stepper and Full Scalar imaging model. Both positive and negative tone features show sloped and re-entrant wall profiles at opposite extremes in focus. This realistic profile dependence on focus is impossible without properly accounting for the image defocus through the resist.

To determine the 3D capabilities and speed advantage of the LPM model over the full physical model a double exposure SRAM gate cell was simulated using a typical 248nm resist and exposure setting. The resist model chosen was for JSR KrF M108Y photoresist as found in the PROLITH 7.2 database. The exposure tool was a 248nm 0.63 NA tool with 0.7σ for the trim Mask and 0.3σ for the dark field phase-shift gate definition mask. The two masks are shown in Figure 9. The 3D LPM model parameters were optimized to match the full physical model results using the same procedure from Smith's paper [9]. The 3D profiles from both the full resist model and the new 3D LPM model are shown in Figure 10. The agreement is very good. The calculation times, using a Pentium III 933mHz machine, were 118s for the full physical model and 15s for the 3D-LPM model. Both results were obtained using PROLITH Speed Factor setting 2 and the Full Scalar imaging model. The calculation times included the Full Scalar image-in-resist calculation for both masks, the LPM model calculation, and the 3D profile extraction and metrology. Figure 11 shows a simulation of the Line End Shortening for the same gate structure as a function of serif size on the trim mask. Again, the agreement between the full physical resist model and the optimized 3D LPM model is very good. The total calculation times were 1023s and 141s for the full physical and LPM models respectively.

The goal for new 3D LPM model is to allow large area simulations of full resist profiles as a function of process variations. As shown in Figure 12 the LPM profile calculation time scales linearly with the total number of surface grid points. The model should be extendable to very large mask areas. These results are for the actual LPM calculation after the three image-in-resist planes are calculated. The calculation times for the non-defocused LPM model (Equation 6) and the defocused LPM model (Equation 13) are both shown. The defocused LPM model is approximately 3 times slower than the non-defocused model. Both models calculate the optimal develop path given the defined develop rate versus position. The 3X speed difference is a result of the extra effort required to determine the optimal path and develop time given a more complicated z dependence of the image-in-resist when defocus affects are included.

Table 2: LPM parameters used to match PAR710 ArF resist for simulations shown in Figures 6 and 7

	Original LPM	New LPM
E_0 (mJ/cm^2)	12.5	12.8
Absorbance α (um^{-1})	0.87	0.904
Contrast γ	11.5	10.57
Diffusion Length L (nm)	39	36
Min Develop Rate R_{min} (nm/s)		0.02

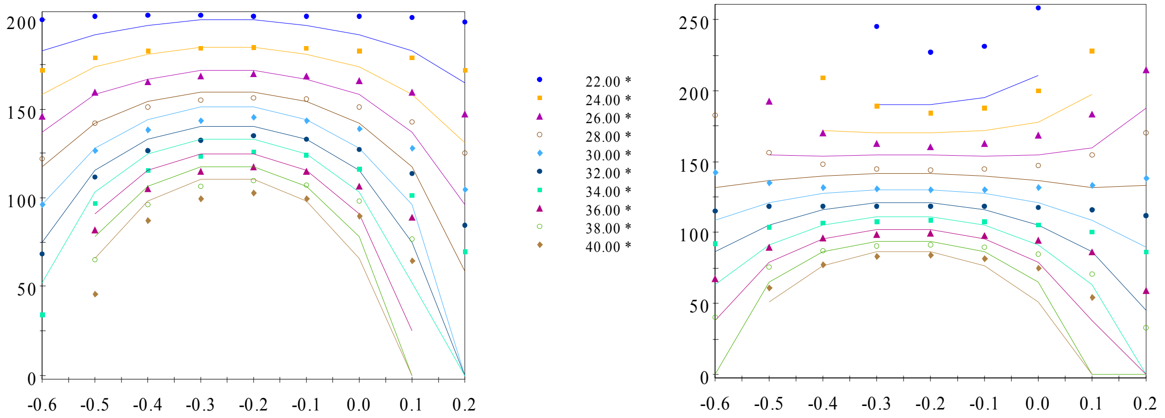


Figure 6: The comparison of focus exposure matrices for 130nm isolated (left = 1300nm pitch) and dense (right = 310nm pitch) lines simulated using a full chemically amplified resist model (symbols) and the original LPM model (lines). The resist model used was PAR710 found in the PROLITH 7.2 database. Imaging tool was 193nm with 0.6NA and 0.7σ illumination. The parameters used for the original LPM model are given in Table 2.

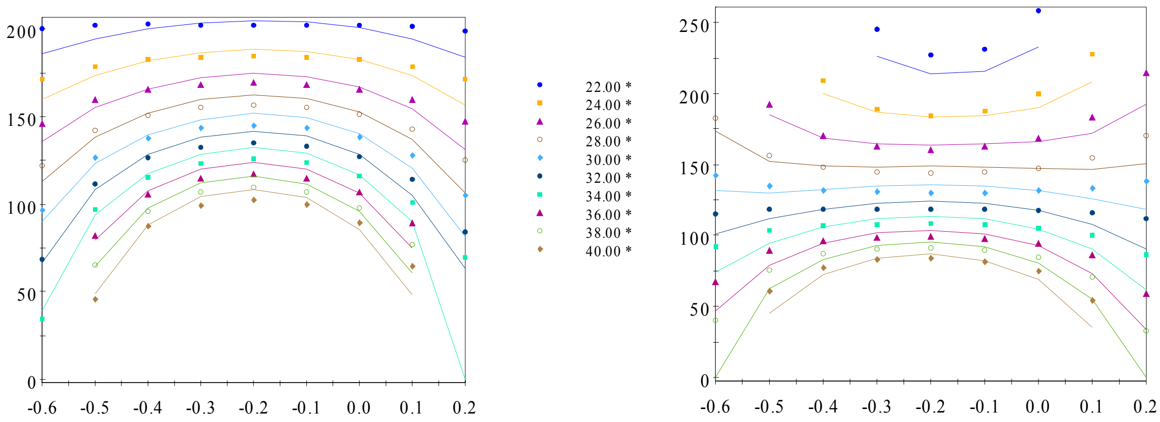


Figure 7: The comparison of focus exposure matrices for 130nm isolated (left = 1300nm pitch) and dense (right = 310nm pitch) lines simulated using a full chemically amplified resist model (Symbols) and the new 3D LPM model (Lines). The resist model used was PAR710 found in the PROLITH 7.2 database. Imaging tool was 193nm with 0.6NA and 0.7σ illumination. The parameters used for the new LPM model are given in Table 2.

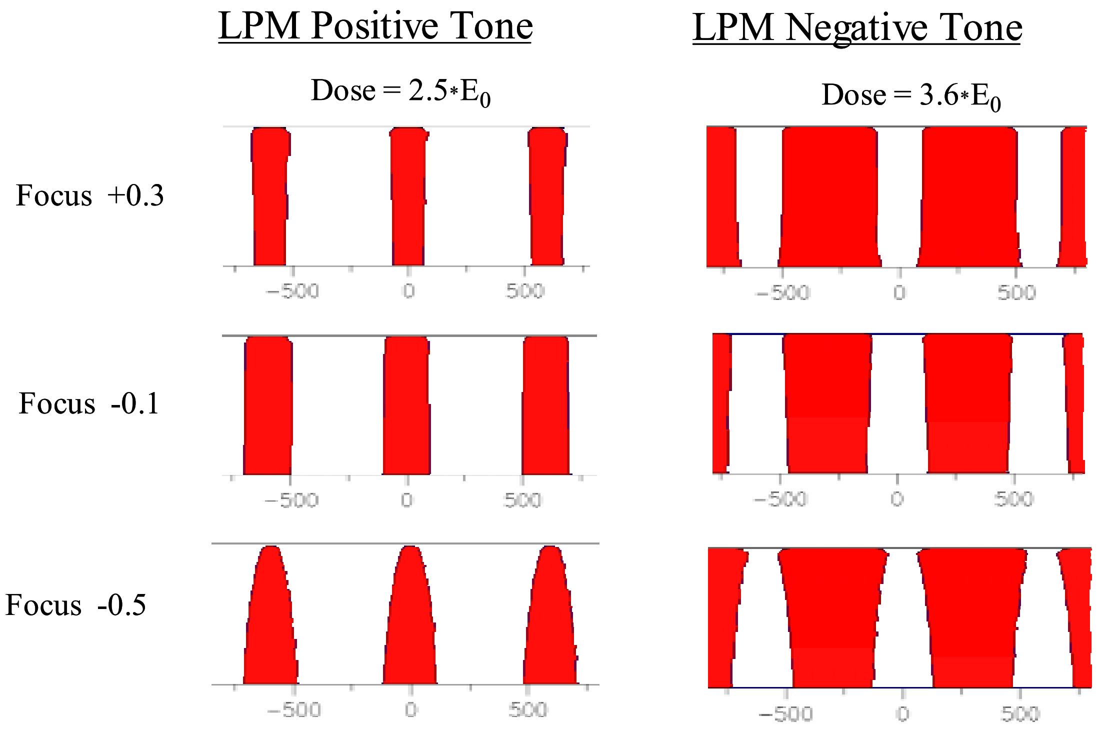


Figure 8: Dependence of LPM profile shapes on focus when the three image term defocus model of Equation 13 is employed. Features simulated are 200nm chrome on 600nm pitch. Imaging tool was 248nm with 0.63NA and 0.7σ illumination.

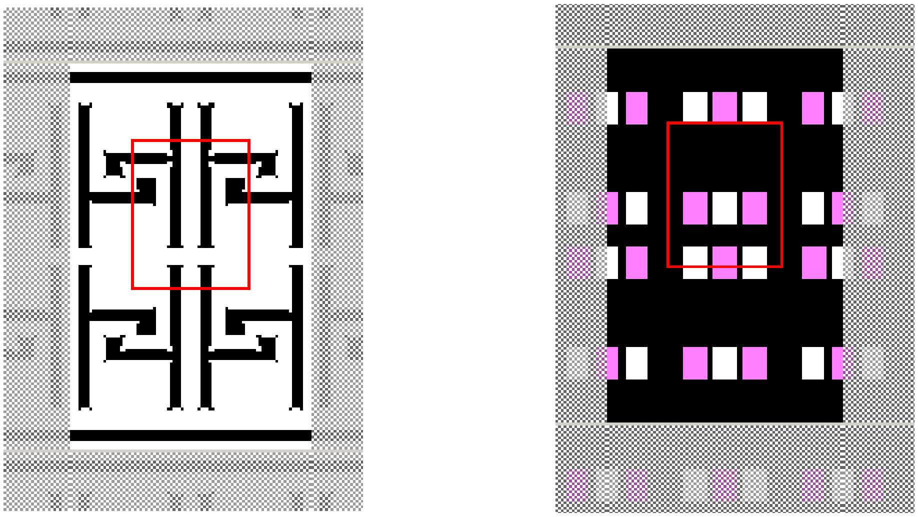
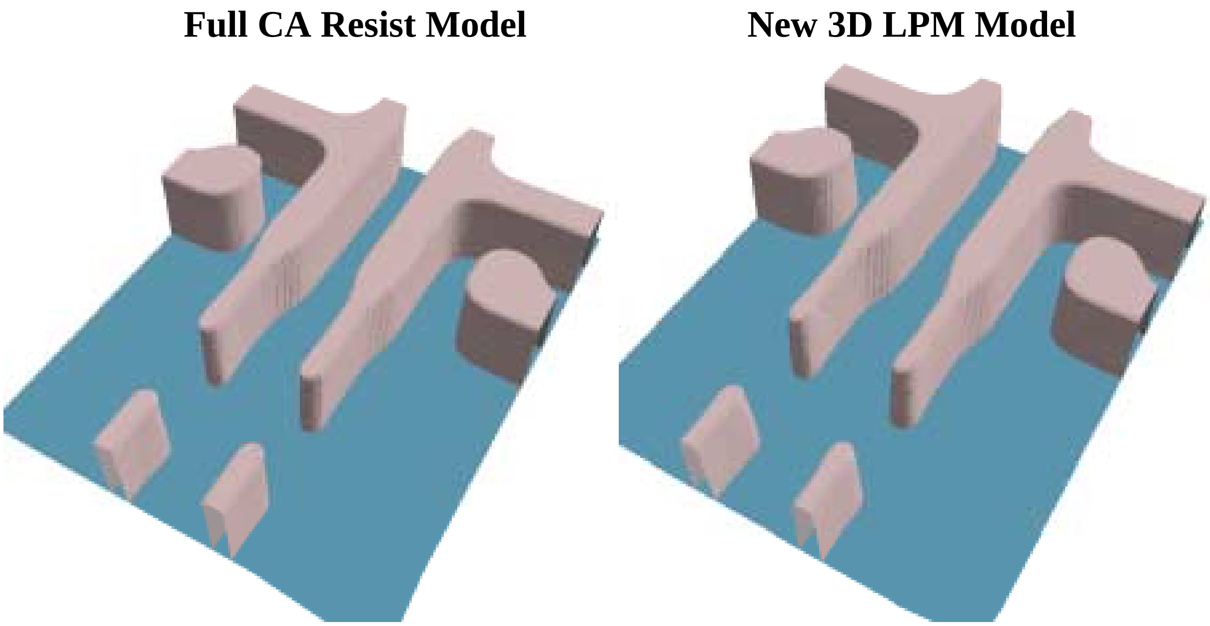


Figure 9: Mask set used for 3D simulations of double exposure SRAM bit cell.



Full CA Resist Model

New 3D LPM Model

Figure 10: 3D Profiles obtained using the full physical resist model (left) and the new 3D LPM model (right). The resist parameters were taken from the PROLITH 7.2 database for JSR KrF M108Y photoresist. Imaging tool was 248nm with 0.63NA and 0.7σ (Trim) 0.3σ (Gate) illumination. The substrate used for M108Y simulations was an optimized ARC.

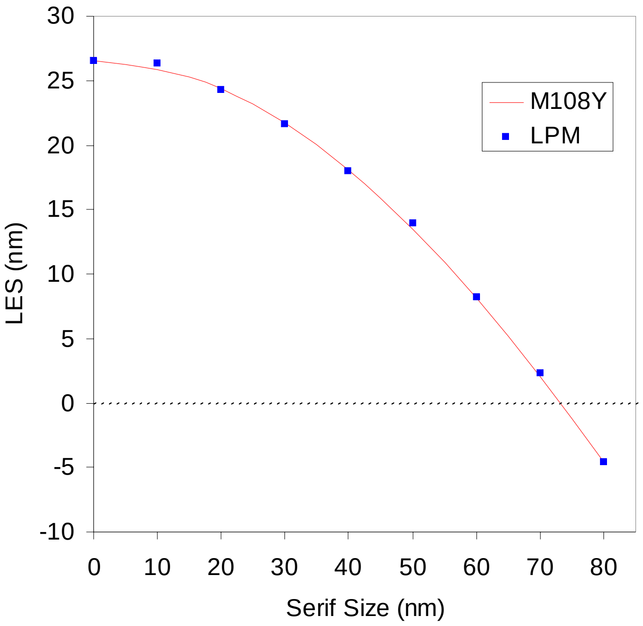


Figure 11: Comparison of Line End Shortening calculation as a function of serif size on trim mask using the full physical resist model (line) and the new 3D LPM model (symbols). The resist parameters were taken from the PROLITH 7.2 database for JSR KrF M108Y photoresist. Imaging tool was 248nm with 0.63NA and 0.7σ (Trim), 0.3σ (Gate) illumination. The substrate used for M108Y simulations was an optimized ARC.

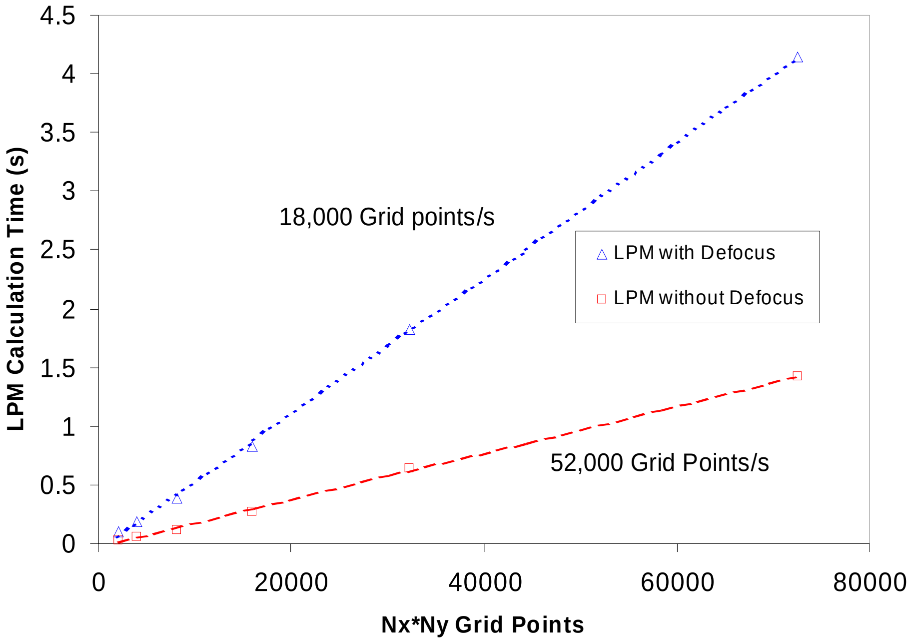


Figure 12: Scaling law for 3D LPM calculation of resist profiles after the image-in-resist calculation is complete. The upper line shows the results using the three term defocus model defined by Equation 13 and the lower line shows the results using the non-defocus model defined by equation 6. The calculation times are shown as a function of the number of surface grid points (mask area).

5. CONCLUSION

In this paper a modified Lumped Parameter Model was proposed and implemented for 3D lithography simulations. The proposed model introduced the minimum develop rate parameter R_{min} for improved matching of develop rate contrast near the final feature edge. The model correctly accounts for the image refraction at the air resist interface and the defocus of the image within the resist. The segmented develop path approximation of the original Lumped Parameter Model was replaced by a numerical solution of the full 3D develop problem. By allowing a negative contrast value, negative tone resists can effectively be simulated using the new model. When the optimal LPM parameters are obtained, the new model matches a full chemically amplified resist model fairly well, yet is considerably faster. Because the new model scales linearly with mask area the model should be extendable to large mask area simulations of the full resist profile.

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