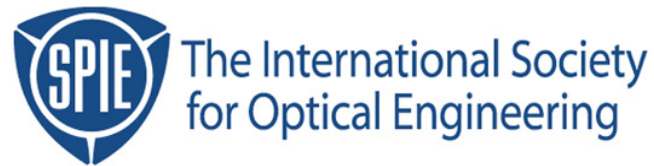


Copyright 1996 by the Society of Photo-Optical Instrumentation Engineers.



This paper was published in the proceedings of
Metrology, Inspection, and Process Control for Microlithography X,
SPIE Vol. 2725, pp. 49-63.

It is made available as an electronic reprint with permission of SPIE.

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

Resist Metrology for Lithography Simulation, Part 2: Development Parameter Measurements

A. Sekiguchi, C. A. Mack*, Y. Minami and T. Matsuzawa
Litho Tech Japan Corp., Kawaguchi, Saitama, Japan
**FINLE Technologies, Inc., Austin, TX*

Abstract

Resist simulation technology began with the presentation of Dill's lithography models over 20 years ago, and in the ensuing years has undergone various improvements. Basic parameters in resist modeling include the exposure parameters, bulk development parameters, diffusion length of the photoactive compound (PAC) due to post-exposure baking (PEB), and surface inhibition factors. (The exposure parameters are discussed in detail in "Resist Metrology for Lithography Simulation, Part 1.") In this report, equipment and data analysis software capable of efficient and accurate determination of development parameters, the diffusion lengths of PAC due to PEB, and surface inhibition factors are discussed. In particular, the construction of equipment for the measurement of development rates is described, and techniques for extraction of development parameters, PAC diffusion lengths, and surface inhibition factors are discussed in detail and examples are given for a high resolution i-line resist.

Keywords: photoresist, development rate, development rate measurement, development parameter, surface inhibition factor, lithography simulation

I. Introduction

The exposure parameters, development parameters, PAC diffusion length due to PEB, and surface inhibition factors are known to be basic to resist modeling. In this paper, the construction of a Resist Development Analyzer (RDA) system capable of efficient and accurate determination of the development parameters, PAC diffusion lengths, and surface inhibition factors necessary for accurate lithography simulations is described, and data analysis software is explained in detail. (The exposure parameters are discussed in detail in "Resist Metrology for Lithography Simulation, Part 1" which appears just prior to this paper.) In order to determine the above parameters, first the development rate distribution in the resist depth direction is measured [1]. Dill's exposure model [2] is used in simulations to determine the PAC concentration distribution in the resist depth direction immediately after exposure. In order to incorporate the effect of PEB, a one-dimensional diffusion calculation is performed for the PAC distribution data [3]. By comparing these two data sets, the relation between PAC distribution and development rate is determined. By fitting the relation to the development rate equation, the development parameters can be found. And by

further adapting this method, the PAC diffusion length due to photoresist PEB and surface inhibition factors can be determined along with the development parameters. In this study, we attempted to determine the values of these parameters for a high-resolution i-line resist, THMR-iP3000 (Tokyo Ohka Kogyo). These values were inputted to PROLITH/2 and profile simulations performed, and the results were compared with SEM observations. It was confirmed that the parameters in question could be accurately determined, and that by using them in simulations the actual process could be reliably reproduced.

II. RDA Equipment and Analysis Software

A. Equipment for development rate measurement and principle of measurement

The rate of photoresist development is measured by making monochromatic light incident on a thin film of resist during development. When monochromatic light is incident on developing resist, the light reflected from the resist surface and the light reflected from the substrate surface interfere. As the resist thickness changes with development, the reflected intensity is observed to vary sinusoidally with time. Figure 1 is a schematic diagram of the unit used to measure development rates. The 950 nm light from an L.E.D. is focused into a beam approximately 3 mm in diameter, and is made incident on a wafer in development. A wavelength of 950 nm was chosen to minimize the effect of absorption by the dissolution products. Reflected light is focused by a receiving lens, converted into an electrical signal by a phototransistor, digitized by an A/D converter, and sent to a personal computer. This device has 18 such measurement channels, and is capable of monitoring the photoresist at 18 different sites simultaneously through high-speed sampling at intervals as short as 10 ms. Automated detection of interference peaks makes the operation quite efficient. The reflection intensities at different positions in the resist are calculated in advance using theoretical equations for multilayer thin films [2]. From this theoretical relation between the reflected intensity at the resist surface and the resist film thickness, the measured relationship between reflected intensity and monitoring time can be used to accurately determine the remaining resist film thickness as a function of development time. From this, the development rate distribution in the resist thickness direction is calculated (Fig. 2). In particular, theoretical calculations for multilayer thin films can be applied to films of up to ten layers. Thus, the dissolution rate of a resist can be accurately found in the presence of a top-layer anti-reflection coating, a bottom-layer anti-reflection coating, or a photoresist on a multilayer film substrate.

B. Method for computing development parameters

The development rate $R(z)$ at an arbitrary depth z in the resist film for a given exposure dose can be measured by the procedure described above. On the other hand, at present there is no method for measuring the concentration $M(z)$ of PAC at an arbitrary depth z in the resist film for a given exposure dose. Hence $M(z)$ must be determined through calculations. Here we assume a plane wave of monochromatic light incident on multilayer thin films consisting of multiple materials with flat interfaces. In accordance with the model of Dill et al. [2], we calculate the distribution of the PAC concentration $M(z)$ at an arbitrary point in time (i.e., for a given exposure

dose). For the most advanced i-line resists, PEB is indispensable. Hence in addition to the above Dill model, we solve the one-dimensional diffusion equation in the z direction (eq. (1) below) to take PAC diffusion due to PEB [3] into consideration, and calculate the normalized PAC concentration distribution $M'(z)$ after PEB.

$$\frac{\partial M}{\partial t} = D \frac{\partial^2 M}{\partial z^2} \quad (1)$$

Here M is the normalized PAC concentration, D is the diffusion coefficient, z is the depth into the resist, and t is the PEB time.

Figure 3 shows the development rate distribution $R(z)$ after PEB and the values of $M(z)$ and $M'(z)$, the PAC concentration distribution immediately after exposure and PEB, respectively, as determined by simulations. A table of the relation $R(M)$ was constructed from the measured development rate in the resist film as a function of depth $R(z)$ (Figure 3(b)) and the normalized concentration distribution $M'(z)$ (Figure 3(a)), with the depth position z eliminated. By fitting the resulting $R(M)$ to the different development rate equations, the development model parameters can be obtained. The development rate equations studied were the rate equations of Dill [4], Kim [5] and Mack [6].

Dill:
$$R = \exp(E_1 + E_2 M + E_3 M^2) \quad (2)$$

Kim:
$$R = \frac{1}{R_1^{-1} (1 - M \exp(-R_s (1 - M))) + R_2^{-1} M \exp(-R_s (1 - M))} \quad (3)$$

Mack:
$$R = R_{\max} \frac{(a+1)(1-M)^n}{a + (1-M)^n} + R_{\min}, \quad (4)$$

where
$$a = \frac{n+1}{n-1} (1 - M_{th})^n$$

C. Method for computing the PAC diffusion length due to PEB

The above-described method was used to calculate development parameters. In this work, we used the Mack model to estimate PAC diffusion lengths due to PEB because the equation fitted best among the models. First, the above Mack equation was applied to convert development rate data of samples subjected to PEB into a PAC concentration distribution. Separately, simulations were carried out to determine the PAC concentration after PEB (Fig. 4). While varying the

diffusion length in the latter calculations, differences in PAC concentrations (residues) between the two methods were calculated, and the value at which the total residue was a minimum was taken to be the estimated diffusion length, σ (Fig. 5). The diffusion length could also be related to the diffusion coefficient at the PEB temperature by

$$\sigma = \sqrt{2Dt} \quad (5)$$

where D is the diffusion coefficient, and t the time over which the system is at temperature T . The assumption here is that only PAC diffusion causes a smoothing out of the standing waves.

D. Method for computing the surface inhibition factors

The method indicated above was used successfully to calculate development parameters and PAC diffusion lengths due to PEB. We next use these values to compute surface inhibition factors. Surface inhibition is a phenomenon in which the development rate is reduced at the resist surface. In the most advanced i-line resists, this phenomenon is utilized to improve the resist profile against defocusing. In PROLITH/2, the surface inhibition effect is expressed as follows [6].

$$R(z)/R_B = 1 - (1 - R_0)\exp(-z/\delta) \quad (6)$$

where R_B is the bulk development rate, R_0 is the development rate at the resist surface relative to R_B , and δ is an empirical constant related to the thickness of the inhibition layer (called the Inhibition Depth in PROLITH/2). Measured dissolution rate data in the z direction were used to determine the surface inhibition factors R_0 and δ by the following method.

First the PAC concentration distribution in the z direction after PEB was calculated. Then this data was used with the previously determined Mack development rate equation to obtain a development rate distribution. This predicted rate as a function of depth was compared with the measured development rate distribution. Surface inhibition results in a measured rate at the surface of the resist which is less than the predicted rate based on bulk measurements (Fig. 6). Then the minimum development rate in the resist surface region relative to the predicted bulk rate was computed as R_0 , and by fitting the measured depth-direction development rate data to eq. (6), δ was determined (Fig. 7).

III. Experimental

Development rate distributions in the depth direction were measured for various exposure doses. The measurement conditions were as follows:

The i-line photoresist THMR-iP3000 (Tokyo Ohka Kogyo) was applied to a thickness of 1.05 μm to a bare silicon substrate. Pre-baking was at 80°C for 90 s, and PEB was performed at 90, 100, 110 and 120°C (with the data for 110°C used to compute bulk development parameters) for 90 s. The exposure system used light of wavelength of 365 nm, and had an NA of 0.50 and

coherence factor of 0.60. Development was by the immersion (dip) method using NMD-W (2.38% tetramethyl ammonium hydroxide with surfactant) at 23°C.

IV. Results and Discussion

A. Raw data

Figure 8 shows the dissolution rate distribution in the z direction for different exposure doses obtained from the RDA system for the 110°C PEB conditions. Note that some residual standing wave behavior is still apparent.

B. Determination of bulk development parameters

Figure 9 shows the results obtained by fitting to the equations of Dill, Kim and Mack, and Table 1 lists the parameter values. For this example, a logarithmic scale for development rate was used when fitting and showing the results. For THMR-iP3000, there exists a strong nonlinear region between $M = 0.5$ and 0.8. The results using the rate equations of Dill and Kim deviate considerably from measured values in this region, whereas Mack's equation provides a good fit. Hence in subsequent calculations we used the Mack equation.

C. Determination of diffusion lengths

Figure 10 shows the calculated PAC diffusion lengths from the development rate data at each exposure dose for different PEB temperatures. There are some differences depending on the PEB temperature, but the diffusion length gradually increases for E_{dose}/E_0 between 0.7 and 0.9, and is nearly constant for E_{dose}/E_0 above 1.0, where E_{dose} is the exposure dose and E_0 is the dose to clear. Hence we conclude that for E_{dose}/E_0 in the range 0.7 to 0.9, the diffusion length depends on the exposure energy (that is, the diffusion coefficient D is not constant). Considering that in actual pattern formation processes an exposure dose of E_{dose}/E_0 greater than one is necessary, we chose the value at $E_{dose}/E_0 = 1.0$ as the diffusion length. Figure 11 shows the resulting estimated diffusion lengths for different PEB temperatures.

D. Determination of surface inhibition factors

Figure 12 shows the surface inhibition factors R_0 and δ for different PEB temperatures. As the PEB temperature rises, the development rate at the photoresist surface declines dramatically, indicating that as the PEB temperature is raised surface inhibition intensifies. On the other hand, δ , the depth at which development rate transition occurs, was found to increase only slightly with increasing PEB temperature.

V. Simulations

Profile simulations were carried out with PROLITH/2 for a 0.4 μm line pattern with defocus conditions varied, and the results were compared with SEM cross-section observations (Fig. 13). The input parameters used for development simulations are shown in Table 2. The resolution versus defocus, standing waves on sidewalls, resist overhang due to surface inhibition and other features of the simulations were found to be in good agreement with the SEM observation results, confirming that accurate values of the parameters were obtained. Simulation can now be used to explore other areas of interest with confidence in the accuracy of the results.

VI. Conclusions

In addition to describing the construction of a Resist Development Analyzer (RDA) system, we have described the use of this system in determining development rate modeling parameters, PAC diffusion lengths due to PEB and surface inhibition factors for use in lithography simulations. Extensive experimental data was collected for a high-resolution i-line resist, THMR-iP3000 (Tokyo Ohka Kogyo), to demonstrate the utility of this system. The results obtained were input into PROLITH/2, profile simulations were performed, and the results were compared with SEM observations. As a result, it was confirmed that the parameters in question were accurately determined, and that by inputting the values into a simulator the process could be reliably reproduced.

Acknowledgments

The authors are grateful to Mr. Hayato Ohno of Tokyo Ohka Kogyo for providing resist materials and SEM photos used in this work.

REFERENCES

1. Y. Minami and A. Sekiguchi, "Defocus simulation using observed dissolution rate in photolithography," *Electronics and Communications in Japan, Part 2*, Scripta Technica, Inc., Vol. 76, No. 11, pp. 106-115, 1993.
2. F. H. Dill, A. R. Neureuther, J. A. Tuttle, and E. J. Walker, "Modeling projection printing of positive photoresist," *IEEE Trans. Electron Devices*, Vol. ED-22, No. 7, pp. 456-464, 1975.
3. D. A. Bernard, "Simulation of post exposure bake effects on photolithographic performance of a resist film," *Philips Journal of Research*, Vol. 42, pp. 566-582, 1987.
4. F. H. Dill, W. P. Hornberger, P. S. Hauge, and J. M. Shaw, "Characterization of positive photoresist," *IEEE Trans. Electron Devices*, Vol. ED-22, No. 7, pp. 445-451, 1975.

5. D. J. Kim W. G. Oldham, and A. R. Neureuther, "Development of positive photoresist," *IEEE Trans. Electron Devices*, Vol. ED-31, No. 12. pp. 1730-1736, 1984.
6. C. A. Mack, "Development of positive photoresist," *J. Electrochem. Soc.*, Vol. 134, No. 1, pp. 148-152, 1987.

Table 1. Development parameters of Dill, Kim and Mack for THMR-iP3000.

Equation	Development parameters
Dill's equation	$E_1=6.53162$ $E_2=-0.14479$ $E_3=-6.71930$
Kim's equation	$R_1=0.0672871$ $[\mu\text{m/s}]$ $R_2=0.00013655$ $[\mu\text{m/s}]$ $R_3=6.38727$
Mack's equation	$R_{\text{max}}=65.5505$ $[\text{nm/s}]$ $R_{\text{min}}=0.025568$ $[\text{nm/s}]$ $n=5.01352$ $M_{\text{th}}=0.30$

Table 2. Diffusion length and the parameters related to Mack model for THMR-iP3000 at various PEB temperature.

PEB Temperature (°C)	σ (nm)	R_0	δ (nm)
90	29.8	0.682	22.0
100	37.6	0.128	27.5
110	49.7	0.0178	30.1
120	68.7	0.0106	32.6

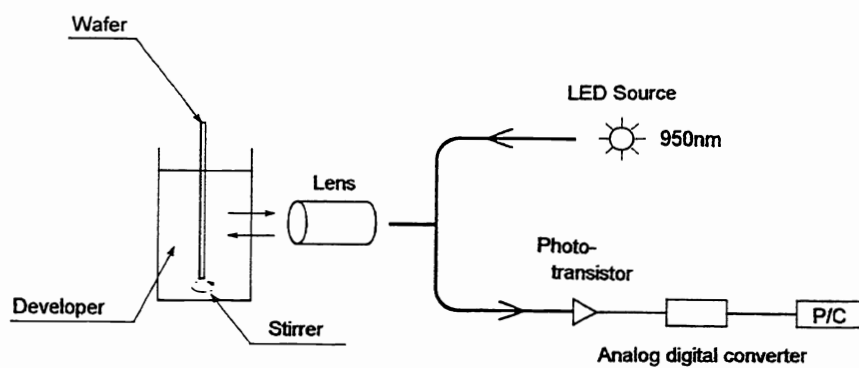


Fig. 1. Schematic diagram of the development rate measurement system.

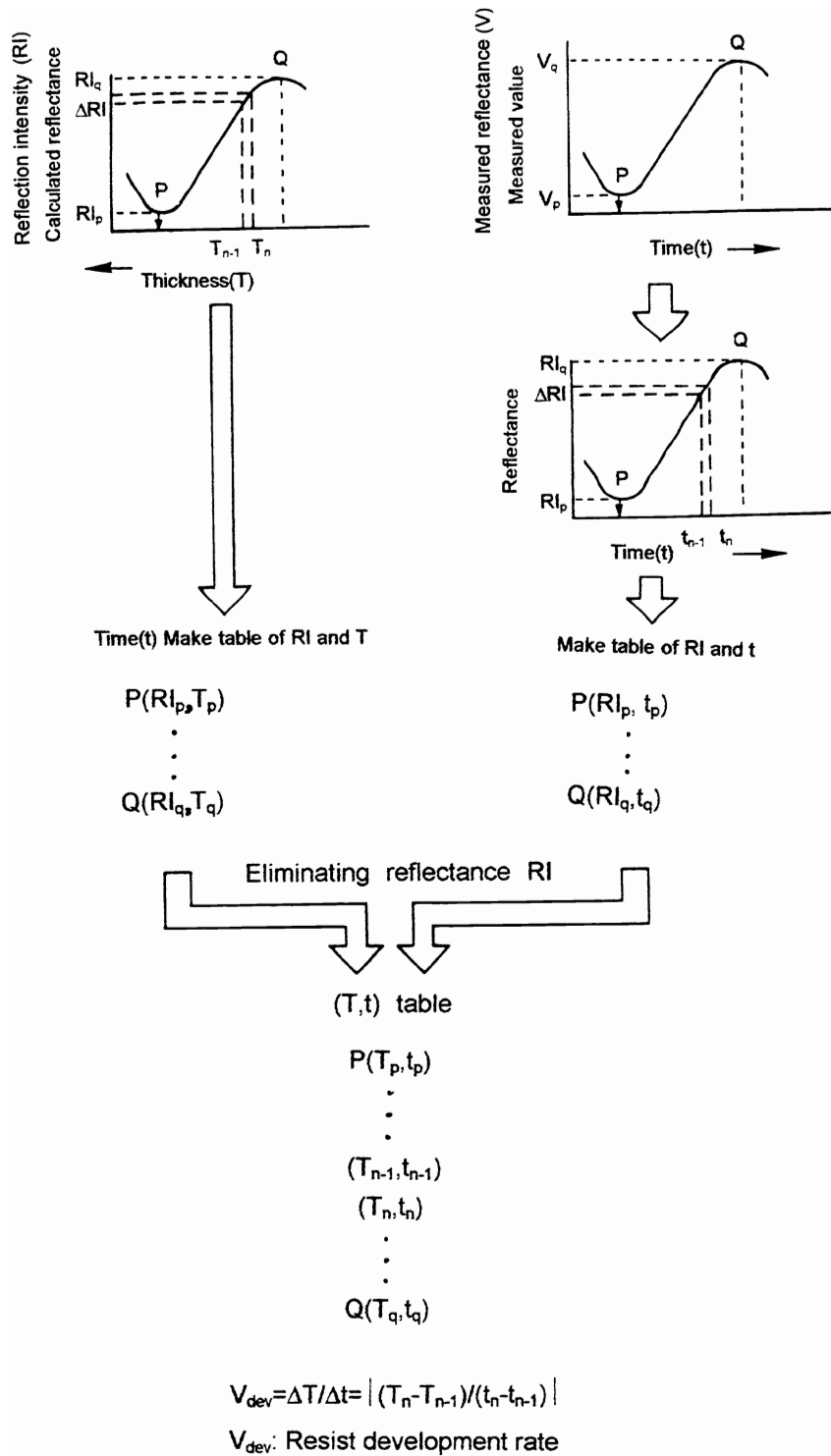
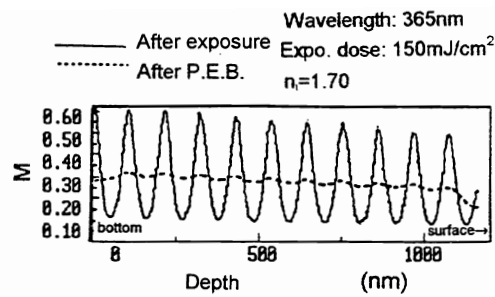
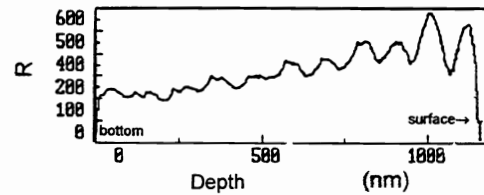


Fig. 2. Procedure for calculating development rates.



(a) Relative normalized PAC concentration (M) distribution in depth direction.



(b) Development rate (R) distribution in depth direction.

Fig. 3. (a) PAC concentration distribution in resist depth direction (calculated),
(b) Development rate distribution in resist depth direction (measured).

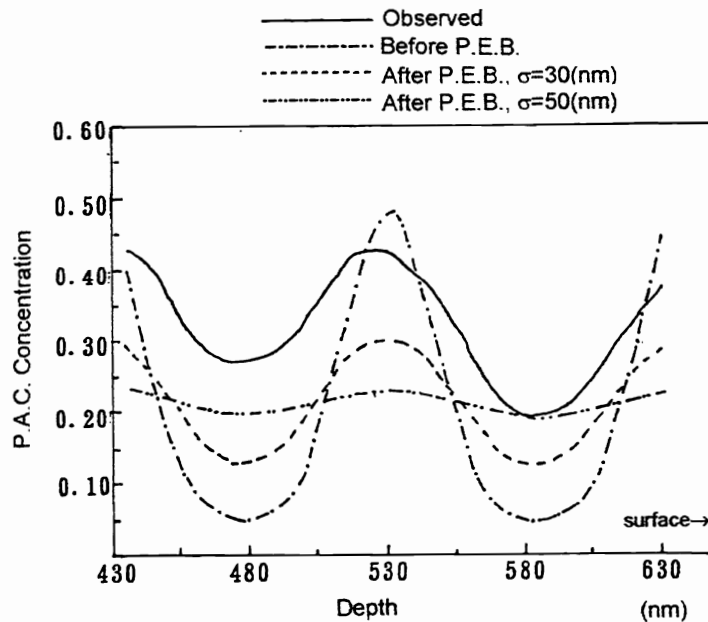


Fig. 4. Comparison of measured and calculated PAC concentration depth-direction distributions.

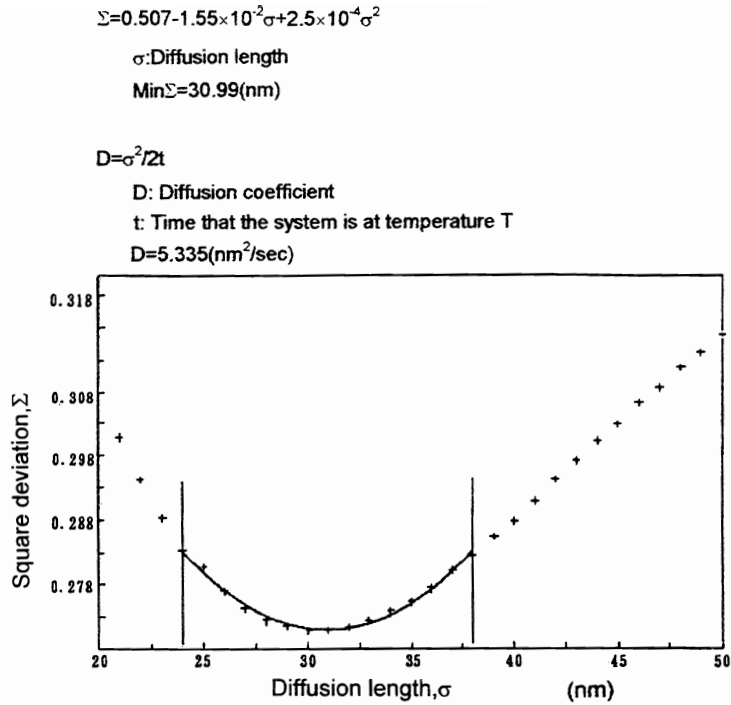


Fig. 5. Relation between residue (square of deviation) and diffusion length.

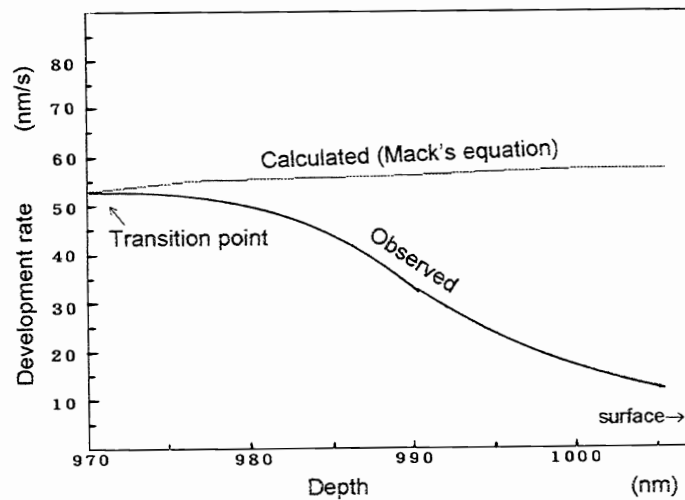


Fig. 6. Deviation of development rate equation from measured development rate in surface region (the figure shows the square of the difference as a function of depth).

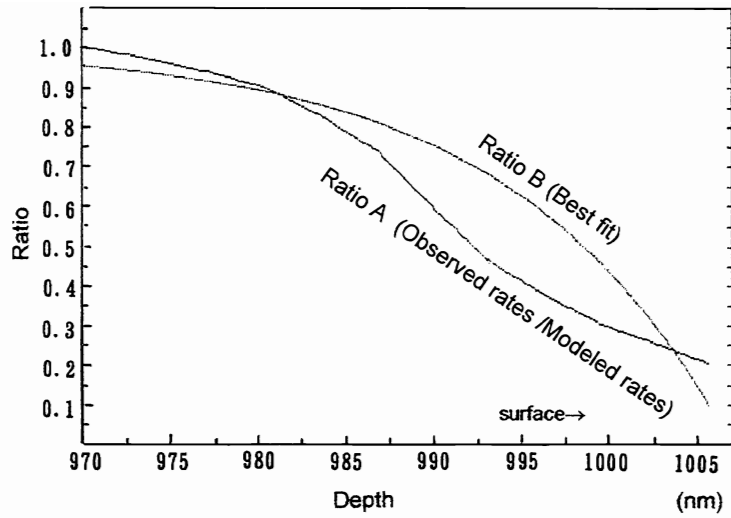


Fig. 7. Ratios of observed rates to modeled rates.
 A: Observed rates/modeled rates
 B: Best fit for observed rates/modeled rates

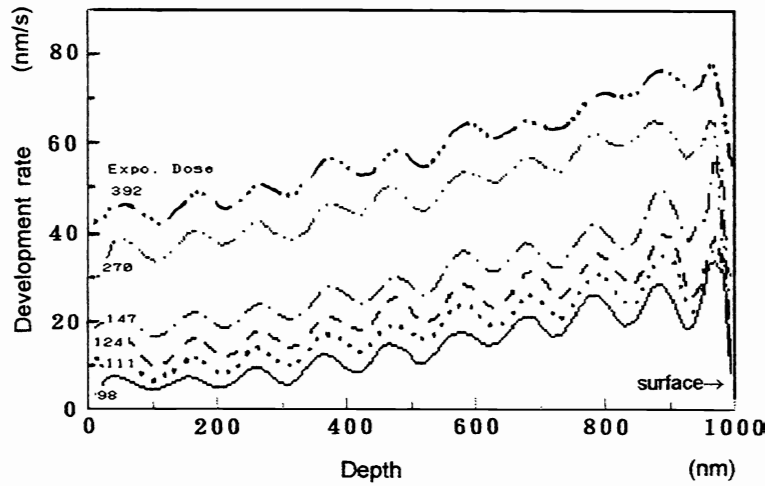


Fig. 8. Development rate distribution in depth direction.

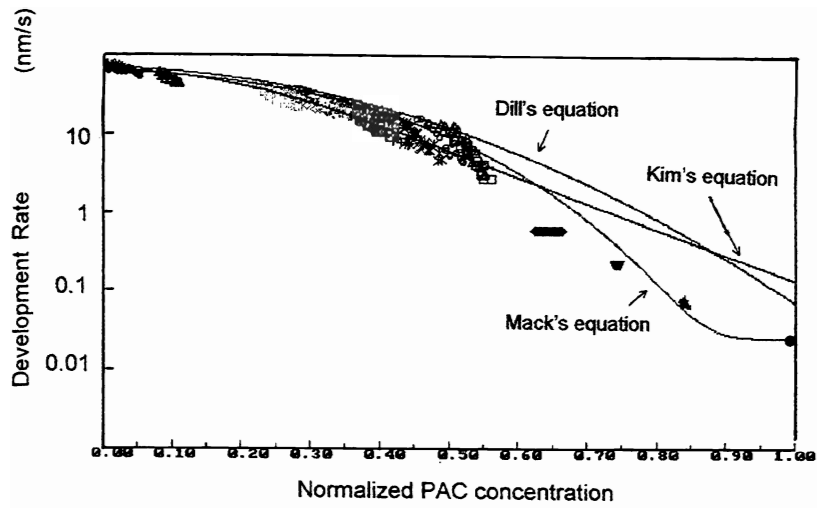


Fig. 9. Relationship between development rate and normalized PAC concentration for THMR-iP3000.

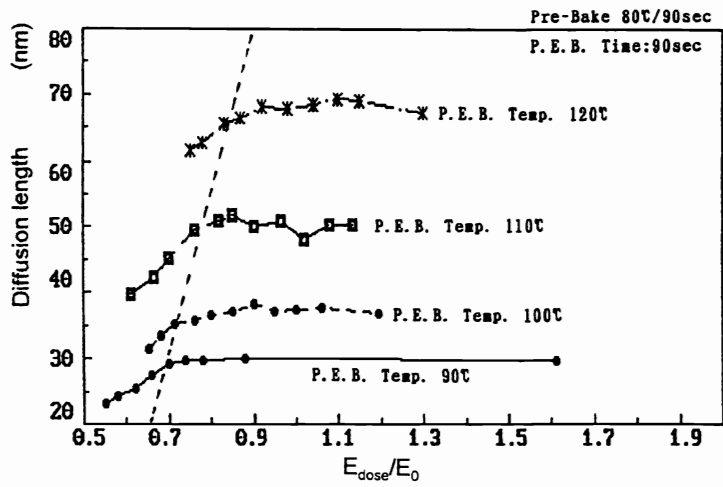


Fig. 10. Relation between diffusion length and E_{dose}/E_0

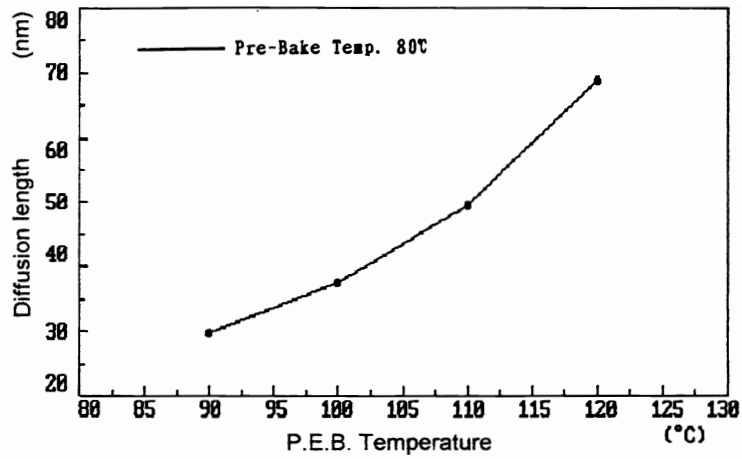


Fig. 11. Relation between diffusion length and PEB temperature.

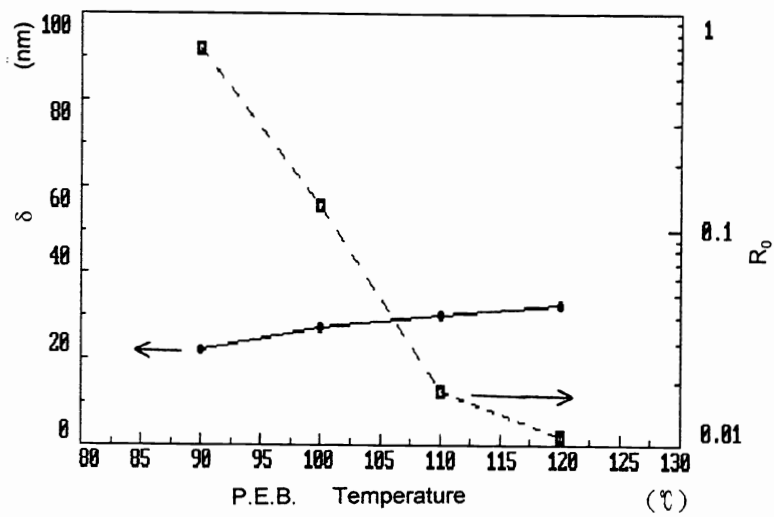


Fig. 12. Dependencies of δ and R_0 on PEB temperature.

P. E. B.		Defocus		
		$-0.6\mu\text{m}$	$\pm 0\mu\text{m}$	$+0.4\mu\text{m}$
90°C	SEM			
	PROLITH/2			
100°C	SEM			
	PROLITH/2			
110°C	SEM			
	PROLITH/2			
120°C	SEM			
	PROLITH/2			

Fig. 13. Comparison of simulation results for resist profiles with SEM observations.