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Extraction of Process Specific Photolithography Model Parameters

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ABSTRACT

In order to truly represent photolithography through simulation, the exposure, bake and development models and model parameters must be accurate. Models for the pre-bake, exposure, post-exposure/pre-development bake, and the development have been developed and are available with most commercial simulators.[1-5] The extraction of the exposure parameters has been established.[1-3] However, the extraction of the bake and development model parameters have been subject to question[6-13] given the immersion type development that has been required for the measurement of the development rate and henceforth the extraction of these parameters.

Using the approach for the measurement of the in-situ development rate, developed in the first paper of this two paper series, the model parameters were extracted for Shipley 812 resist with Shipley MF312 developer. Development rates for exposures of 66, 90 and 114mJ/cm^2 were measured. It was discovered that the set of Kim model parameters, R_1 through R_6, were highly correlated with the combination of the Dill exposure parameters. Thus, for A=0.581µm^{-1}, B=0.082µm^{-1}, C=0.013cm^2/mJ, the parameters R_1=25.559µm/min, R_2=10.451µm/min, R_3=1.879, R_4=0.112, R_5=1.586, R_6=0.000µm, and σ=0.0016µm were extracted. A comparison of simulated data using the extracted model parameters with the measured data demonstrated the quality of the fit.

1.0 INTRODUCTION

As the drive for smaller line-width geometries at the expense of increasing cost and process development time continues in semiconductor manufacturing, the value and convenience of accurate, process specific modeling parameters is becoming increasingly vital. Time and money invested up-front in the determination of the model parameters can be realized and compensated in subsequent process optimizations or process trouble-shooting.

In the case of the photolithographic transfer of a desired pattern onto the wafer surface, resist and development parameters have been obtained using the Perkin Elmer Development Rate Monitor (DRM).[6-13] The DRM requires an immersion development. This detracts from the validity of these parameters since production wafer processing is usually performed individually on a wafer track with a dispense or spray type development.

We propose a technique by which a set of model parameters can be extracted from in-situ measured development rates. Through simulation it was discovered that the set of exposure parameters were highly correlated with the combination of development parameters in terms of the resist image after development. As a result, the group of extracted parameters were reduced to a fundamental and independent set.

This parameter extraction was applied to the development rates calculated in the preceding paper of this two paper series. A comparison of the simulated development rate using the extracted model parameters and the development rate measured from the wafers demonstrated the success of this approach.

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2.0 METHOD

The extraction of photolithography model parameters presents a challenging predicament since there are four models serially contained within. Measurement the photo-active compound (PAC) concentration is not obtainable on the microscopic level, however, the PAC concentration can be obtained for the bulk resist using the resist transparency technique proposed by Dill.[2] This allows the exposure parameters to be extracted but unfortunately the effect of the pre-bake and post exposure bake (PEB) parameters on the PAC cannot be determined from this approach. Because the development models are provided in a closed form, the extraction of these parameters can be straightforward to obtain via non-linear regression algorithms. In order to do so, the PAC concentration as a function of depth in the resist must be known. Since the bake model parameters are not known, the PAC concentration is not available.

It was theorized that the development parameters were highly correlated with the exposure parameters in terms of the developed image. Given the development rate of the resist as a function of depth, an arbitrarily selected set of exposure parameters can be used to generate the PAC concentration as a function of depth in the resist. Then, the development rate parameters can be extracted using non-linear regression by iteratively searching for the appropriate parameters to match the calculated PAC to the measured development rate. In terms of the resist image after development, inaccurate exposure parameters are of little consequence since the development parameters have suitably compensated for them.

In order to substantiate this theory, the development rate versus depth in the resist was generated with an in-house one dimensional photolithography simulator. The first test examines the situation of an exposure and development but without either of the two bake simulations. The second test accommodates the pre-bake and PEB models in the parameter extraction approach.

Using the arbitrarily selected, though realistic parameters listed in table 1, the rate versus depth was simulated for three values of exposures (66, 90, and 114 mJ/cm^2) in order to obtain a larger range of development rates and to demonstrate the correlation of exposure and development parameters across a range of exposure doses.

Table 1: Parameters used to generate simulated development rates versus depth

Parameter	Value
A	0.5198 μm^{-1}
B	0.2700 μm^{-1}
C	0.014 cm^2/mJ
Resist thickness	1.10 μm
Refractive index magnitude	1.68
R_1	14.4 μm/min
R_2	0.03 μm/min
R_3	8.1
R_4	0.24
R_5	0.76
R_6	0.55 μm

In the same way that development rate data would be gathered from wafers subsequently in this research, the development rates were simulated as a function of depth in the resist for three different exposure doses. Three doses were chosen to accumulate a wide range of PAC concentrations, and although there already exists a range of PAC concentrations within a single wafer, three wafers guaranteed a wider range of values.

Extraction of the modeling parameters was pursued using the Marquardt-Levenberg algorithm[14-17] which uses a compromise of two separate techniques: steepest descent and a linearization. The linearization uses the first partial derivatives of the proposed model with respect to the extracted parameters to find the first two terms of the Taylor series expansion. For each new combination of R_1 through R_6, a new linear approximation of the non-linear model is established and operated on. As such, the first partial derivative with respect to the extracted model parameters was required. Since the Dill exposure model is not in a closed, analytic form, it cannot be inserted into the development model or in the bake models. This prevents nonlinear regression being used to extract these parameters, but this is of little consequence. Non-linear regression can be used to extract the parameters of the development models.

Given the development rates curves simulated with the data in table 1, development rate parameters were extracted assuming the exposure parameters, A=0.781μm^{-1}, B=0.082μm^{-1}, and C=0.013cm^2/mJ were correct. The program used for this extraction did not extract the PEB diffusion length constant since neither of the bakes were included in the simulation data. The parameter extraction was able to converge, the ANOVA table for which is given in table 2. Judging by the residual sum of squares, the parameter extracted from this routine provide an excellent fit to the simulated data. The extracted development rate parameters are listed in table 3 along with 95% confidence intervals where appropriate. Plots of the original simulated data and data simulated with the extracted set of parameters in figures1 through3 demonstrate the closeness of fit.

Table 2: ANOVA table for the extraction of model parameters. Development rate data was simulated using the parameters in table 1.

Source	DF	Sum of Squares	Mean Square
Regression	6	13473.597275	2245.599546
Residual	744	2.721391	0.003673
Uncorr. Total	750	13476.318667	

Table 3: Extracted parameters for the simulated development rate versus depth data

Parameter	Estimate	Asymptotic Std. Error	Asymptotic 95% CI Lower	Asymptotic 95% CI Upper
R1(µm/min)	13.914284	0.045504	13.824950	14.003618
R2(µm/min)	0.035789	0.000420	0.034965	0.036613
R3	8.357614	0.24256	8.309995	8.405233
R4	0.238234	0.003429	0.231503	0.244965
R5	0.803234	0.006400	0.790670	0.815797
R6 (µm)	0.487934	0.012305	0.463777	0.512091
A(µm-1)*	0.781			
B(µm-1)*	0.082			
C(cm^2/mJ)*	0.013			

* Assumed for extraction.

Next, it was necessary to incorporate the Mack pre-bake model and the PEB model. With a closer look at the pre-bake model, it was evident that the pre-bake model manifests itself as a modification of the Dill A and B parameters. Therefore, since the Dill parameters are highly correlated with the combination of development parameter, for a given set of pre-bake conditions, the pre-bake can be removed from consideration for the parameter extractions.

If the PEB conditions are fixed, only one parameter, the PEB diffusion length constant, σ, is required for the PEB model if time and temperature are constant. The extraction of σ is straightforward since it is the only parameter outside of the closed form of the development models. A practical approach for the search on the value of was to perform a three point minimization of the develop model regression SSE.

Table 4: Simulation parameters for the generation of development rate data. Simulation included both the pre-bake and the PEB models.

Parameter	Value
A	0.5198 μm^{-1}
B	0.2700 μm^{-1}
C	0.014 cm^2/mJ
R_1	14.4 $\mu m/min$
R_2	0.03 $\mu m/min$
R_3	8.1
R_4	0.24
R_5	0.76
R_6	0.55 μm
Resist thickness	1.1 μm
Refractive index magnitude	1.68
$E_{a\text{-pre-bake}}$	29.5 Kcal/mol
$\ln(A_r)$	35.3 $\ln(min^{-1})$
f_{PAC}	1.5
$E_{a\text{-PEB}}$	62.0 Kcal/mol
ln(Do)	87.5 $\ln(nm^2/min)$
Pre-bake time	0.5 min
Pre-bake temperature	363 Kelvin
PEB time	0.5 min
PEB temperature	363 Kelvin

The three point minimization was performed as follows. First upper and lower limits for the parameter to be estimated are established. The SSE for the two limits and for the median between the two limits are found. The range between a limit and the median is successively cut in half by finding the SSE for the fit of the development model when the mean of the two σ's is

used. If the new SSE is lower than the SSE for the median, then the median was modified. Otherwise, the limit was modified. Eventually, the limits have been paired down to a reasonable tolerance which is the best estimate. The initial lower limit of σ can be taken to some very small value, slightly
larger than zero. An upper limit was selected based upon the periodicity of the standing wave effect.

Using the parameters listed in table 4, a simulation of development rates for three different exposures was performed as above, but this time it incorporated the pre-bake and PEB models.

Development parameters R_1 through R_6 were extracted assuming values for A, B, and C of 0.781μm^{-1}, 0.082μm^{-1}, and 0.013cm^2/mJ respectively. The exposure parameters used to generate the development rate data were intentionally different from the exposure parameters in the extraction to demonstrate that they may be selected arbitrarily. The ANOVA table for the non-linear regression of the development model is given in table 5. It was worth noting, the agreement in the fit of the data as is evident by the very small SSE. A value for σ of 0.02406μm was found with the extraction routine. The extracted values are listed in table 6 along with confidence intervals where applicable.

Table 5: ANOVA table for the extraction of model parameters from simulated data. Simulated data included the pre-bake and PEB models.

Source	DF	Sum of Squares	Mean Square
Regression	6	6731.065291	1121.844215
Residual	744	2.065702	0.002788
Uncorr. Total	750	6733.130993	

Table 6: Extracted parameters from simulated development rate vs. depth. Simulation included pre-bake and PEB models.

Parameter	Estimate	Asymptotic Std. Error	Asymptotic 95% CI Lower	Asymptotic 95% CI Upper
R_1 (μm/min)	13.531180	0.118355	13.298824	13.763536
R_2 (μm/min)	0.037330	0.000467	0.035925	0.038246
R_3	8.152274	0.029600	8.094163	8.210385
R_4	0.266616	0.007312	0.252262	0.280970
R_5	0.781953	0.013353	0.755737	0.804356
R_6(μm)	0.709424	0.017686	0.670758	0.740200
A(μm^{-1})*	0.781			
B(μm^{-1})*	0.082			
C(cm^2/mJ)*	0.013			

These extracted values were then used to simulate the development rate as a function of depth for comparison with the original development rate data. In figures 4 through 6, both plots of development rate versus depth are shown to demonstrate that the resist image after development is virtually the same.

Hence, for the extraction of the modeling parameters of the resist image after development, given a proposed A, B, and C and a known refractive index for the resist, only the development rate parameters and the PEB diffusion length constant need to be extracted to sufficiently model the resist.

3.0 APPLICATION

In order to examine the applicability of this technique to real-life photolithography, the model parameters for DNQ/Novolac positive Shipley 812 resist with Shipley MF312 developer were sought. Three wafers were coated with about 1.2μm of resist. Wafers were exposed with GCA 6700 G-line stepper with 66, 90 and 114 mJ/cm^2 each. All three wafers were pre-bake and PEB at 100C for 45sec. A patterned reticle was chosen to demonstrate that the in-situ development rate can be measured from patterned resist. Exposure parameters used for the extraction were taken from Finle Technology's Prolith photolithography simulator for Shipley System 8 resist at 436nm. These parameters were A=0.581μm-1, B=0.082μm-1, and C=0.013cm^2/mJ. The ANOVA for this regression is given in table 7 and the converged parameter set was listed in table 8.

Table 7: ANOVA table for the extraction of model parameters for Shipley 812 resist.

Source	DF	Sum of Squares	Mean Square
Regression	6	72280.498519	12046.749753
Residual	391	2412.489870	6.170051
Uncorr. Total	397	74692.988389	

Table 8: List of parameter estimates for Shipley 812 resist

Parameter	Estimate	Asymptotic Std. Error	Asymptotic 95% CI Lower	Asymptotic 95% CI Upper
R1 (μm/min)	25.559337	2.295053	21.047083	30.071591
R2 (μm/min)	10.451110	0.311492	9.838692	11.063528
R3	1.878882	0.477362	0.940351	2.817413
R4	0.111717	0.013289	0.085590	0.137844
R5	1.586487	0.136965	1.317203	1.855771
R6 (μm)	0.000000	0.046279	-0.090989	0.090989
A (μm^{-1})	0.581**			
B (μm^{-1})	0.082**			
C (cm^2/mJ)	0.013**			
σ (μm)	0.0016			

** Estimates were taken from Finle Technology's Prolith software for Shipley System 8 resist at G-line exposure.

Using the extracted parameters in table 8 and the conditions used for processing the wafers, the development rates were simulated in order to verify the extraction routine. Plots of the development rates, simulated and measured are given in figures 7 through 9. All three plots appear to fit, particularly for the upper portions of the resist layer. It should be emphasized that only depths less than 0.7µm were used for the extraction since there is less confidence in the measured results for the bottom 0.4µm of resist.

It appears as if the models used for the simulation perhaps do not sufficiently describe the development mechanisms. For all three exposures, the predicted development rate does not seem to oscillate as far as the measured data. The predicted localized minima in the standing wave effect appears to be higher than the measured data. On the other hand the predicted maxima is lower than the measured data. Clearly, a more extensive analysis of the exposure, bake and development models needs to be performed in order to discern model inadequacies or bias from anomalous behavior.

4.0 CONCLUSION

The value and convenience of a process specific simulation model is advantageous for timely process development. A method was proposed by which process specific modeling parameters can be extracted for photolithography modeling.

Next a one-dimensional photolithography simulator was used to examine the relationship between model parameters. A difficult challenge was presented in how to extract the exposure parameters, but after simulation it was discovered that the set of exposure parameters were highly correlated with the development parameters. This meant that for a proposed set of exposure parameters, regardless of the accuracy, a set of development parameters could be extracted that would describe the resist profile after development.

With this extraction approach in mind, the parameters for Shipley 812 resist were extracted. It was found that for a proposed A = $0.581\mu m^{-1}$, B = $0.082\mu m^{-1}$, and C = $0.013 cm^2/mJ$, the development parameters, R1 = 25.559µm/min, R2 = 10.451µm/min, R3 = 1.879, R4 = 0.112, R5 = 1.586, R6 = 0.000µm, and = 0.0016µm, were found. A plot comparison of measured and simulated development rate demonstrated the closeness of the simulation fit. The models appear to fit to the first order but a more extensive evaluation is required to examine model adequacy.

5.0 ACKNOWLEDGEMENTS

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6.0 REFERENCES

1. F. H. Dill, "Optical Lithography," Trans. Electron Dev., Vol. ED-22, No. 7, (July 1975) pp. 440-444.

2. F. H. Dill, W. P. Hornberger, P. S. Hauge, J. M. Shaw, "Characterization of Positive Photoresist," Trans. Electron Dev., Vol. ED-22, No. 7, (July 1975) pp. 445-452.

3. F. H. Dill, A. R. Neureuther, J. A. Tuttle, E. J. Walker, "Modeling Projection Printing Positive Photoresists," Trans. Electron Dev., Vol. ED-22, No. 7, (July 1975) pp. 456-464.

4. C. A. Mack, "Modeling the Effects of Prebake on Positive Resist Processing," Kodak Microelec. Interface '85 (Nov. 1985) pp. 155-158.

5. C. A. Mack, "A Diffusion Model for Post-Exposure Bake," source unknown.

6. P. D. Flanner III, "Semi-automated Measurements of Photoresist Optical Parameters," Philips Research Laboratories, internal technical report.

7. P. D. Flanner III, "Improved Methods of Photoresist Development Characterization," Philips Research Laboratories, internal technical report.

8. M. Exterkamp, W. Wong, H. Damar, A. R. Neureuther, C. H. Ting, W. G. Oldham, "Resist Characterization: Procedures, Parameters, and Profiles," Optical Lithography, SPIE Vol. 334 (1982) pp. 182-187.

9. C. Zee, W. R Bell, A. R. Neureuther, "Effect of Developer Type and Agitation on Dissolution of Positive Photoresist," Adv. in Resist Tech. and Processing V, Proc., SPIE, Vol. 920, (1988) pp. 154-161.

10. W. R. Bell II, P. D. Flanner II, C. Zee, N. Tam, A. R. Neureuther, "Determination of Quantitative Resist Models from Experiment," Adv. in Resist Tech. and Proc. V, Proc., SPIE, Vol. 920, (1988) pp. 382-389.

11. A. S. Chiu, et al., "Resist Parameter Extraction (PARMEX) with Graphical Interface in X," Adv. in Resist Tech. and Proc. VIII, Proc., SPIE, Vol. 1466, (1991) pp. 641-652.

12. R. A. Ferguson, et al., "Modeling and Simulation of Multiple Chemical States in Photoresist Materials," Adv. in Resist Tech. and Proc. VI, Proc., SPIE, Vol. 1086, (1989) pp. 262-273.

13. C. A. Spence, R. A. Ferguson, "Some Experimental Techniques for Characterizing Photoresists," Adv. in Resist Tech. and Proc. VIII, Proc., SPIE, Vol. 1466, (1991) pp. 324-335.

14. N. R. Draper, H. Smith, Applied Regression Analysis, John Wiley and Sons, New York, 1981, pp. 458-517.

15. G. A. F. Seber, C. J. Wild, Nonlinear Regression, John Wiley and Sons, New York, 1989.

16. SAS/STAT User's Guide, Version 6, Fourth Edition, Volume 2, SAS Institute, Cary, NC, 1990, pp. 1135-1193.

17. D. W. Marquardt, "An Algorithm for Least-Squares Estimation of Nonlinear Parameters," J. Soc. Indust. Appl. Math., Vol. 11, No. 2, (June 1963) pp.
431-441.

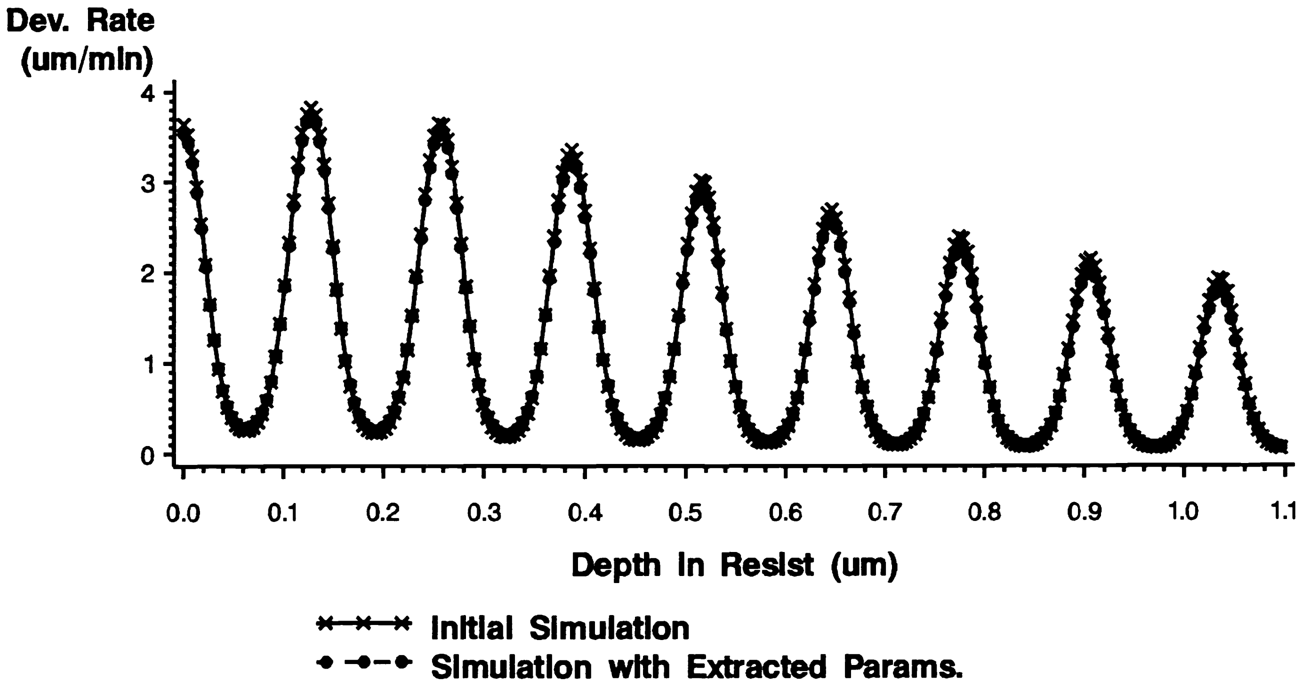

Figure 1: A comparison of simulations. The first simulation was performed on an arbitrarily selected group of parameters and the second used the extracted model parameters from the first. Dose = 66mJ/cm2. No prebake or PEB.

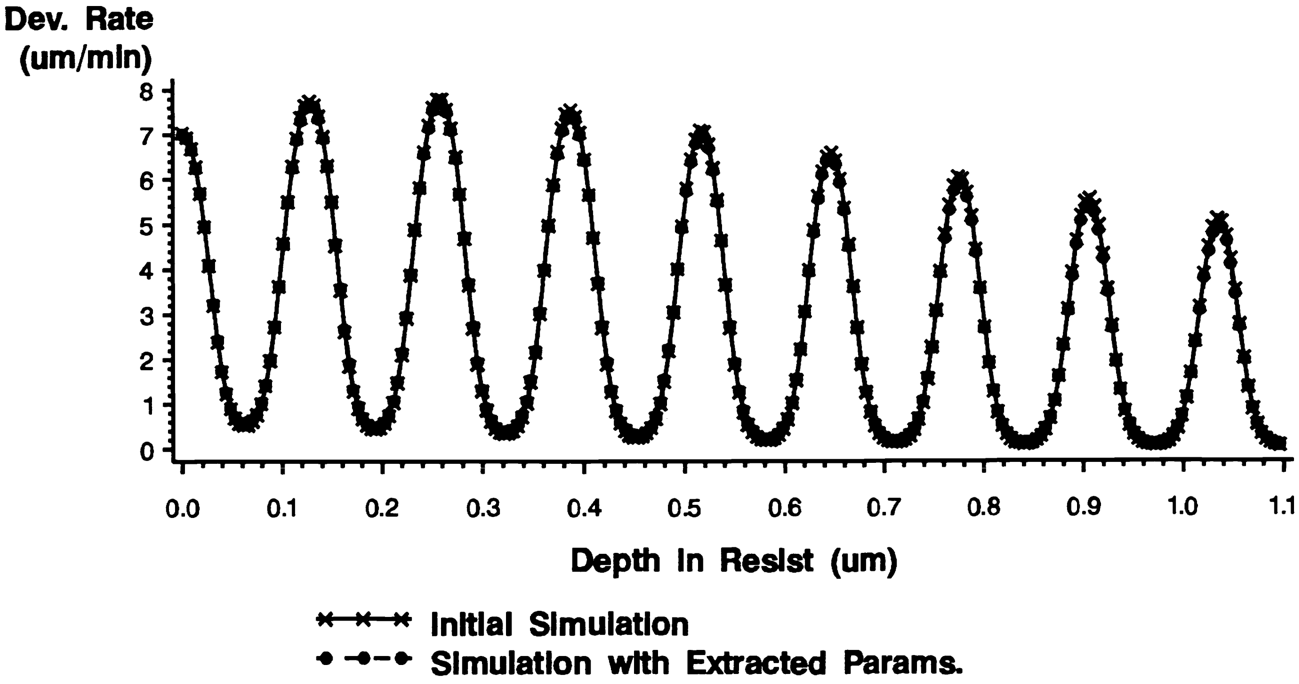

Figure 2: A comparison of simulations. The first simulation was performed on an arbitrarily selected group of parameters and the second used the extracted model parameters from the first. Dose = 90mJ/cm2. No prebake or PEB.

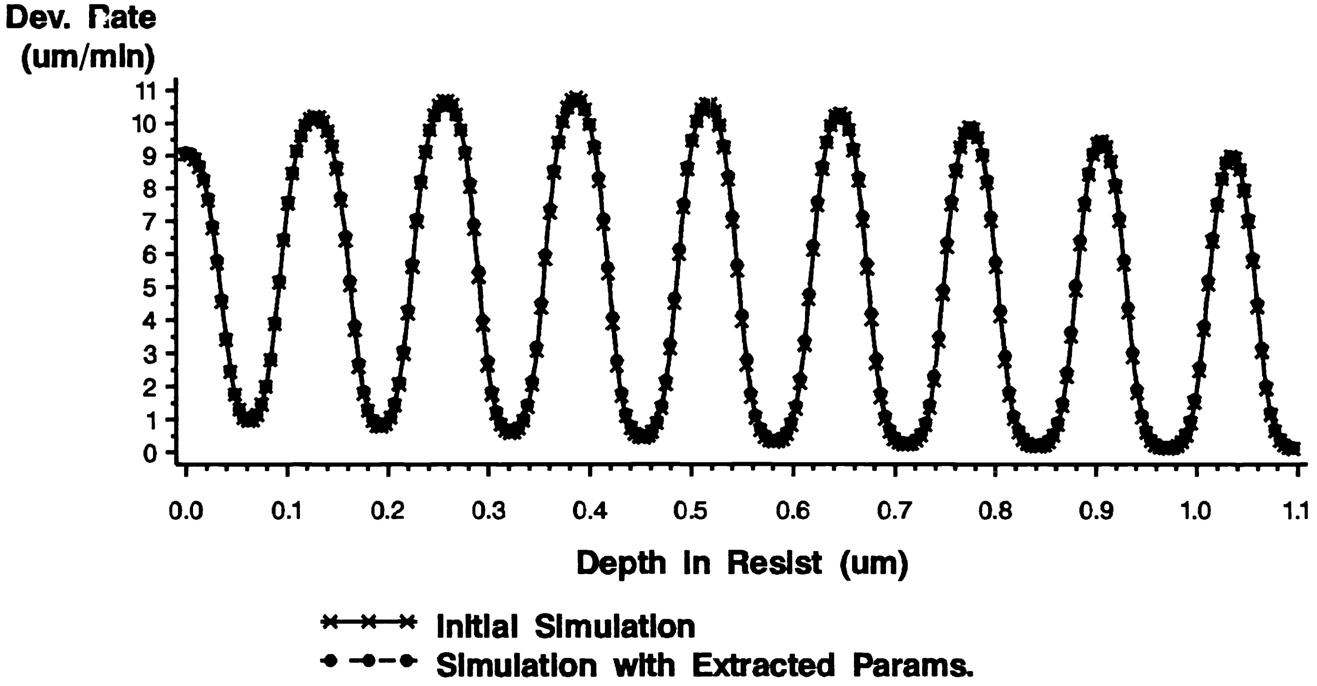

Figure 3: A comparison of simulations. The first simulation was performed on an arbitrarily selected group of parameters and the second used the extracted model parameters from the first. Dose = 114mJ/cm2. No prebake or PEB.

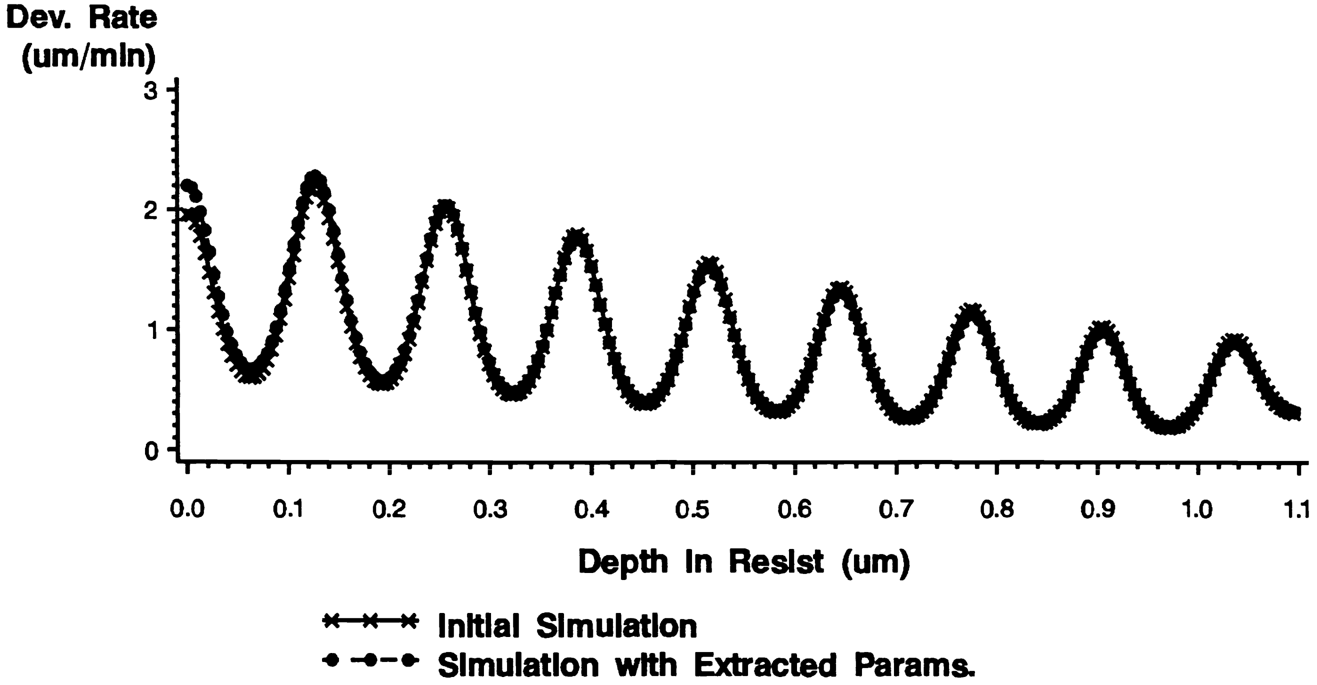

Figure 4: A comparison of simulations. The first simulation was performed on an arbitrarily selected group of parameters and the second used the extracted model parameters from the first. Dose = 66mJ/cm2. See tables 4 and 6 for conditions.

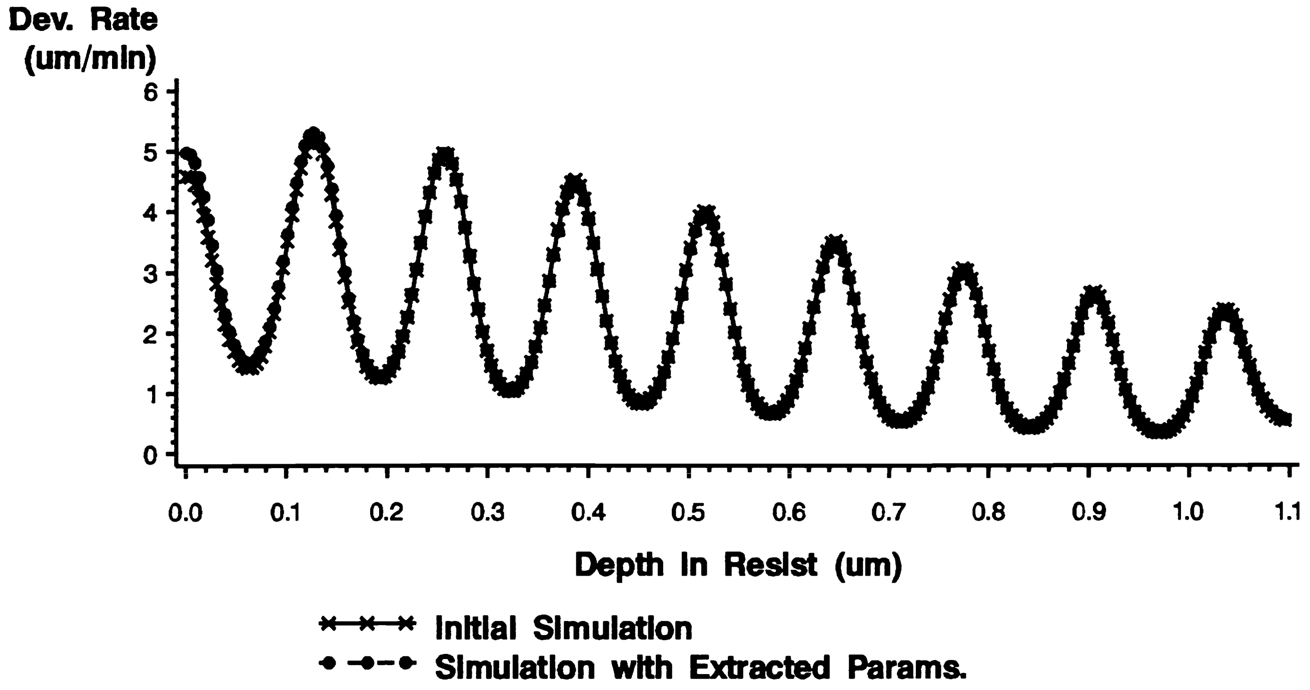

Figure 5: A comparison of simulations. The first simulation was performed on an arbitrarily selected group of parameters and the second used the extracted model parameters from the first. Dose = 90mJ/cm2. See tables 4 and 6 for conditions.

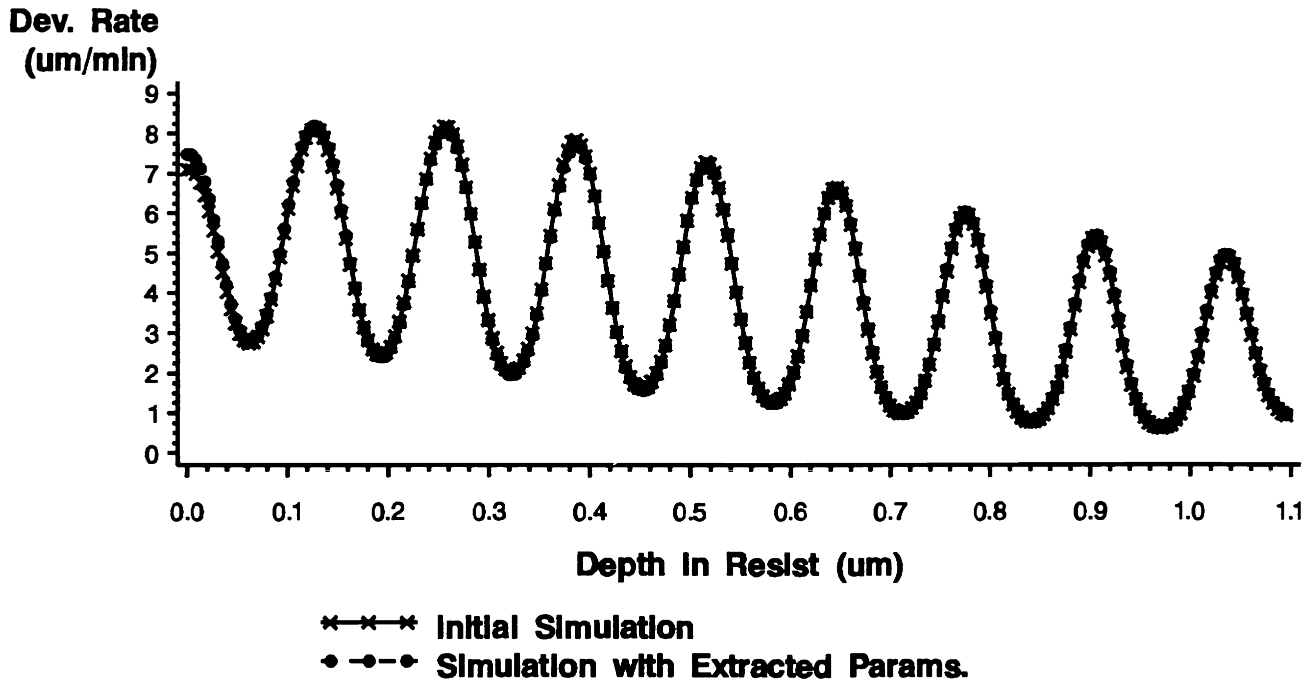

Figure 6: A comparison of simulations. The first simulation was performed on an arbitrarily selected group of parameters and the second used the extracted model parameters from the first. Dose = 114mJ/cm2. See tables 4 and 6 for conditions.

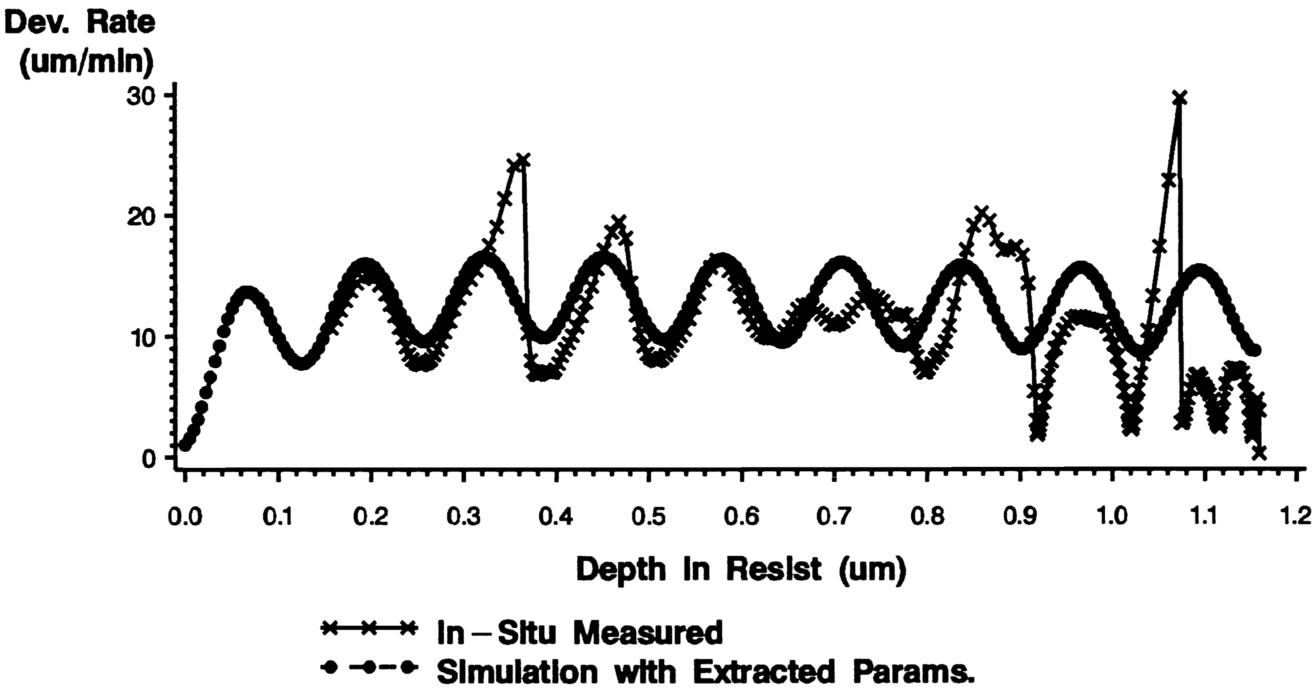

Figure 7: A comparison of the measured development rate from the first paper in this series with simulated development rate using the extracted parameters listed in table 8. Dose = 66mJ/cm2.

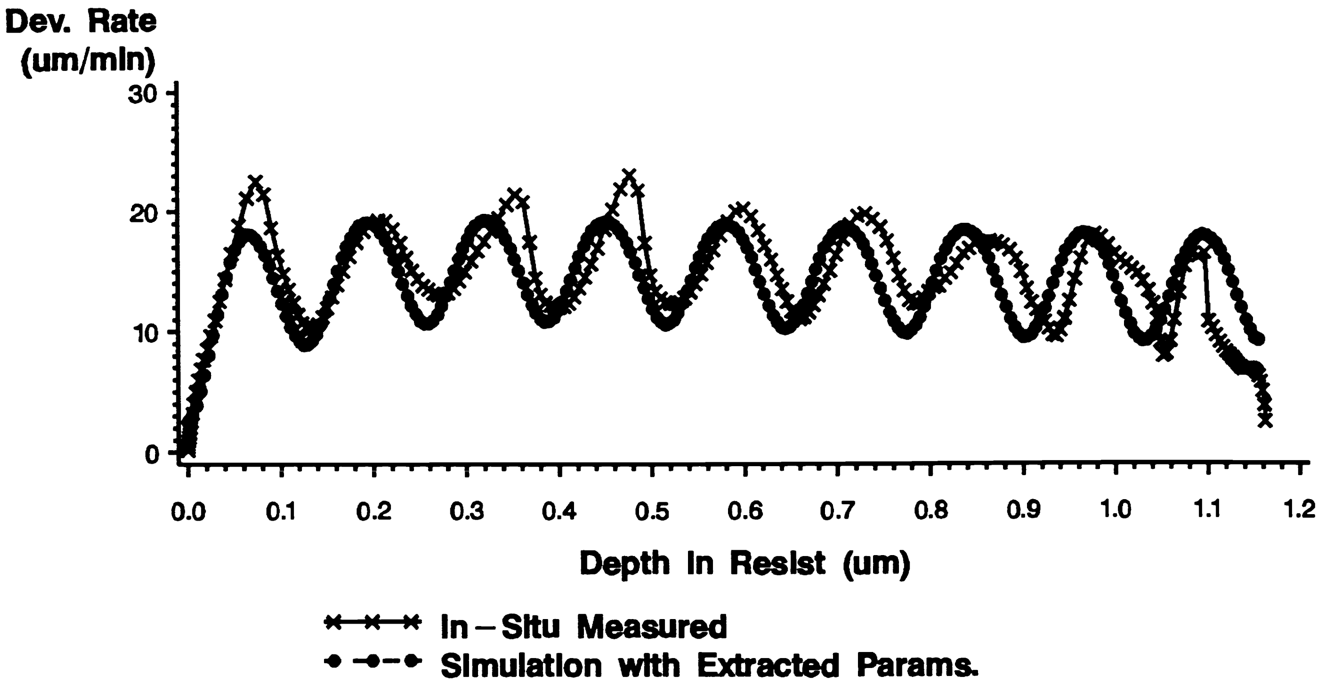

Figure 8: A comparison of the measured development rate from the first paper in this series with simulated development rate using the extracted parameters listed in table 8. Dose = 90mJ/cm2.

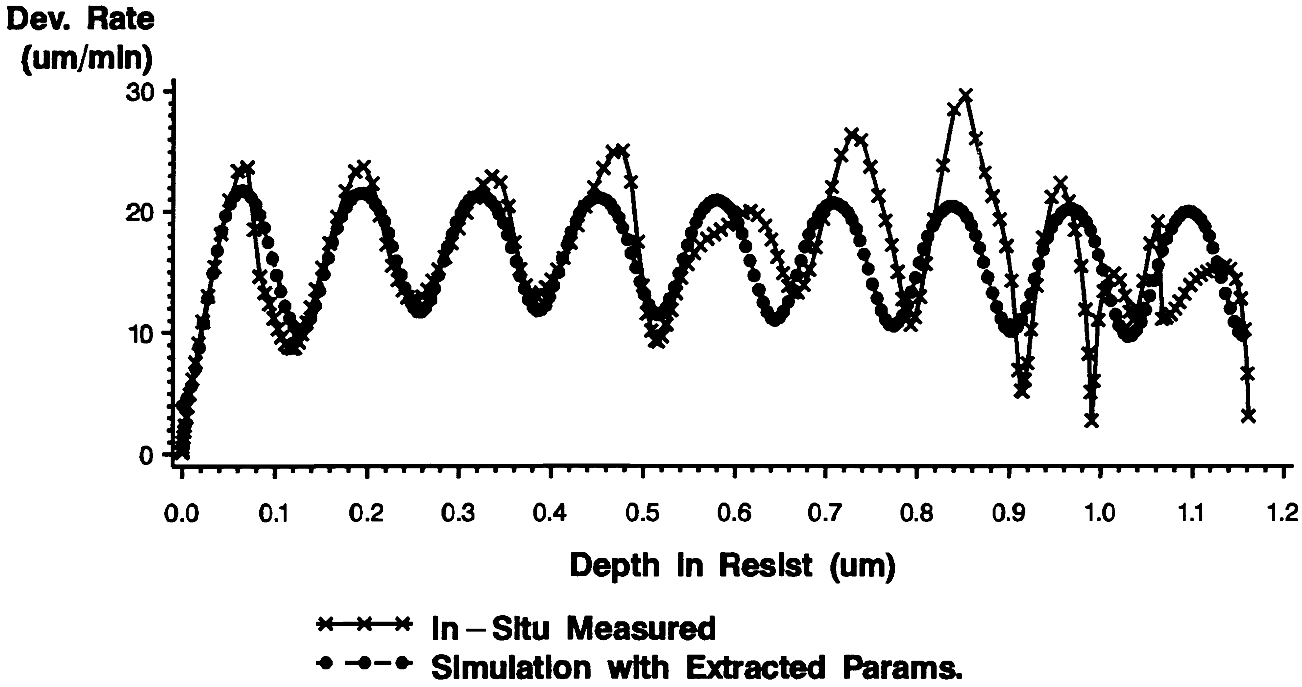

Figure 9: A comparison of the measured development rate from the first paper in this series with simulated development rate using the extracted parameters listed in table 8. Dose = 114mJ/cm2.