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Microelectronic Engineering 61–62 (2002) 89–95

MICROELECTRONIC ENGINEERING

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Abstract

In this paper a systematic approach to calibrating resist parameters will be provided. The calibration procedure couples nonlinear least squares fitting algorithms with a lithography simulator to achieve the best match between lithographic data and simulation. The importance of calibrating resist parameters using multiple data sets to achieve a unique and predictive model will be discussed. Several examples will be given for chemically amplified resists. © 2002 Published by Elsevier Science B.V.

Keywords: Calibration; Resist parameters; Lithography simulator

0167-9317/02/$ – see front matter
PII: S0167-9317(02)00438-0

Automatic Calibration of Lithography Simulation Parameters Using Multiple Data Sets

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In this paper a systematic approach to calibrating resist parameters will be provided. The calibration procedure couples nonlinear least squares fitting algorithms with a lithography simulator to achieve the best match between lithographic data and simulation. The importance of calibrating resist parameters using multiple data sets to achieve a unique and predictive model will be discussed. Several examples will be given for chemically amplified resists.

1. Introduction

For many applications, lithography simulation has proven extremely effective at predicting or explaining important lithographic trends, providing insight and direction for problem solving, and extrapolating lithographic technology into the future. For some applications, however, the usefulness of lithography simulation depends on its ability to quantitatively match experimental results for a specific process.

When simulation and experiment do not match, there are three possible reasons. First, the experimental results could be wrong due to setup, process, and/or measurement errors. Second, the models used in the simulator may not adequately describe the physical realities present in the experiment. And third, the input parameters used for the simulation may not adequately describe the experimental conditions. Of these three, incorrect input parameters is by far the most common source of simulation to experiment mismatch in optical lithography modeling.

Over the past decade fairly accurate physical models have been developed to describe chemically amplified resist processing. Unfortunately, these models have up to 25 physical parameters. Every parameter must be set to the appropriate value or errors in the simulations may result. Most semiconductor manufacturing facilities do not have the specialized capability to measure each parameter individually and therefore rely on resist vendors, universities, or other sources for resist parameters. Also, because of process (developer temperature, etc.) and tool variability (dose calibration, film thickness methods, etc.) some of the known resist parameters do not transfer perfectly from one facility to another. Therefore, parameters measured at a resist vendor's site often must be calibrated before simulation results can be obtained that match processes elsewhere. The purpose of this work is to show how users of lithography simulation tools can calibrate resist parameters for a given resist using standard lithographic data obtained from the target manufacturing process and toolset.

Recently, a systematic approach to matching simulation to experiment for a given process, called "tuning" the model, was proposed [1-3]. This approach was based upon the systematic but manual adjustment of individual parameters to match certain prescribed experiments. It is reliable for only a few of the resist model parameters. Subsequently, the number of different dataset types and adjustable parameters was expanded by the implementation of numerical algorithms to perform the tuning process [4]. In this paper, the approaches described earlier will be expanded. A systematic approach to calibrating specific parameters for chemically amplified resists will be provided. Very importantly, the ability of a simulator to match multiple sets of experimental data (different numerical apertures, multiple pitches, different feature types, etc.) with one set of simulation parameters enables many important applications of simulation that go beyond trend analysis. In this paper, the ability to match multiple data sets will be explored under a wide range of conditions.

2. Model Calibration Procedure

The systematic and automated calibration of simulation parameters requires adoption of a metric that measures the agreement between experimental and simulation data as well as the algorithms that improve the agreement with data for a given set of simulation parameters. The standard approach is to use the chi-squared (χ^2) function to determine the "goodness of fit" connecting real and modeled data. χ^2 is expressed as

$$c^2(\mathbf{a}) = \sum_{i=1}^{N}\left[\frac{y_i - y(x_i,\mathrm{a})}{s_i}\right]^2 \qquad (1)$$

where N = number of data points,
$\{y_i,x_i\}$ = the experimental data set
y = predicted value
$\mathbf{a}$ = the simulation parameter set
s_i = the uncertainty between y_i and the true data point.

The goal is to minimize χ^2, which in turn equates to better agreement between real and simulated data. The methods introduced in the previous work [4] minimize the merit function in equation (1) using standard nonlinear optimization algorithms and a lithography simulation package to calculate the predicted value $y(x_i,\mathrm{a})$. An acceptable solution is found when the RMS deviation between the simulation and experimental data is on the order of or less than the expected noise in the experimental dataset.

When fitting a single dataset such as an FE matrix for a single feature size and pitch it is observed that typically more than one acceptable solution exists. This is a result of the dataset not sampling enough parameter space to distinguish the multiple solutions. An error can then arise when the resulting "calibrated" model is applied to another input condition (e.g., a different pitch or stepper setting). The model calibration is under-determined for the range of data sampled. This situation is analogous to fitting a straight line through a single point or several closely spaced but noisy data points. More data points covering a larger range must be added to determine the unique model parameters describing the given process with reasonable certainty.

This problem is illustrated for lithography simulation in Figures 1 and 2. In Figure 1 the Focus-Exposure data for an isolated line is shown with a simulation of the process using modeling parameters calibrated using only this dataset. The agreement between the simulation and experimental data is good considering the expected repeatability of the data. Unfortunately, when this set of parameters is used to simulate a dense feature image with the same resist and compared to experiment the result is shown in Figure 2. As can be seen the simulation has considerable mismatch with the experimental data (especially for low doses). By calibrating to more than one dataset this problem can be alleviated.

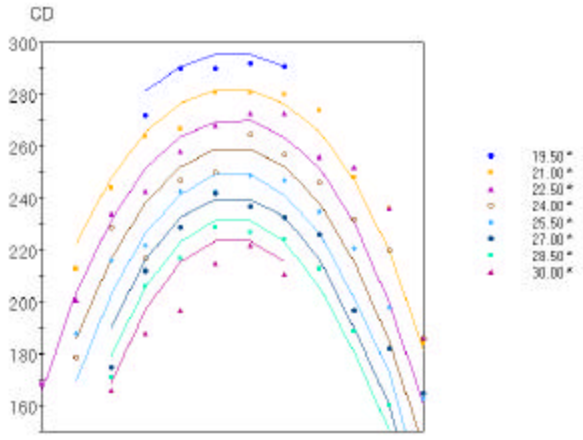

Figure 1: Comparison of isolated line experimental Focus-Exposure data with simulation results using parameters calibrated using only this dataset.

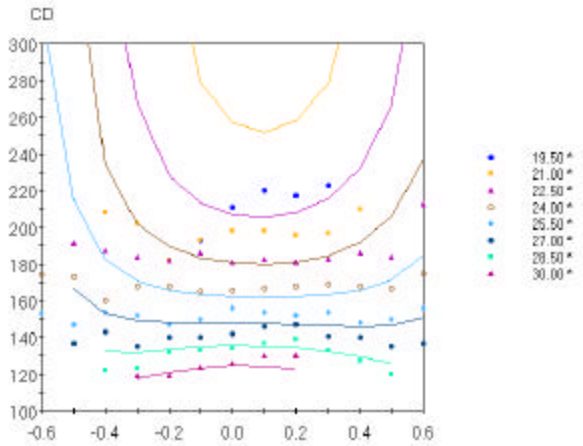

Figure 2: Comparison of 180 dense line experimental focus-exposure data with simulation results using parameters calibrated from the isolated line data of Figure 1.

3. Tuning Examples

In this section two examples of resist model calibration are demonstrated using coupled fits of Focus Exposure matrix data for isolated and dense features. The first example demonstrated is for the JSR KrF resist M91Y.

The lithographic data was obtained using a 0.63NA KrF stepper and 0.8/0.4 annular illumination. The mask was a chrome on quartz binary mask. The isolated features were 300nm (wafer dimension) and the dense features were 180nm/360nm pitch. Both PAB and PEB temperatures were 130°C for 90s. The substrate used was an optimized inorganic ARC stack. The resist thickness was 415nm.

For calibration the optical parameters were fixed at A = 0, B = 0.9μm^{-1}, n = 1.78. These parameters were obtained from a separate calibration using CD swing curve data. The base quencher loading was also fixed at 0.1 relative to the PAG loading. Because the PEB temperature was held fixed the activation energy parameters for diffusivity and deprotection were held constant at 25.869 kcal/mol and not adjusted. The develop model was chosen to be the Original Mack model with R_{max} = 1090nm/s, R_{min} = 0.11nm/s, and m_{th} = 0.67.

Selecting the correct resist parameters to calibrate is an important first step. The parameters chosen for calibration were acid yield C, Diffusion Coefficient pre-exponential $\ln(Ar_D)$, Deprotection Rate pre-exponential $\ln(Ar_a)$ and Develop Contrast R_n. These parameters are the standard set of parameters most commonly used for calibrating to FE matrix data from chemically amplified resists. The initial values were C = 0.07cm^2/mJ, $\ln(Ar_D)$ = 36.0, $\ln(Ar_a)$ = 27.8 and R_n = 8.0, which yield the results shown in Figures 1 and 2.

By simultaneously minimizing the combined χ^2 of the fit to both data sets (dense and isolated features), multiple data set tuning was achieved. The final optimized parameters obtained were C = 0.043, $\ln(Ar_D)$ = 35.62, $\ln(Ar_a)$ = 29.0 and R_n = 15.65. The resulting agreement between simulation and experiment for both datasets is quite good as shown in Figures 3 and 4.

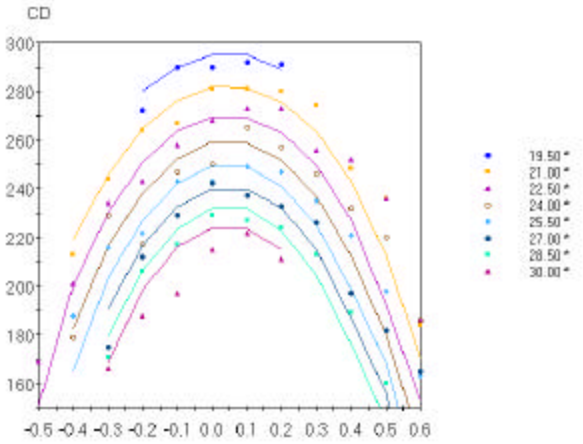

Figure 3: Comparison of experimental Focus-Exposure data with the multi-data set calibrated simulation results for 300nm isolated lines using M91Y photoresist.

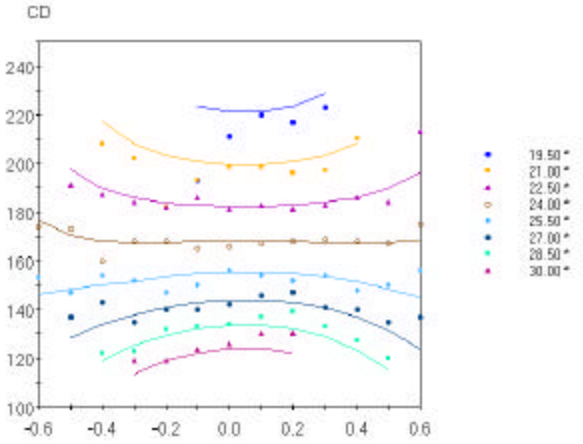

Figure 4: Comparison of experimental Focus-Exposure data with the multi-data set calibrated simulation results for 180nm nested lines using M91Y photoresist.

The second calibration example using multiple datasets involved the Shipley trench/contact hole KrF resist UV210. The lithographic data was obtained using a 0.7NA KrF stepper and 0.85 sigma partially coherent illumination. The mask was a chrome on quartz binary mask. The isolated features were 160nm (wafer dimension) trenches and the dense features were 160nm trenches at 320nm pitch. Both PAB and PEB temperatures were 130°C for 90s. The substrate used was Shipley organic ARC AR2 on silicon. The resist thickness was 393nm.

When calibrating a new resist, a common approach is to start with parameters from a similar resist. In this case, the optical parameters were initially fixed at A = 0, B = 0.5, n = 1.746, values previously measured for UV6, a similar resist manufactured by Shipley. The base quencher loading was also fixed at 0.16 relative to PAG. As with the M91Y case the activation energy parameters were held constant. The develop model was chosen to be the Original Mack model with R_{max} = 4050nm/s, R_{min} = 0.4nm/s, and m_{th} = 0.6. These values are similar to those found for UV6.

The parameters originally chosen for calibration were acid yield C, Diffusion Coefficient pre-exponential $\ln(Ar_D)$, Deprotection Rate pre-exponential $\ln(Ar_a)$ and Develop Contrast R_n. The initial values were C = 0.063, $\ln(Ar_D)$ = 33.0, $\ln(Ar_a)$ = 27.0 and R_n = 23.0. After calibration failed to yield reasonable agreement for both datasets simultaneously the absorbance parameter B was allowed to fluctuate from its initial guess of $0.5\mu m^{-1}$.

With this change the calibration converged to a satisfactory solution as shown in Figures 5 and 6. The final optimized parameters obtained were C = 0.0375, $\ln(Ar_D)$ = 31.55, $\ln(Ar_a)$ = 27.023, R_n = 34.4 and B = 0.38.

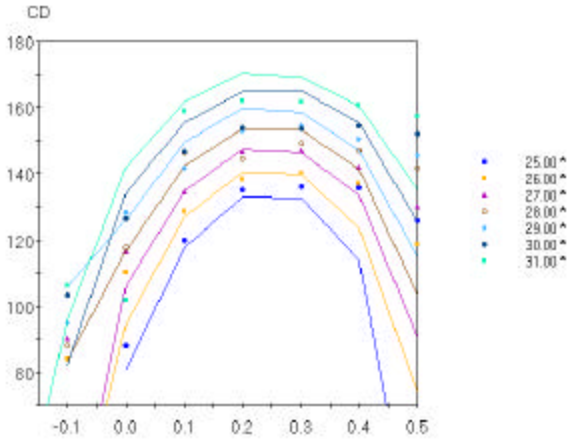

Figure 5: Comparison of experimental Focus-Exposure matrix CD data with the multi-data set calibrated simulation results for 160nm isolated trenches using UV210 photoresist and the process conditions given in text.

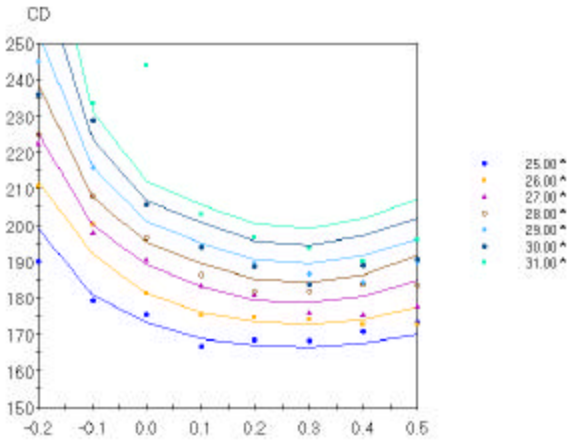

Figure 6: Comparison of experimental Focus-Exposure matrix CD data with the multi-data set calibrated simulation results for 160nm dense trenches using UV210 photoresist and the process conditions given in text.

4. Conclusions

As has been shown, resist parameters can be calibrated using measured lithographic data. However, the quantitative predictive capability of any set of parameters calibrated from a single dataset is suspect. It is important to use several datasets that sample different regions of parameter space. A good start is to use both isolated and dense feature Focus–Exposure data to calibrate the resist model.

5. References

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