Accuracy of 3-D Optical Lithography Simulation for Advanced Reticles

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Optical lithography over the next few product generations will demand the use of various types of advanced reticles (OPC, attenuated phase shift, alternating phase shift, etc.). Planning for these generations relies ever more heavily on simulation to make intelligent choices among the options in exposure wavelength, numerical aperture, reticle type and design, etc. Simulation of resist exposures of 2-dimensional reticle patterns becomes increasingly important, since some 2-D reticle patterns (and resulting 3-D resist patterns) are crucial to the device structure and at the same time the most sensitive to resolution limitations.

Simulation of arbitrary 2-D mask structures is also a much more difficult task than for 1-D reticle patterns, requiring not only more computing power but more complex algorithms. These structures pose a severe challenge to the calibration of a simulation tool: however, this is also an opportunity to make a simulation program more useful by demonstrating more predictive power.

We present experimental data and simulations illustrating progress towards calibration accuracy on some key 3-D resist patterns for a 0.25 μm lithography process. Careful calibration of the model provides for accurate simulation under a wide variety of conditions, thus allowing the use of simulation for critical feature mask design.

Introduction :

As leading edge manufacturing lithography progresses from 0.35 μm minimum feature sizes to 0.25 μm, 0.18 μm and 0.15 μm over the next few years, required improvements in feature resolution will actually outstrip the progress in optical lithography tools. Traditionally, reductions in minimum feature size have been accomplished through decreasing exposure wavelength and increasing lens numerical aperture (NA) according to the well known Rayleigh relation :

$$\text{minimum feature size} = k_1 \lambda / NA$$

This scaling rule essentially defines k_1 as a parameter indicating the "difficulty" of the lithographic process : i.e., the smaller k_1, the more difficult the process. The progress in recent process generations has resulted from wavelength reductions from 436 nm (mercury g-line) to 365 nm (mercury i-line) to 248 nm (KrF excimer laser), and increasing lens numerical apertures to 0.6 or higher.

The next few process generations will have the benefit of further NA increases to around 0.7, and the availability of 193 nm (ArF excimer laser) exposure systems. However, as shown in Figure 1, even with these changes k_1 decreases steadily over the next few years, to a value of 0.47 that would have been considered totally impractical for manufacturing 10 years ago. Enor-

mous efforts have been made in all areas to cope with this increasing "difficulty" : improved process controls, the introduction of scanners to reduce the impact of lens aberrations, off-axis illumination methods, and higher contrast chemically-amplified resists, to name a few.

New photomask technologies are also becoming necessary to carry out the lithography process with diminishing k_1. These include optical proximity correction (OPC), attenuated phase shift, and alternating phase shift. Through the 0.15µm process generation, it is likely that all of these methods will be in use, at 365 nm, 248 nm and 193 nm exposure wavelengths. Planning for the upcoming lithography generations requires sorting through a huge array of possible configurations of wavelength, illumination, resist, mask types and OPC methods. Experimental evaluation of every case is unwieldy, expensive and, for some cases, not possible. In spite of this, choices of technology direction must be made well ahead of time. There is therefore a crucial need for lithography simulation tools with the flexibility to deal with all of the feature types of interest for the performance of real devices, and most importantly, predictive power.

Two dimensional simulation, i.e. profiles of lines and spaces extending infinitely in one axis, is not sufficient to deal with the device features that are most sensitive to a reduction in k_1. There are many important 2-D mask features which require full 3-D simulation of their resist images. A single contact can, in principle, be dealt with by a 2-D simulation, taking advantage of the rotational symmetry. However, two or more contacts in close proximity, or a metal landing pad near a conductor, are resolution-sensitive features which cannot be adequately simulated in two dimensions.

Another example, which will be dealt with in this study, is line end pullback. Pullback on polysilicon gates can cause leakage current in transistors, so the polysilicon lines must be extended by a safety margin beyond the active area to compensate for both misalignment and pullback. If this margin is greater than actually necessary, there will be an avoidable sacrifice in device density. OPC can be applied to line ends in the form of assist features (serifs or hammerheads) to reduce pullback. It is important to be able to model pullback accurately, in order to prescribe the safety margin required for future processes and to determine the optimum OPC assist features.

Experimental :

A set of wafers was exposed using a pattern with several resolution-sensitive features, for comparison with simulation over a range of parameter space. A chemically amplified DUV resist and a bottom ARC were used on a polysilicon substrate, and the exposures were made on an ASML PAS 5500 /300 deep UV stepper. Exposures were carried out with resist thickness at both maximum and minimum reflectivity (749 nm and 787 nm, respectively). For the present and future studies, exposures were made with NA of 0.4 and 0.57, with three different illumination conditions (high σ, low σ, and annular), and with both Cr and attenuated phase shift masks. A focus-exposure matrix was run for each set of conditions.

For the present study, dense and isolated lines and a simple pullback test pattern were examined (Figure 2). This is a "T" pattern with a gap, simulating a gate in proximity to a wordline (as might be found in an SRAM cell), in this case a 1.625 µm long "dummy" wordline. Pull-

back can be observed by measuring the actual gap in the developed resist, and also by measuring the actual length of the "dummy" wordline. Additional copies of this pattern with OPC assist features (serifs and hammerheads) on the gate ends were present on the mask.

Measurements were obtained from top-down inspection on a Hitachi 7280H SEM, using a "middle" algorithm for edge definition.

Results and analysis :

For calibration of PROLITH to resist data, it is particularly useful to display the resist measurements in the form of a correlation plot. Figure 3 is an example of such a plot, in which the gap between the gate end and the wordline is plotted against the isolate line width. This data, collected for a range of exposures, tends to fall along a characteristic line. In Figure 3 there is one such locus for NA = 0.4 and another for NA = 0.57. It is apparent from the figure that, while there is a distinct dependence on NA, data plotted this way is insensitive to the difference between conventional and annular illumination. It is also insensitive to resist thickness variations (the data shown includes resist thicknesses at both maximum and minimum reflectivity), and has been found to be insensitive to the algorithm used to identify edges in SEM measurements (as long as the algorithm is applied consistently to both features).

In simulations, plotting one feature type against another makes it possible to focus on those few input parameters which are crucial to the calibration. In other words, while many input parameters (such as the resist sensitivity, for example) can be adjusted to fit the simulation to the data for one feature type, most will affect two features types similarly and will not change the relationship between the simulation and the data on a correlation plot. Since the plot of gap vs. isolated linewidth is linear, the difference between linear fits of the data and the simulations serves as a figure of merit for calibration.

The first attempt at predicting the experimental pullback data of Figure 3 was to use an overly-simplified 2-D modeling. Although it was expected that 2-D simulation could not adequately describe this obviously 3-D effect, the magnitude and direction of the inaccuracy was of interest. To apply 2-D simulations to this problem, a "cut" line was drawn through the center of the gate pattern and across the gap. The 2-D aerial image was simulated for the whole mask, but only the 1-D image along this cut was used to expose the resist. 2-D diffusion and development then provided a 2-D approximation to the actual gap width. Carrying out these simulations for the 0.57 NA, 0.8 σ case with a chrome binary mask and the 787 nm resist thickness, exposure was varied and the results plotted against the data of Figure 3. The results are shown in Figure 4. Although the trend is correct, when the 2-D simulator matches the isolated linewidth correctly, it underestimates the amount of line-end pullback by about 60 nm. Obviously effects such as 3-D diffusion and development cannot be ignored.

The second attempt at matching the experimental data was to use full 3-D modeling with PROLITH/3D. Thus, 3-D diffusion and development were used to better predict the actual conditions near the line end. Figure 4 also shows these results. The use of 3-D models for diffusion and development had the intended effect of better matching the experimental data.

The first attempt at 3-D simulation used a simplified model for chemically amplified resists. Instead of solving the full set of reaction-diffusion equations in three dimensions, an approximate calculation method of 3-D diffusion followed by reaction was employed. To further improve PROLITH/3D, a newly developed 3-D reaction-diffusion solver is being incorporated. This new calculation engine offers the high accuracy of proven reaction-diffusion models for chemically amplified resists with the needed capability for 3-D simulations. For the full 3-D reaction-diffusion calculations, we assume a non-linearly varying acid diffusivity and the use of a significant amount of base quencher. An example of the resulting 3-D resist profile is shown in Figure 5. Additional work will be required to optimize this improved 3-D model, using measurements from many other mask features and exposure conditions.

Conclusion :

With production lithography becoming progressively more challenging over the next few process generations, and the multiplicity of mask variations available to apply to these processes, there is a growing need for lithography simulation capability which is flexible enough to simulate the most sensitive 2-D mask patterns (and resulting 3-D resist profiles), and accurate enough to have predictive power. We have begun a program to calibrate the simulation package PROLITH/3D based on resist data over a large matrix of exposure conditions, including attenuated phase shift masks and OPC features. Calibration based not only on dense and isolated lines, but also on line end pullback, is much more challenging than calibration based on 1-D mask patterns alone.

We have introduced the use of feature correlation plots as an efficient means of checking simulations against measurements. Correlation plots, for example line end pullback against isolated line width, are insensitive to a wide range of experimental conditions and simulation parameters, and make it possible to identify and optimize the most crucial simulation parameters.

The results show quite clearly that a 3-D lithographic effect, such as line end pullback for chemically amplified resists, can be a complicated function of many parameters. Accurate simulation requires accurate physical models for reaction, diffusion and development, and appropriate 3-D algorithms which implement these models. Attempts at using simplified versions of full physically-based models, as shown in this study, can sometimes be less than adequate.

Further work will refine and improve this model by comparison with the resist data over the full range of experimental conditions. The goal is to use the existing data to achieve a consistent calibration applicable to 3-D effects such as pullback, over variations in resist thickness, stepper NA and illumination, and mask type (chrome vs. attenuated phase shift).
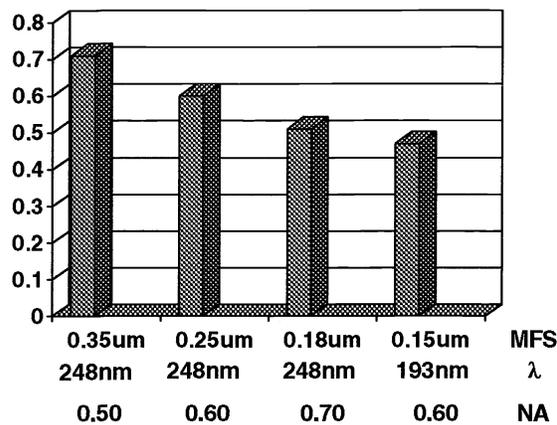
Figure 1. Decrease in k_1 factor (from the Rayleigh relation) with process generation. A smaller k_1 indicates more challenging lithography, i.e., the need for greater resolution relative to the basic capability of the optical system.
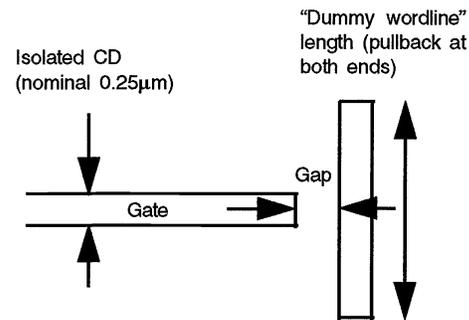

Figure 2. Test pattern containing features for measuring pullback. Nominal CD is 0.25µm. Drawn features are polysilicon : on the mask, they are opaque on a clear background
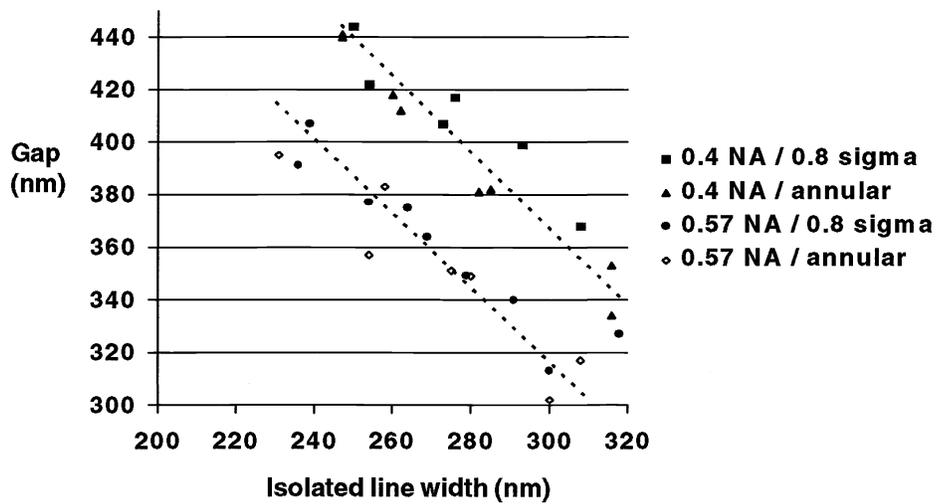

Figure 3. Feature correlation plot of gate end to wordline gap vs isolated line width. Measured values are shown for 4 different exposure conditions.
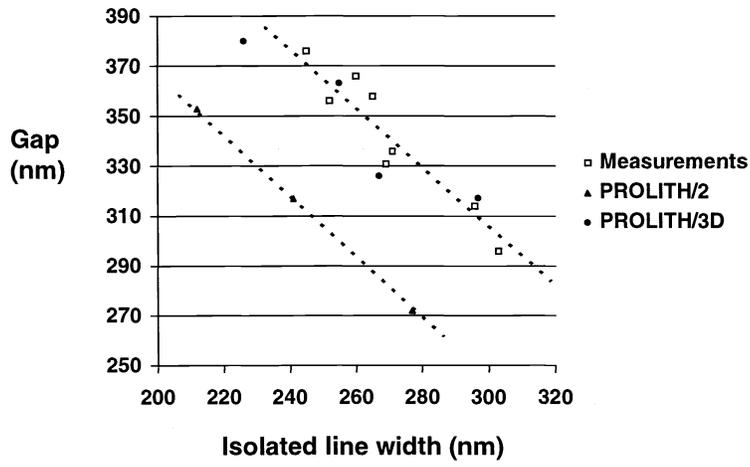
Figure 4. Correlation plot for one exposure condition (0.57 NA, 0.8 σ), comparing measurements with PROLITH/2 and PROLITH/3D simulations.
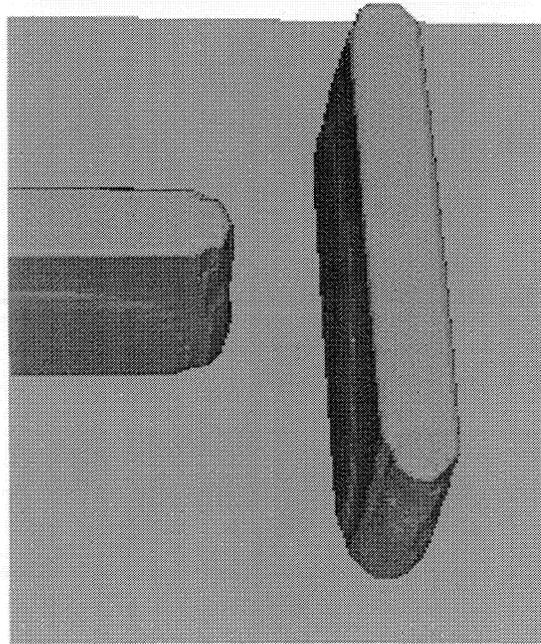

Figure 5. 3-D profile of pullback test structure generated by PROLITH/3D.