Impact of mask three-dimensional effects on resist-model calibration

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Abstract. We report on a comparison between a full-physical resist model that was calibrated to experimental line/space (L/S) critical dimension (CD) data under the flat-mask (also called "thin-mask" or "Kirchhoff") approximation with the model obtained when using a mask 3-D calculation engine (i.e., one that takes into account the mask-topography effects). Both models were tested by evaluating their prediction of the CDs of a large group of 1-D and 2-D structures. We found a clear correlation between the measured-predicted CD difference and the magnitude of the mask 3-D CD effect, and show that the resist model calibrated with a mask 3-D calculation engine clearly offers a better CD predictability for certain types of structures. © *2009 Society of Photo-Optical Instrumentation Engineers.* [DOI: 10.1117/1.3158356]

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Calibration of full-physical resist models[1–4] has a long record of use and is constantly being refined to offer better predictability to rigorous simulators, such as Sentaurus Lithography™ of Synopsys or Prolith™ of KLA-Tencor. We used a large experimental critical dimension (CD) data set, which was generated for the purpose of optical proximity correction (OPC)-model building, to assess the importance of mask 3-D (or mask-topography) effects in resist-model calibration. The CD data was measured with a top-down Hitachi H9380 scanning electron microscope from a 120 nm TOK TArF-Pi6-001-ME resist on 95 nm ARC29SR Barc on Si wafer exposed with an NA=1.20 ASML XT:1700i immersion scanner, using cQuad20 $\sigma_{outer}/\sigma_{inner}=0.96/0.60$ *XY*-polarized illumination. The experimental CD data consisted of two types. The first type consisted of Bossung (i.e., through-dose and -focus) data for 30 L/S structures, with pitches between 100 and 400 nm. The resist models were essentially calibrated using (part of) these L/S Bossungs only. The second CD-data group (~5000 different structures) was measured at a single dose-focus setting only and was used for verifying the resist models. It consisted of more 1-D-type data (L/S structures with and without SRAFs, isolated lines and trenches and line and trench doublets and triplets), end-of-line (EOL) gap-CD data and of CDs measured from more complicated 2-D structures (which we shall call the Generic 2-D or G2D structures). Most of the structures in this data set are located on the mask in a locally clear-field area, but others are located in a locally dark-field area. The resist-model quality is then quantified by first calculating the measured-predicted CD difference, $\Delta CD \equiv CD_measured\text{-}CD_simulated$, for all individual verification structures. In view of the very large number of structures in the verification set (>5000), we reduced this ΔCD data set by calculating the mean value [Mean(ΔCD)] and the standard deviation [StDev(ΔCD)] for a number of—somewhat arbitrarily chosen—subsets of this verification-structure group.

In Fig. 1, we represent such a verification result, by plotting these Mean(ΔCD) values for each of the selected structure subsets (the labels we use for these subsets are explained in the caption of Fig. 1). The error bars in Fig. 1(b) actually stand for the $\pm$StDev(ΔCD) values (i.e., they are not actual error bars but represent the variation of the ΔCD values in each structure subset. Figure 1(b) shows the raw ΔCD data for four such subsets). We made a separate calculation with a Prolith10.2 and a Sentaurus Lithography (or S-Litho) resist model, both calibrated under the Kirchhoff- or flat-mask-approximation to the experimental Bossung data, and Fig. 1(b) shows the result for both. Although both simulators (most likely) do not use identical resist-modeling equations, there is a striking similarity in the result of Fig. 1(b): some structure groups are clearly less well predicted, which is best recognized in Fig. 1(b) as a larger |Mean(ΔCD)|. This seems to occur primarily in the CDs measured from the locally dark structures [i.e., the isolated trenches, trench doublets, and trench triplets (which are labeled as ISO_Inv, B2Inv, and B3Inv, respectively)].

One could surely think of a number of reasons why these locally dark structures would be predicted less well, and some of these would point to the resist-model equations or the calibration structures used, but a correlation shown in Fig. 2 has led us to believe that mask 3-D or (mask topography) effects[5] take a large part in the explanation. This correlation plot compares the measured-simulated CD difference (i.e., the ΔCD data, used above) to the mask 3-D CD contribution [simulated while not using the Hopkins approximation[6], i.e., solving the diffraction equations at the "correct" angles of incidence on the mask]. This mask 3-D CD contribution is calculated as follows. Using the resist model calibrated under the Kirchhoff approximation, we switched the simulator to one of the available mask 3-D calculation engines (RCWA in Prolith and FDTD in S-Litho) and recalculated the CDs of all verification structures: the difference with the original CD (i.e., the CD obtained under the Kirchhoff approximation) was then taken as the above mentioned mask 3-D CD contribution. Note that these CD recalculations using the mask 3-D solver were done after also adjusting the simulation dose, such that a chosen "anchor structure" prints at the same CD as in the Kirchhoff-calculation case. We, somewhat arbitrarily, took a pitch 100-nm mask linewidth 43.5 nm L/S

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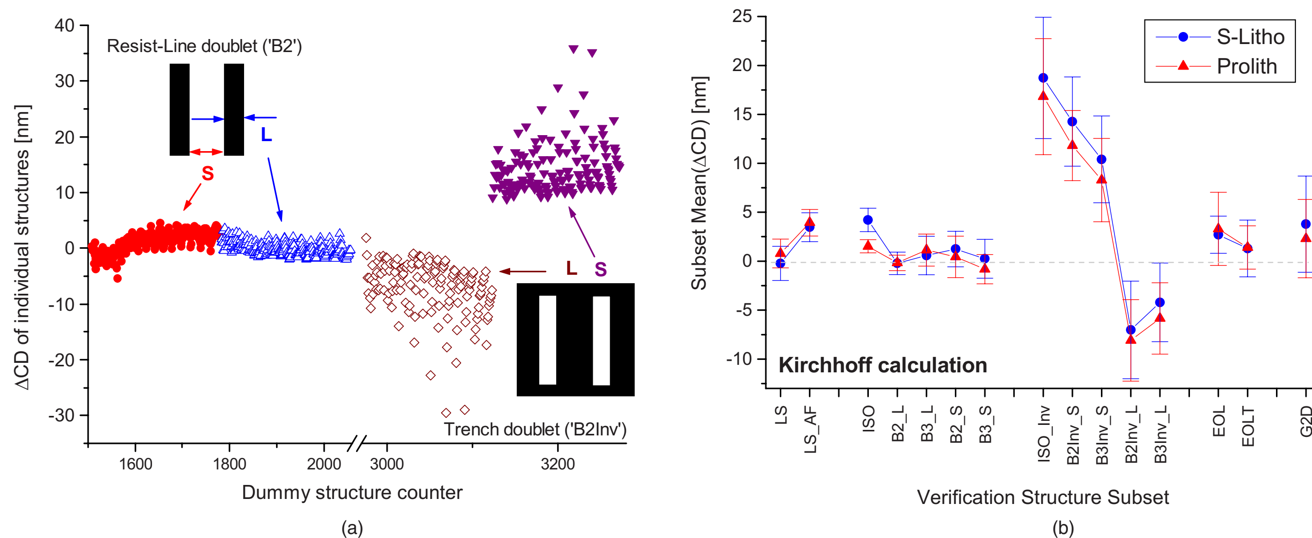

Fig. 1 (a) Example of ΔCD≡CD_measured-CD_simulated results for four subsets of the verification structures, namely the line and space data of line-doublet and trench-doublet–type structures (labeled further on as B2_L, B2_S, B2Inv_L, and B2Inv_S). (b) Mean(ΔCD), i.e., the subset-average value of ΔCD-, obtained with two different Kirchhoff resist models, one from Prolith and one from Sentaurus Lithography. The error bars correspond to ±StDev(ΔCD), i.e., the variation of ΔCD around the mean value. Structure groups used here include L/S structures with and without SRAFs (labeled LS and LS_AF, respectively, on the horizontal axis), line doublets and triplets (labeled as B2 and B3), isolated lines (ISO) and isolated trenches (ISO_Inv), trench doublets and triplets (labeled as B2Inv and B3Inv), end-of-line gaps [(EOL) and (EOLT); in the latter, the line end faces a perpendicularly oriented line], and more complex Generic 2-D structures (G2D). In the line and trench doublets and triplets, all the different line- and trench- or space-CDs were measured/simulated. The _L suffix indicates the CD of a resist line; _S the CD of a space between resist structures.

structure as the anchor structure. We calculated this mask 3-D CD contribution for all 1-D structures in the verification-structure set. Figure 2 shows that this mask 3-D CD contribution correlates well with the ΔCD measured-simulated difference, at least for those structures for which the mask 3-D CD contribution is relatively large (say larger than ∼10 nm); for structures with a smaller 3-D effect, there is no correlation any more. This explains why the resist models calibrated under the Kirchhoff approximation do not predict certain structures as well because they simply do not incorporate this mask 3-D CD contribution effect.

What, then, can we do to further improve the resist model? The simplest way to try to incorporate mask 3-D effects in the full-physical resist model simulations would be to keep the resist model as fitted to the experimental Bossung data under the Kirchhoff approximation (we shall call this the Kirchhoff resist model) and simply switch the mask-diffraction solver to the 3-D calculation engine, adjusting the dose again to keep the anchor structure at the same CD, but without any further changes. The resulting Mean(ΔCD) verification data are shown as the open-triangle curve of Fig. 3; plotting ±StDev(ΔCD) again as "error bars." It is clear that this approach makes the measured-simulated agreement worse for most structures.

The better—though more time-consuming—approach is to replace the Kirchhoff-approximation-based resist model with a completely new one, obtained from a refit of the experimental Bossung data with the simulator set to the mask 3-D engine already in the calibration step, thus obtaining what we shall call a Mask 3-D resist model. The second curve of Fig. 3 shows that verification now drastically improves for those structures that were most deviating in Fig. 1(b), while retaining the agreement for the others. (Note that we applied this Mask 3-D resist model to all the 1-D and EOL structures of our verification set; the more complex G2D structures were not tried because of the excessive calculation time they would require.)

Conclusion

The data presented in this paper make it clear that mask 3-D effects also play a role in resist calibration at hyper NA. Usually, resist calibration is done under the flat-mask or Kirchhoff assumption. From a calculation-effort point of view, this is a logical choice, in view of the larger CPU- and/or memory-consumption when doing mask 3-D calculations, but one must realize that when doing so, mask 3-D effects will be *absorbed* into the resist parameters. In cases where mask 3-D effects are not too high, this can still be an acceptable practice. Taking the data of this paper, if we exclude the locally-dark structures from the verification set, our Kirchhoff models would have done the job well. Including these more mask 3-D sensitive structures, however, makes the Kirchhoff models much less convincing. It is therefore necessary to be aware of the mask 3-D sensitivity of the target structures, if accurate CD prediction is intended. (A more detailed discussion of *why* it are the locally dark-field structures that seem to "suffer" most from the absence of mask 3-D effect in the resist-model calibration, e.g., by considering differences in mask-diffraction spectra or image-intensities in resist between the Kirchhoff and mask 3-D calculation would obviously be interesting, but falls outside the scope of a letter. To be noted also is that as in all cases we adapt the simulation dose to fix the CD of the anchor structure, part of the mask 3-D effect is also *absorbed* in this dose retargeting, which further compli-

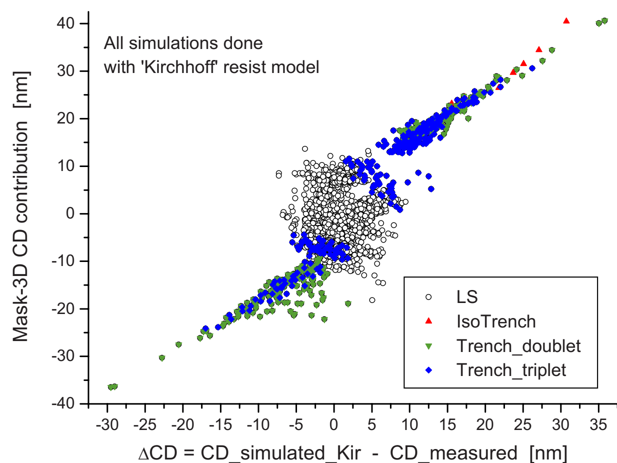

Fig. 2 Correlation of the mask 3-D CD contribution (calculated as the difference between the mask 3-D simulated CD to the Kirchhoff-simulated CD for each individual structure) with the simulated-measured CD difference (ΔCD).

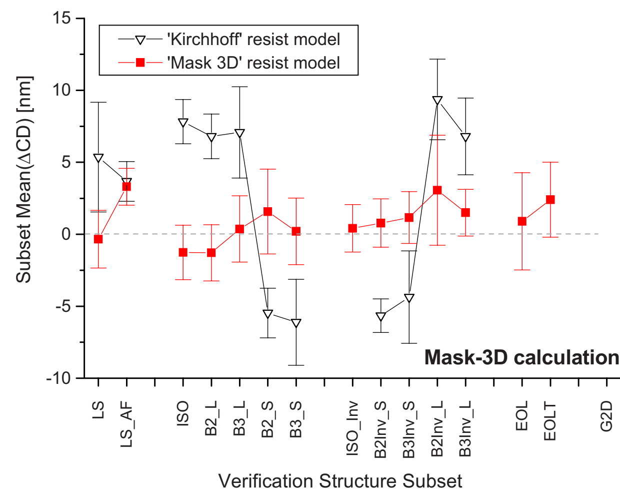

Fig. 3 Resist-model verification (similar to Fig. 1), now using a mask 3-D calculation engine, first while keeping the Kirchhoff resist model (open triangles) and second after refitting the resist model under mask 3-D conditions also (filled circles).

cates the detailed interpretation of our result.)

Do our results mean that we always should calibrate resist models under mask 3-D conditions? Unfortunately, rigorous mask 3-D effects are not feasible in many practical cases. The absence of mask 3-D simulated CD data in Fig. 3 for the G2D structures of our study illustrates this point painfully well: the calculation time required for rigorous 3-D simulations over mask areas of several microns in both X and Y becomes exceedingly large. (Note that isolated 1-D structures or EOL structures can be calculated within a very reasonable time because the simulated mask area in X or Y remains submicron.) This calculation-time limitation explains why attempts have been made to come up with a mask 3-D equivalent Kirchhoff mask, in which, e.g., transmission, phase, or the mask dimensions were altered such that the resulting CDs approximate the CD-values obtained from rigorous mask 3-D calculations. Although these approaches have had some success,[7,8] their applicability has been demonstrated for specific structure sets only. Thus, more work would be required in proving general applicability as well as the absence of artifacts before such equivalent Kirchhoff masks could be safely employed for a wide variety of structures.

We would like to conclude with a final note on OPC modeling of the verification CD data of this paper: We were able to obtain a very good OPC-model fit to the entire CD data set (i.e., including both dark- and bright-field structures) while still using a Kirchhoff calculation engine (we obtained an rms value of 1.6 nm). Thus, apparently, the OPC model contained *enough* degrees of freedom to largely *absorb* the mask 3-D effects in this case. Nevertheless, we are currently also investigating to which extent OPC model accuracy could improve if mask 3-D effects would be incorporated, because some improvement should be expected, especially for the type of extended hyper-NA data sets dealt with in this letter.

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