

# Comparative study of simulations and experiments for contact array patterns on attenuated phase shifting mask

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## ABSTRACT

Experiments and full resist simulations of contact patterns using both infinitely thin masks (2D) and 3-dimensional mask topography (3D) were performed to examine the quality of prediction by simulation. Experimental data were acquired by CD-SEM measurements of contact patterns in resist which were generated using a 193 nm scanner with a numerical aperture of 0.75, circular illumination ( $\sigma=0.5$ ), and an attenuated phase shifting mask with 6% transmission. Analysis of the data is performed in terms of dose to size, process window, mask error enhancement factor (MEEF), and printed critical dimension (CD) in resist. Furthermore, an error analysis is performed with respect to mask CD, illumination source, dose and focus error.

A parabola like dependence of the mask contact length on contact width was found by experiment and simulation for the same contact size in resist. Fair agreement between 2D and 3D simulation was obtained above 180 nm mask CD whereas a strong difference was observed below this region. Especially the location of the minimum at around 140 nm mask CD can be reasonably described only by 3D simulation. Thus, the prediction of accurate mask biases and process windows below 120 nm mask CD is only possible by 3D simulation. Simple corrections of the 3D effect like the consideration of a mask CD or dose offset fail. Apart from that, 2D simulation in conjunction with a well calibrated resist model is sufficient for delivering reliable predictions for process window, MEEF, and CD.

**Keywords:** lithography, contact holes, simulation, 3D mask, mask error

## 1. INTRODUCTION

Due to increasing pressure on DRAM manufacturers with respect to production cost, electronic devices have been scaled down in order to reduce chip area resulting in reduced cost per chip. Thus, lithographic structures on the wafer become smaller and smaller. Knowledge about size and statistical deviations of the CD of such structures is essential for improvement of lithographic processes in production and development. Despite the availability of modern CD-SEM measurement tools, accurate measurement of small structures in resist, especially contact patterns, is however difficult and time consuming. This limits not only the optimization of a specific lithographic process but also the comparison of processes with different illuminations and/or mask technologies by experiments. Consequently, there is a growing trend to apply simulation in order to get ideas how to optimize the process and how to interpret experimental results.

Recently it was shown that only full resist simulation may predict the correct mask bias for contact holes, in contrast to aerial image and resist image simulations [1]. In that study an infinitely thin mask (Kirchhoff approach) was applied. However, such a simplified model cannot be used in general. From a recent study on mask topography effects in 2D simulation of line-space patterns it is clear that significant 3D mask effects can also be expected for contact holes [2]. On the other hand, full resist simulations require a large simulation area, and are therefore very time consuming, in particular when using a 3D mask topography. Therefore, the goal of this study is to find out how to get reliable predictions in terms of CD, MEEF, and process window by simulation. Thus, it is investigated how resist simulations fit to experimental data when using either 2D or 3D masks. Further on, significant differences between 2D and 3D simulation are revealed and discussed. Analysis of the data is performed in terms of dose to size, process window, MEEF, and of printed CD in resist. In addition, an error analysis is done by considering mask CD, illumination source, dose and focus errors in simulation.

## 2. DATA ACQUISITION

Silicon wafers were spin-coated using commercially available bottom antireflective coating (ARC), ArF positive tone resist, and top ARC. Exposures were performed using an 193 nm scanner with a numerical aperture (NA) of 0.75 and circular illumination ( $\sigma=0.5$ ). An attenuated phase shifting mask with 6% transmission was used which contains contact patterns of different pitches and sizes. Contact hole structures in resist were developed using state-of-the-art bake and development conditions of a pilot line. Experimental CD data were then acquired by top-down CD-SEM and X-SEM measurements in resist. All experimental CD's were corrected by a constant value of 18 nm in order to account for the offset between top-down CD-SEM and X-SEM. Design of experiment (DOE) software (Design-Expert<sup>TM</sup>) has been used to obtain interpolated dose to size and mask CD values for which the CD in resist is perfectly on target.

For error analysis of simulation, additional information on the performance of the mask and illumination source of the exposure tool is required. Therefore, the illumination source distribution of the scanner was measured using a commercially available sensor technique. Moreover, patterns on mask were measured at Advanced Mask Technology Center (AMTC) using CD-SEM and surface nanoprofilng (SNP).

Simulations were performed by use of the commercially available lithography simulator SOLID-CTM<sup>TM</sup> (version 6.5.1) in combination with SOLID-C batch language and in-house scripts written in MATLAB<sup>TM</sup>. These scripts were developed based on an algorithm which controls the case to be simulated. This ensures a considerable reduction of simulation time compared to simulations using simple batch processing or a graphical user interface. General simulation parameters, which were kept constant during simulation, are provided in Table 1. Either an infinitely thin mask or a 3D mask topography has been used. In the following, the first case will be referred as "2D simulation", and the second one as "3D simulation". SOLID-CTM<sup>TM</sup> uses a fast Finite Difference Time Domain (FDTD) algorithm for rigorous calculation of the EM field of 3D masks. Further details of this method can be found elsewhere [3]. The resist model applied was calibrated previously to line/space patterns using a 2D mask.

Simulation Parameter	2D simulation	3D simulation
<b>Illumination</b>		
Mode	circular	
NA	0.75	
$\sigma$	0.5	
Wavelength	193 nm	
<b>Imaging</b>		
Model	Transfer Matrix, Vector	
Pupil Mesh Points	10	
Normalization	Open Frame	
Flare	constant (2%)	
<b>Mask</b>		
Stack	n.a.	MoSi / SiO <sub>2</sub>
Transmission / Phase	6% / 180°	
Pattern	regular contact array	
Pitch-x / Pitch-y	300 nm / 380 nm	
Resolution x/y/z	n.a.	0.5 / 0.5 / 1 nm
<b>Resist</b>		
Stack	250 nm Resist / matched substrate*	
Resolution x/y/z	1-2 / 1-4 / 4 nm	

Table 1: General simulation parameters used in 2D and 3D SOLID-CTM<sup>TM</sup> simulation

\*matched substrate: material with same optical properties (n,k) as of the resist in order to suppress standing waves

### 3. RESULTS AND DISCUSSION

The pattern investigated in this study is a regular contact hole array of 11 x 5 contacts with always the same pitches as stated in Table 1. Nominal mask parameters and mean mask CD's calculated using CD-SEM and SNP data measured at AMTC are given in Table 2. According to these CD-SEM measurement results, small contacts were printed too small on mask, whereas the biggest one was almost on target. Thus, the mask CD deviation decreases with increasing size, and is almost zero for the biggest contact. This result demonstrates a high quality of the attenuated phase shifting mask which was previously manufactured by the mask shop of Infineon Technologies in Munich. Moreover, there is a CD offset between CD-SEM and SNP, i.e. the CD of the contact width obtained by SNP is always higher by about 3nm compared to CD-SEM (see Figure 1). We believe that the CD obtained by CD-SEM is closer to the real size of the contact since only the CD-SEM measurement tool was previously calibrated to requirements of Infineon technologies.

nominal mask CD		mean CD by CD-SEM		mean CD by SNP	
X (nm)	Y (nm)	X (nm)	Y (nm)	X (nm)	Y (nm)
80	300	74.9	286.8	78.4	282.8
90	300	85.9	289.3	89.2	289.3
100	300	97.0	291.9	100.1	291.9
105	290	102.2	282.5	105.1	282.9
110	290	107.6	283.4	110.8	285.9
120	280	118.2	274.8	121.2	278.2
130	280	128.4	275.7	131.9	279.8
140	280	138.9	277.1	141.8	280.3
150	280	148.8	277.3	152.5	281.5
160	280	159.0	278.4	162.9	281.9
180	290	180.1	289.7	183.3	294.2

Table 2: Nominal and mean mask CD's (1X) by CD-SEM and SNP for contact array patterns used in this study

Figure 2 shows SEM images of the smallest and biggest contact used in this study. Images were taken from the center of the pattern. A significant corner rounding can be seen which radius has been estimated as about 40nm for all contacts.

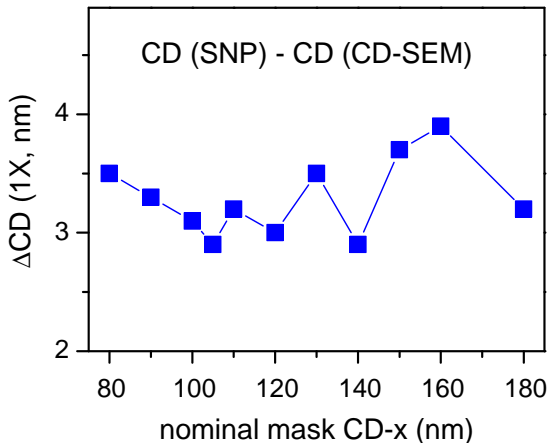


Figure 1: Difference between mask CD measured by SNP and mask CD measured by CD-SEM for contact hole widths.

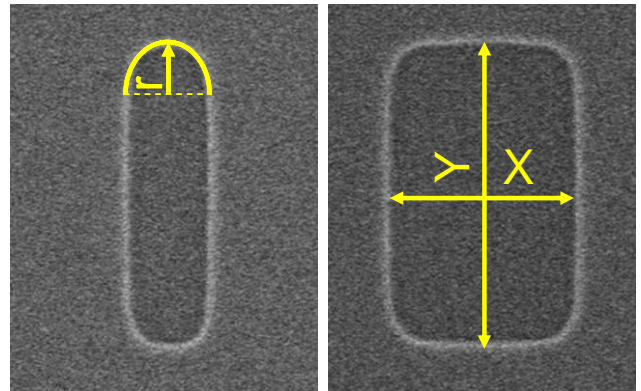


Figure 2: SEM images of center contacts with a size of 80 nm x 300 nm and 180 nm x 290 nm, respectively.

First of all, the CD of the contact array pattern in resist as a function of its corresponding CD on mask has been investigated by experiment and simulation. Figure 3 illustrates for the contact width an increase in CD in resist with increasing mask CD while the contact length was kept constant. There is a linear relation between printed CD and mask

CD in the upper mask CD range, and a strong deviation from this behaviour in the lower mask CD range. As can also be seen, there is a slight mismatch between experiment and 2D simulation, especially at small contact widths. This can be explained by the fact that the resist used in the experiment was slightly different to the one used in calibration. Possible causes might be differences in the chemical composition of the resist, bake temperatures, thicknesses of the stack layers etc. Figure 4 demonstrates the same behaviour for the contact length, except for the mismatch which is generally smaller in the mask CD range investigated.

Since a 2D mask was used for resist model calibration in the past, the CD in resist obtained from 3D simulation must be smaller than the CD provided by 2D simulation. In other words, the dose to size must be higher for 3D than for 2D simulation. The reason is that interaction of light with the side walls of the 3D mask decrease the amount of light entering the projection lens system. Figure 3 and 4 show that the CD as obtained from 3D simulation is indeed smaller than the one resulted from 2D simulation when using the same dose as applied in the experiment. Moreover, the CD offset between 2D and 3D simulation is not constant but increases with decreasing mask CD.

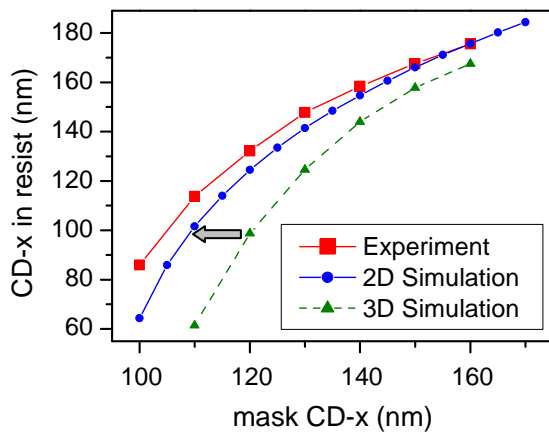


Figure 3: Printed CD of contact width in resist vs. mask CD (width) using a constant mask CD for the length (270 nm) and a constant dose (19 mJ/cm<sup>2</sup>)

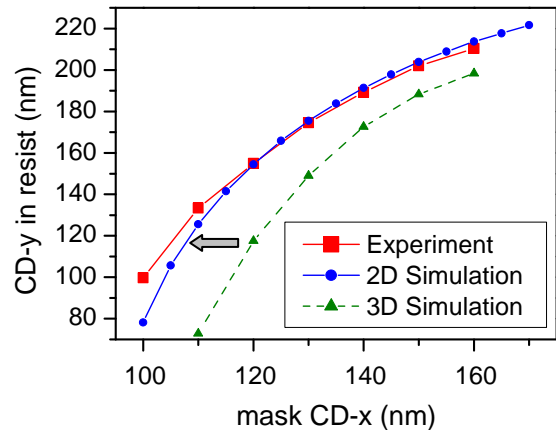


Figure 4: Printed CD of contact length in resist vs. mask CD (width) using the same conditions as in figure 3

In general, 3D simulation should normally match with experiment. The question arises what can be done to get this agreement, and what would be the consequence for 2D simulation. This issue is of some academic nature because resist models are usually calibrated using 2D masks. This is mainly due to computer run time limitations when calibrating the model as well as when doing simulations for lithography applications later on. Though a very fast 3D simulator is under development, however, this tool was not available for this study [4]. Nevertheless, an established correlation between 2D and 3D simulation would help to understand 3D mask effects when interpreting simulation results.

Under the assumption that the resist model has been calibrated to experiment by use of a 3D mask, one would theoretically have the following possibilities to obtain the same CD by 2D simulation as in experiment (or 3D simulation):

- I) decrease width and length on mask using individual (or same) CD offsets
- II) decrease the exposure dose by an offset

To examine the first proposal, the mask CD difference between 3D and 2D simulation has to be known. As an example, the offset for the contact width can be extracted from Figure 3 and 4 keeping in mind the assumption stated above. That is, each point of the 3D simulation curve correlates with one specific point of the 2D simulation curve which belongs to the same printed CD in resist (see arrows in Figure 3 and 4). Then the mask CD offset between 3D and 2D simulation for the contact width on mask can be plotted as a function of 3D mask CD-x (see Figure 5). To close the gap between 2D and 3D simulation with respect to the printed contact hole width, at least the introduction of a mask CD offset for the contact width is necessary when keeping mask CD-y and dose unchanged. However, this offset increases slightly with decreasing contact width on mask. On the other hand, the same mask CD offset has to be reduced with decreasing contact width in order to match the contact hole length in resist. Thus, it is not possible to match 2D with 3D simulation just by changing one mask dimension (width or length) only. Instead, individual CD offsets for width and length are

required. These offsets were determined by adjusting the mask parameters (width and length) in 2D simulation to get the same CD for width and length in resist as in 3D simulation. The calculated CD offsets are given in Figure 6. As can be seen, the offset for the contact width increases slightly with decreasing mask CD, however, the absolute values are lower compared to those provided in Figure 5. As for the contact length, not only the offset but also the uncertainty of its determination increases with decreasing mask CD. This is in contrast to the contact width, which offset can be determined with a significant smaller uncertainty. This is shown by the error bars illustrating the CD offset range for which the difference between 2D and 3D in terms of mean RMS error is  $\leq 1$  nm. In addition, contour plots of the calculated RMS error show that the optimum CD offset is very confined to a small mask CD region for a 3D mask CD of 160 nm, whereas this region is very elongated with respect to the length for 110 nm mask CD (s. Figure 7). Hence, printing of small contacts in resist is much more insensitive to the contact length on mask. The reason for this behaviour is given later on. To summarize the results, the introduction of a mask CD correction in 2D simulation (method I) may give predictive results for the CD in a limited range of proximity, mask biases, and imaging settings. However, some calibration work is necessary to achieve this. On the other hand, the second proposal, i.e. the introduction of a dose offset, does not work. In general it is not possible to get the printed CD of both width and length simultaneously on target just by correcting the exposure dose (not shown here). It should be noted however that this method may work for squared contact holes.

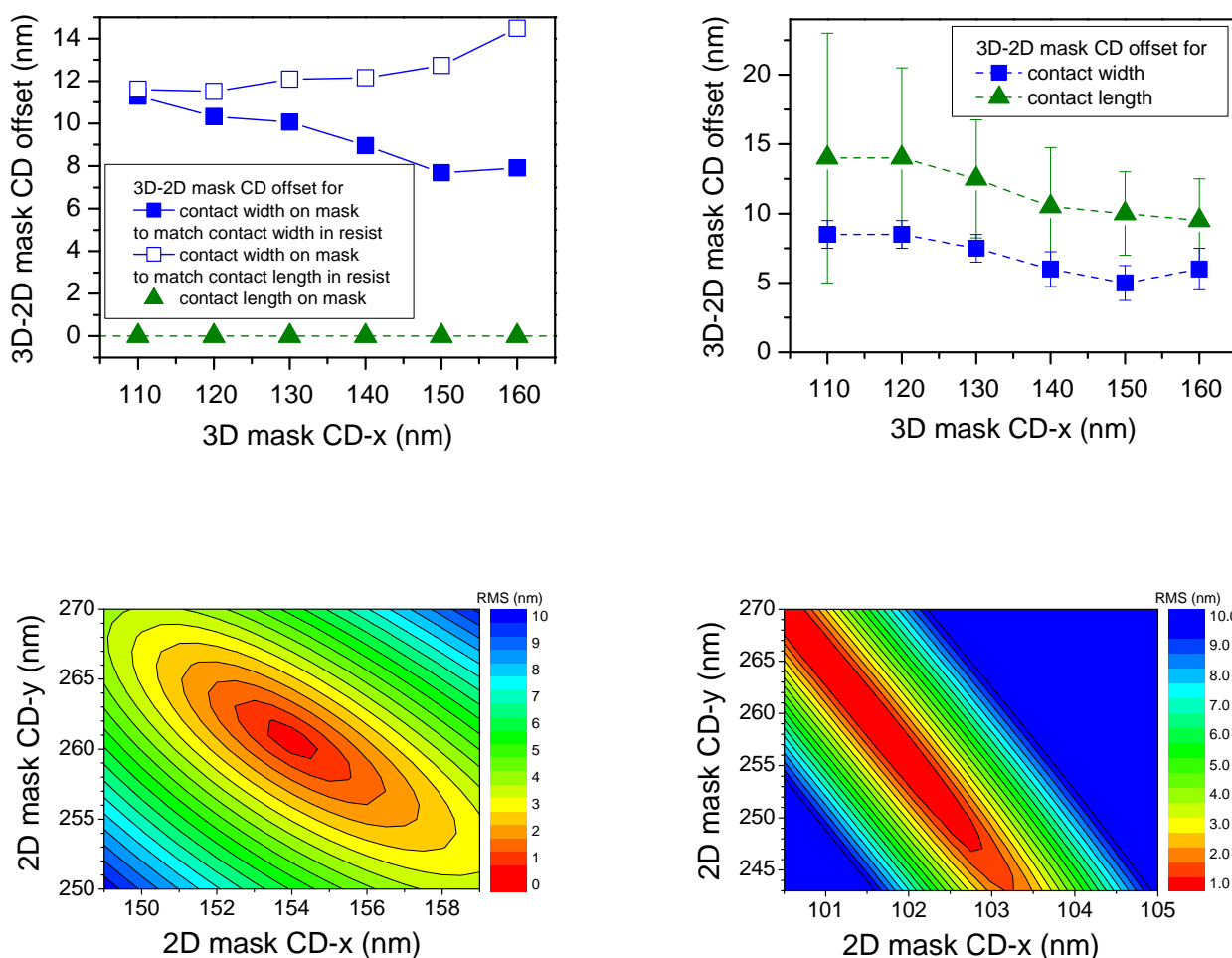


Figure 7: Difference between target CD provided by 3D simulation and printed CD obtained by 2D simulation with adjusted mask CD for width and length (in terms of mean RMS error) as calculated for a 3D mask CD-x of 160 nm (left) and 110 nm (right).

The mask error enhancement factor can be obtained just by calculating the first derivative of the curves shown in Figure 3. It should be noted that this calculation does not take into account a variation of the length on mask, i.e. MEEF is

defined here for the contact width while applying a constant length. This simplifies work. As expected, the MEEF increases with decreasing mask CD (see Figure 8). There is a good agreement between experiment and 2D simulation except for small printed CD's. The discrepancy at 80 nm can be explained by the high error of the top-down CD-SEM measurement in resist. One reason could be the irregular shape of the contact hole seen in the SEM image. The applied CD-SEM measurement algorithm fits an ellipse to that shape whose axis determine the CD for width and length. Thus, it might be that the fitted ellipse covers a bigger area than the contact actually has. Consequently, the CD is over- and the MEEF is underestimated. Another issue could be the constant offset between top-down CD-SEM and X-SEM applied. It is not unreasonable to assume that this offset depends on contact size, i.e. the CD offset is smaller for small contacts and v.v. Following this argumentation, the X-SEM CD is overestimated and therefore the MEEF also underestimated in this case.

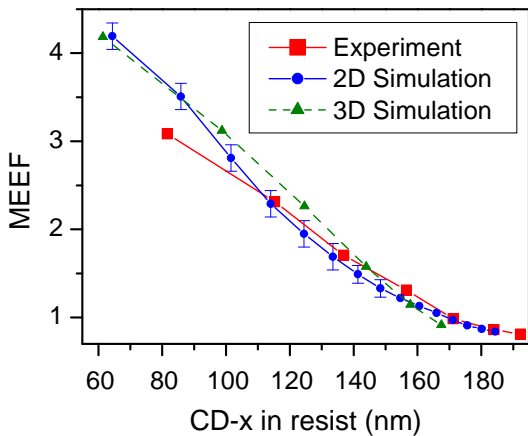


Figure 8: MEEF of contact hole width as a function of the CD in resist (width) as derived from figure 3

In contrast to CD determination in resist, 3D simulation yields almost the same result (MEEF) as 2D simulation, except for a medium CD range between 100 and 140 nm where the MEEF is slightly higher predicted by 3D simulation. It is not clear whether this is to be ascribed to a systematic difference between 2D and 3D simulation or to deficiencies of the resist model. Further investigations are ongoing to clarify this issue. It should be emphasized however, that the experimentally determined MEEF is well within the uncertainty of 2D simulation if illumination, focus and dose errors are considered (see error bars in figure 8).

2D and 3D Simulations were performed in order to calculate dose to size and mask CD necessary to print the CD for width and length at best focus on target. That is, for a given contact width on mask the dose and contact length on mask were varied within an optimization loop until the final CD in resist was, within a given tolerance of  $\pm 0.5$  nm, on target. As for the target CD, 115 nm and 142 nm were chosen for contact width and length, respectively. The final values for dose to size and contact length on mask are plotted as a function of contact width on mask (see Figure 9).

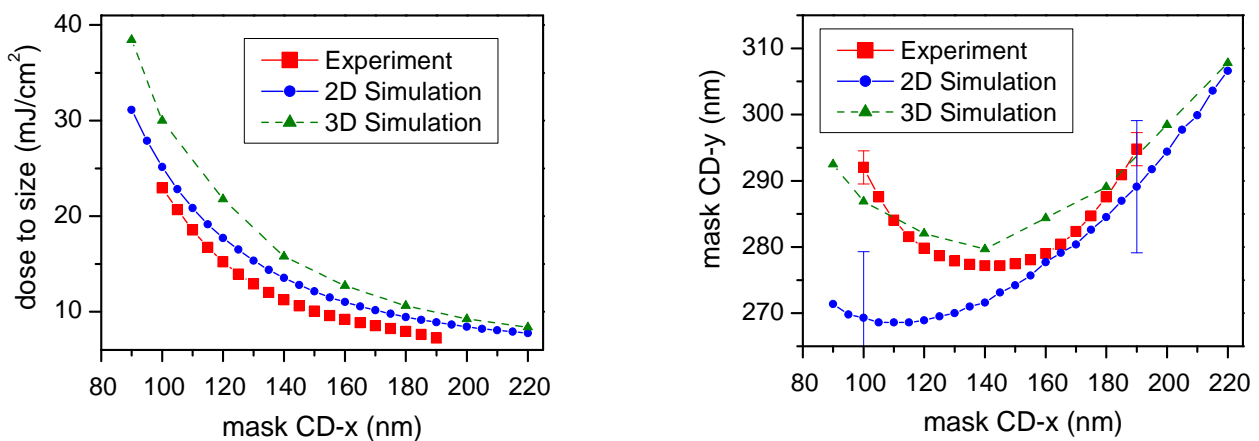


Figure 9: Dose to size (width and length on target) as a function of contact width on mask (left). The corresponding contact lengths on mask (mask CD-y) are displayed vs. contact width (mask CD-x) (right).

Experimental dose to size and mask CD values cannot be obtained with the same precision as in simulation. This is due to limited CD-SEM measurement accuracy at the one hand and higher dose and mask CD stepwidths in experiment on the other hand, compared to simulation. Therefore, final experimental values as plotted in the figures were obtained by interpolating experimental data using standard DOE analysis. As expected, the dose to size is higher for 3D than for 2D simulation. In addition, the ratio between dose to size for 2D and 3D simulation is not constant but changes by about 15% in the mask CD range examined.

As can also be seen, the contact length on mask decreases almost linearly with decreasing contact width in the upper mask CD range. With further decrease of the width the length approaches a minimum until it increases again. This behaviour is observed both in simulation and experiment.

The existence of this minimum can be simply explained by the fact that printing of contact holes, which are smaller than about  $0.6\lambda/NA$  ( $\sim 150\text{nm}$  in this study), is controlled by the point spread function of the optical system and not by the mask dimension [5]. This implies that only the peak intensity of light is reduced when reducing the contact size. At the minimum of the curve, the light passing through the contact is just sufficient to print width and length on target. However, the length in resist cannot be kept on target if the width on mask is further reduced. Therefore, the length has to be increased when continuously scaling down the width. As for 2D simulation, the agreement between simulation and experiment is fair in the upper mask CD range, and rather unsatisfactory in the lower range. Especially the minimum is predicted at a 35 nm smaller width and 9 nm smaller length on mask. On the other hand, 3D simulation predicts fairly well the location of the minimum as well as the overall trend. However, there is still some improvement possible with respect to quantitative agreement to the experiment.

An error analysis was performed in order to examine whether measurement and simulation errors may have a significant impact on the curves shown in Figure 9. As for the experimental data, a CD-SEM measurement error of  $\pm 3$  nm has been taken into account. As for simulation, two points were again simulated applying real mask layouts (CD and corner rounding) as obtained by CD-SEM, a real illumination source distribution (instead of a top hat distribution) as well as dose and focus offsets. The result of this analysis is provided in terms of error bars in Figure 9. Clearly, the overall error found in the upper mask CD range may, at least partly, account for the mismatch between 2D simulation and experiment. However, this is not the case for the lower mask CD range. Thus, 2D simulation completely fails in predicting the correct mask bias for contact hole widths on mask well below 160 nm.

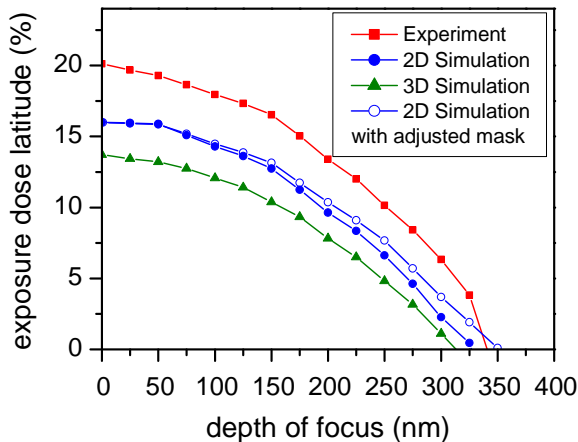


Figure 10: EDL of the contact width as a function of depth of focus for 100 nm contact width on mask (length was adjusted to match the target CD).

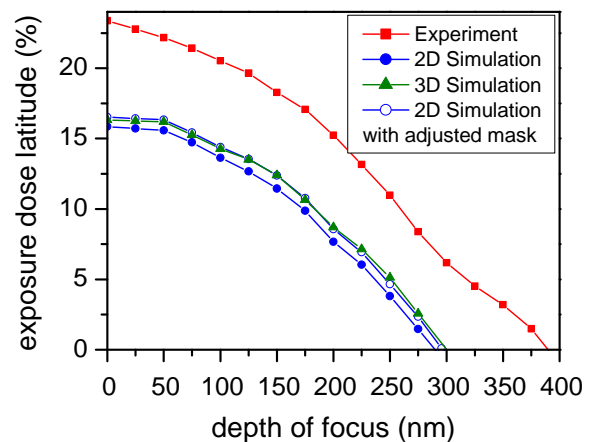


Figure 11: EDL of the contact width as a function of depth of focus for 140 nm contact width on mask (length was adjusted to match the target CD).

Finally, process windows (PW), i.e. the exposure dose latitudes (EDL) as a function of depth of focus (DoF), were calculated for several contact widths using measured and simulated CD data. A target of 115 nm and a tolerance of  $\pm 10\%$  were applied for the CD of the contact width. Mask errors were not included in simulation. As an example, PW's are shown in Figure 10 and 11 for a contact width on mask of 100 and 140 nm, respectively. Obviously, there is a discrepancy between simulation and experiment, which is very likely due to an inconsistent resist model. The interesting fact is however, that 2D simulation almost coincides with 3D simulation in the higher mask CD range, as demonstrated for 140 nm width. This implies here that the mask CD offset between 2D and 3D simulation does not have a significant

impact on PW. However, this behaviour changes when looking at smaller contact widths. 3D simulation delivers a lower PW for 100 nm width than 2D simulation. So far, diffraction effects on the small mask pattern are believed to be responsible for the loss in PW. Moreover, an additional contribution may arise from deficiencies of the resist model used. The question is whether 2D simulation can be applied using a mask CD correction in order to get the same results as in 3D simulation. Thus, 2D simulations were repeated using the mask CD offsets as given above. As for 140 nm contact width, the result matches perfectly with the one obtained by 3D simulation. In case of 100 nm contact width however, the discrepancy between 3D and 2D (with adjusted mask) is even higher than before. This is probably due to a systematic difference between 3D and 2D simulation which can be seen more clearly in Figure 12. It shows the calculated DoF at 5% exposure dose latitude as a function of mask CD. When looking at results obtained without considering mask errors first, the DoF calculated by 2D simulation increases steadily with decreasing mask CD, and is very similar to the one obtained by 3D simulation for mask CD's above 120 nm. Below this value however, agreement is no more given. The difference in DoF increases when further decreasing the mask CD. This cannot be avoided by a mask CD correction in 2D simulation, as also shown in Figure 12.

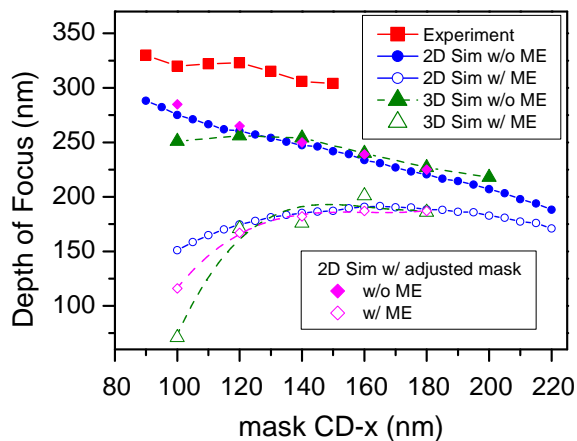


Figure 12: Process window (depth of focus at 5% exposure dose latitude) of the contact width, with and without considering a mask CD error (ME) of  $\pm 2$  nm (1X), as a function of mask CD (width). A target CD of 115 nm and a CD tolerance of  $\pm 10\%$  were applied.

When considering a constant mask error of  $\pm 2$  nm (1X) during calculation, a rather different curve with a weakly pronounced maximum was obtained for the overlapping process window by 2D simulation. Again, there is a fair agreement between 2D and 3D simulation down to about 120 nm mask CD. Below this limit however, the DoF declines much faster with decreasing mask CD if a mask topography is used in simulation. This discrepancy cannot be resolved by introducing a mask CD correction although such a correction reduces the difference in DoF between 2D and 3D simulation (s. Figure 12).

#### 4. CONCLUSIONS

Full resist simulations of contact patterns using both 2D and 3D attenuated phase shifting masks were carried out to examine the quality of prediction with respect to printed CD in resist, MEEF, and PW in comparison to experimental results. It has been demonstrated that there are significant differences between 2D and 3D simulation in terms of the printed CD in resist in dependence on mask CD and exposure dose. The behaviour observed in 3D simulation can however be described by 2D simulation if a mask CD correction is applied for both contact width and length. In case of rectangular contact holes, the CD offset between 2D and 3D simulation is different for width and length, and exhibits a non-linear function on 3D mask CD, i.e. increases with decreasing mask CD. As for the prediction of MEEF, a good agreement has been found between simulation and experiment. In particular, only minor differences between 2D and 3D simulation were observed in the mask CD range of 100 - 140 nm which can be resolved by applying the same mask CD correction in 2D simulation. As for the prediction of PW's, 2D and 3D simulation deliver very similar results above 120 nm mask CD independent of the mask error included in simulation. With decreasing mask CD below this limit however, PW's are more and more overestimated by 2D simulation in comparison to 3D simulation. Furthermore, a mask CD correction does not help to bring 2D simulation in accordance with 3D simulation in the lower mask CD range. It has been shown by experiment and simulation that for the same contact size in resist there is a minimum of the contact length on mask in dependence on the width. Fair agreement between 2D and 3D simulation was obtained above 180 nm mask CD whereas a strong difference was observed below this region. Especially the location of the experimentally observed



minimum at 145 nm mask CD is reasonably described only by 3D simulation. Thus, 2D simulation fails to predict the correct mask bias in the lower mask CD region. In addition, a mask CD correction would not help in this case.

Summarizing, the prediction of realistic mask biases and PW's in the lower mask CD range is only possible by 3D simulation, and not by introducing mask CD offsets in 2D simulation. 2D simulation in conjunction with a well calibrated resist model is sufficiently reliable in the higher mask CD range. It would be interesting whether the mask CD limits given above will change with pitch, mask type, and imaging settings. It is, for example, expected that the impact of a 3D mask on the simulation result increases with decreasing pitch. Since the mask CD for small pitches of future technology nodes cannot be as large as the CD of pitches of current nodes, the 3D effect will become even more important.

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