Photoresist 3D profile related etch process simulation and its application to full chip etch compact modeling

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ABSTRACT

The optical proximity correction (OPC) model and post-OPC verification that takes the developed photoresist (PR) 3D profile into account is needed in the advanced 2Xnm node. The etch process hotspots caused by poor resist profile may not be fully identified during the lithography inspection but will only be observed after the subsequent etch process. A complete mask correction that targets to final etch CD requires not only a lithography R3D profile model but also a etch process compact model. The drawback of existing etch model is to treat the etch CD bias as a function of visibility and pattern density which do not contain the information of resist profile. One important factor to affect the etch CD is the PR lateral erosion during the etch process due to non-vertical PR side wall angle (SWA) and anisotropy of etch plasma source. A simple example is in transferring patterns from PR layer to thin hard mask (HM) layer, which is frequently used in the double pattern (DPT) process. The PR lateral erosion contributes an extra HM etch CD bias which is deviated from PR CD defined by lithography process. This CD bias is found to have a nontrivial dependency on the PR profile and cannot be described by the pattern density or visibility. In this report, we study the etch CD variation to resist SWA under various etch conditions. Physical effects during etch process such as plasma ion reflection and source anisotropy, which modify the local etch rate, are taken into considerations in simulation. The virtual data are generated by Synopsys TCAD tool Sentaurus Topography 3D using Monte Carlo engine. A simple geometry compact model is applied first to explain the behavior of virtual data, however, it works to some extent but lacks accuracy when plasma ion reflection comes into play. A modified version is proposed, for the first time, by including the effects of plasma ion reflection and source anisotropy. The new compact model fits the nonlinear etch CD bias very well for a wide range of resist SWAs from 65 to 90 degrees, which covers the resist profile diversities in most real situations. This result offers a potential application for both resist profile aware and etch process aware mask correction model in the mask synthesis flow.

Keywords: etch model, R3D model, OPC, pattern density, etch retargeting, RIE, plasma ion reflection

1. INTRODUCTION

In the semiconductor micro-fabrication, wet etch and plasma etch processes are used to transfer the patterns from previous layer (usually the photoresist) to underlying layer. Unlike the wet etch process which is isotropic in all directions, plasma etch is anisotropic and highly material selective that performs a nearly vertical etching as shown in figure 1. The plasma etch is used to produce a profile with very high aspect ratio.

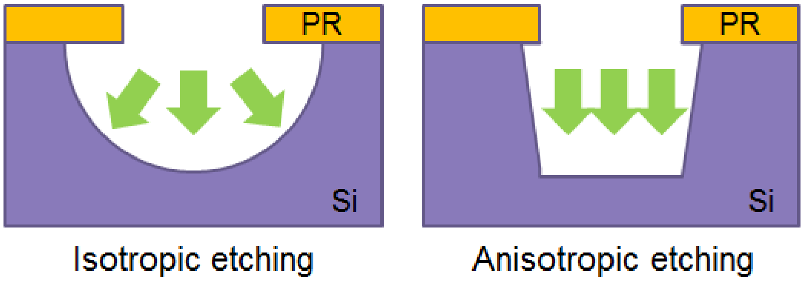

Figure 1. Wet etching (isotropic) and plasma etching (anisotropic) processes. The plasma etch such as reactive ion etching (RIE) system can also contain a fraction of isotropic component in the etch chamber.

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Capability of modeling the critical dimension (CD) of etched layer is much more important since its physical size directly affects the device electrical performance. In practice, the pattern transfer from photoresist lithography CD to etch CD is not ideal, and a good lithography model does not imply a good etch CD prediction. In the Deep Reactive Ion Etching (DRIE) system, the CD of etched layer usually shows a nonzero and non-constant bias to original mask (photoresist) CD. The CD bias varies from pattern to pattern and has complicated dependency on etch process conditions such as plasma ion energy, angular distribution, gas components, pressure, material etch rate, etc…

The mask correction model that targets for etch CD is more difficult than lithography resist CD. Due to lack of physics-based compact model, a rule-based etch bias approach, which needs extensively experimental works, is adapted for years over several technology nodes. The existing empirical model relates the etch bias to pattern density and visibility, however, it is a simplified empirical approach that may not meet the desired accuracy requirement for the advanced nodes. The empirical etch bias model is also not a etch process aware compact model and does not contain the information of resist 3D (R3D) profile.

With the continuing drive towards smaller feature sizes, the developed resist profile after lithography process can have severe resist top loss and tilted sidewalls. This non-perfect resist profile cannot be easily inspected by top-down CDSEM but can be well calibrated by R3D model. Although it may or may not cause failures in the subsequent etch process, it will always modify the etch CD bias from ideal situation that the PR profile is usually assumed to be perfect. For example, the PR lateral erosion during etch process, due to finite PR etching rate and profile SWA, is one of the most important factor to change the etch CD bias. This local change could be a few nms, which cannot be ignored for advanced nodes. The PR lateral erosion is a dynamic process during etching and the etch CD bias from it cannot be modeled by pattern density or visibility. Figure 2 shows this schematically. A complete etch bias model must consider the effect of PR erosion under various etch process conditions to improve the model accuracy.

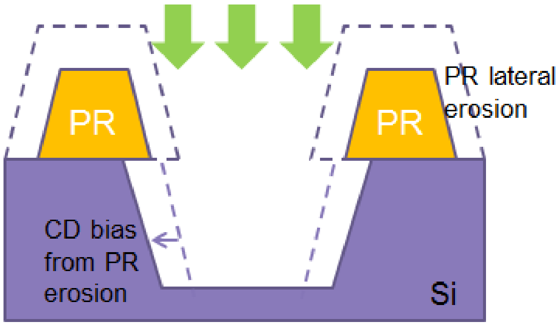


Figure 2. Schematic diagram of etch CD bias resulted from PR lateral erosion during etch process. This CD bias cannot be modeled by pattern density or visibility.

2. PLASMA ETCH PROCESS

Before constructing the compact model, we would like to give a brief introduction to plasma etch process. This helps us to gain some physical insights in building the compact model, and to understand the root cause of etch CD bias variation. The fundamental physics of plasma etching involves a sequence of physical-chemical surface reactions that is too complicated to be simulated rigorously even from the first principle approach. What actually happened on the etched surface is not just material etching. It also includes sputtering, re-deposition, passivation, re-emission, and reflection process, simultaneously. All of these processes are both material and geometry dependent. The plasma source distribution, material selectivity, chamber pressure, and gas components are controlling factors in an etch module. This diversity of combinations create various etch recipes for every specific purposes.

Alternatively, a topography model that utilizes the macroscopic etch rate avoids the microscopic complexity but also keeps the fundamental features of plasma etching. In the topography model, the time evolution of etched profile is calculated by specifying the etch rate at all surface points. Therefore, the problem is reduced to model the geometry dependent etch rate from plasma source. The etch rate at a given surface point is proportional to the next flux which is contributed from several particle sources, as shown in figure 3.

The plasma source in the etching chamber is considered to consist of two kinds of particles: the neutral particles and charged particles (ions). These two particle sources are assumed to be independent and do not interact with each other. However, they can interact with material in various ways and contribute both direct and indirect flux to material surface. The neutral particles are assumed to be isotropic source that is characterized by $\cos(\theta)$ angular distribution, where θ is the angle between the particle path left from source region and vector normal to wafer plane. It has a probability to directly react with material (modeled by sticking probability) when the neutral particle hit the surface and thus triggered the etch event. If the etch event does not happen, the neutral particle is re-emitted to other surface point and reacts with material locally. The neutral particle re-emission is also assumed to be isotropic with $\cos(\theta)$ angular distribution, and thus it is possible to have multiple re-emissions. The net flux of neutral particles to a certain surface point is the summation of direct flux plus the indirect flux due to re-emission from all surrounding points.

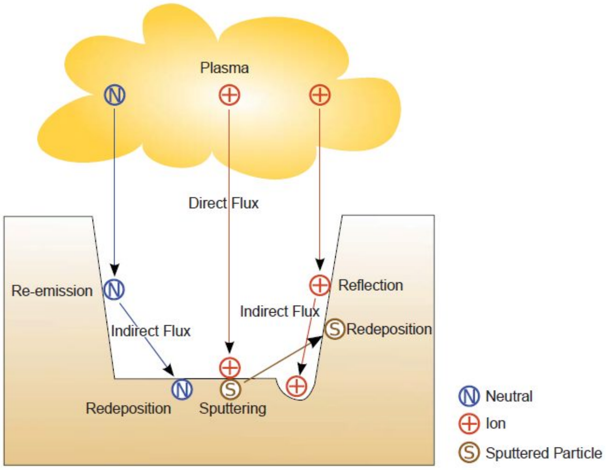


Figure 3. Plasma etch process. The neutrals (isotropic) and ions (anisotropic) are two particles in the plasma source that can directly etch at material surface. There indirect flux from re-emission, re-deposition, and ion reflection that cause a local change of etch rate and result in various etch profile.

The ion flux source is characterized by a directional angular distribution: $\cos^{m}(\theta)$, where m is the exponent to control the ion source anisotropy. The exponent m is usually larger than 100 in the RIE system, therefore the ion flux is highly anisotropic with nearly vertical direction to wafer plane. The ions interact with material in several ways depending on the ion energy. The high energy ions coming from plasma source not only etch the surface directly but also sputter the material and cause re-deposition on other locations. The re-deposition material could be the reaction byproduct which is quite different from the etched material. It is possible to form a passivation layer, which adds resistance to the etching process, and therefore complicate the etch process.

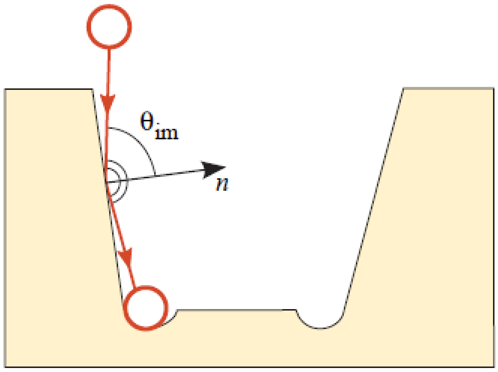


Figure 4. Low energy plasma ions can be reflected by surface and cause local change on the surface etch rate.

On the other hand, the low energy ions can be reflected by the surface depending on the incident angle, surface profile and ion energy. The reflected ions contribute an indirect flux to the etched profile, as shown in figure 4, and play an important role in an RIE system. The ion reflection probability is given by [1],

$$P_{reflection}(\theta_{in}) = \min\left\{1, k\left[\frac{1}{2\pi} + \left(\frac{\pi}{4}-\frac{1}{3}\right)\left(\frac{\pi}{2}-\theta_{in}\right)^{-2} + \frac{5}{\pi^3}\left(\frac{\pi}{2}-\theta_{in}\right)\right]\right\}$$

The constant k, which depends on the atomic number of surface material and ion energy, is the fitting parameter (normalize to 0 ~ 1) in the etch model. Once the ion is reflected and hit the material surface, it is assumed to etch the surface and there will be no subsequent reflections. Table 1 summarizes all effects in plasma etching.

Plasma source	Angular Distribution	Material Interaction
Ion flux (anisotropic)	$\cos^m \theta$	
		Reflection
		Sputtering
		Re-deposition
Neutral flux (isotropic)	$\cos \theta$	
		Re-emission

Table 1. Physical effects in plasma etch process and parameters in the etch topography model.

The total etch rate at any surface point is proportional to the sum of neutral flux and ion flux, that is, [2]

$$R_{etch}(x,y,z) = R_0\big((1-an) * \Gamma_{neutral}(x,y,z) + an * \Gamma_{ion}(x,y,z)\big)$$

where an (= 0 ~ 1) is anisotropy parameter to specify the percentage of two source particles between neutral flux $\Gamma_{neutral}$ and ion flux Γ_{ion}. R_0 is the etch rate on an unshadowed flat surface. As described above, neutral flux consists of direct (isotropic) flux and re-emission flux. Ion flux consists of direct (anisotropic) flux as well as indirect re-deposition and reflection flux.

3. SIMULATION SETUP

To study the etch CD variation due to PR lateral erosion, a profile in figure 5 is considered with fixed PR space CD and height and varying SWA from 65 degree to 90 degree. We use a tri-layer film stack setup that consists of PR / hard mask (HM) / Silicon. The thickness of HM (=20nm) is chosen to be much thinner than the thickness of PR that is set to 100nm in our simulation. This is for the purpose of reducing the vertical visibility of HM layer during etching process, therefore the difference between top and bottom CD of HM layer can be ignored. This structure is frequently used in DPT process that the pattern is transferred first from PR to HM and then from HM to Si.

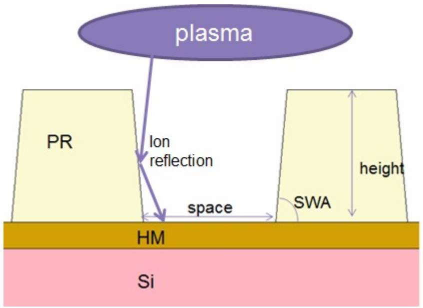


Figure 5. Film stack structure used in Monte Carlo simulation. PR space bottom CD and height are fixed, and SWA is varying from 65 to 90 degree. PR to HM etch rate is set to 1:10. Etch process conditions are modeled by ion reflection and source anisotropy. Etch stop when plasma hit the Si surface. Etch CD is extracted from HM bottom CD and CD bias is defined by the difference between HM bottom CD and PR space bottom CD.

The simulation is done with Synopsys TCAD tool Sentaurus Topography 3D using Monte Carlo engine. The etch rate between PR and HM is set to 1:10. The plasma source contains neutral and ion flux whose relative weights are controlled by the anisotropy factor. In this case study, only the ion reflection is considered. Neutral particle re-emission, ion sputtering and re-deposition are ignored. The grid mesh is set to 2nm in all dimensions. The etch process stops when the plasma hits the Si surface, and the etch CD is extracted from the HM bottom. The etch CD bias is defined by the difference between PR space bottom CD and HM bottom CD.

4. RESULT AND COMPACT MODEL FITTING

A simple etch bias compact model to account for the contribution from PR lateral erosion can be written down by, based on the geometrical argument [3],

$$Model\ \#1\text{: CD}_{\text{bias}} = c_0 + \frac{c_1}{\tan\,(SWA)}$$

This is the geometrical compact model where the PR profile is approximated to a trapezoidal shape characterized by SWA, the sidewall angle. The parameters c_0 and c_1 are the fitting parameters that depend on the etch process conditions. This model assumes the plasma flux is uniform over the PR surface and no ion reflection. To account for the effect of ion reflection and source anisotropy, the model is modified to [3],

$$Model\ \#2\text{: CD}_{\text{bias}} = c_0 + \frac{c_1}{\tan\,(SWA)} + f\left(P_{refleciton}(SWA)\right)$$

where $\text{P}_{reflection}$ is the reflection probability that depends on the ion energy and SWA. The anisotropy parameter is included in the function form of f() that depends the etch system and material selectivity. Conceptually, the ion reflection reduces the PR erosion but enhances the speed of HM etching. In the presence of a fraction of isotropic plasma source, the PR lateral erosion is no more constant scale with tan(SWA). The resulting etch CD bias becomes a nonlinear function of resist SWA. A reason to choose the SWA as the model variable is that SWA can be easily calculated from a calibrated full-chip compact R3D model. The etch bias model utilizing the resist profile SWA is the key to accurate compact etch modeling and provides a tighter link from lithography model to etch model.

The virtual data from Monte Carlo simulations are fitted with these two compact models under various anisotropy and ion reflection conditions. Figure 6 shows the etch CD bias vs. the SWA without ion reflection and fully anisotropic source. The virtual data are fitted by compact model #1 and #2 and show not much difference between these two models. In this etch condition, all ions hit to resist surface and proceed to etch the material without reflection, and the etch CD bias basically follows the geometrical model as described in model #1.

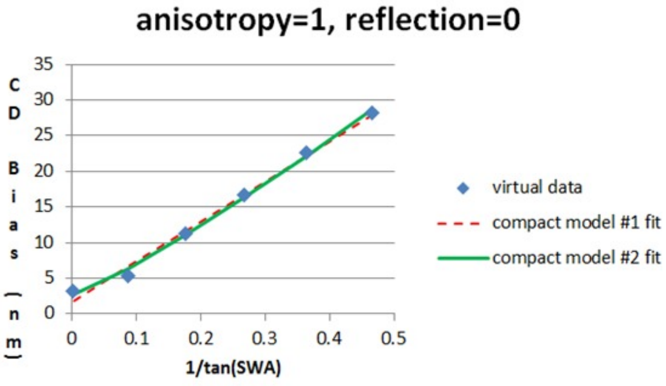


Figure 6. Etch CD bias vs. PR SWA at the conditions of no ion reflection and no isotropic flux. The virtual data are fitted by two compact models and show no much difference. The etch CD bias can be modeled by simple geometrical model. SWA is from 65 to 90 degree.

In reality, ion reflection cannot be neglected in modeling an RIE process.In general, the plasma source contains a fraction of neutral particles. By considering a finite ion reflection probability and a fraction of isotropic neutral flux, figure 7 shows that the etch bias has a nonlinear dependence on the SWA.

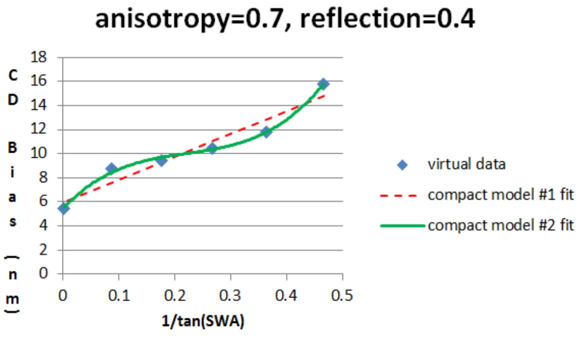
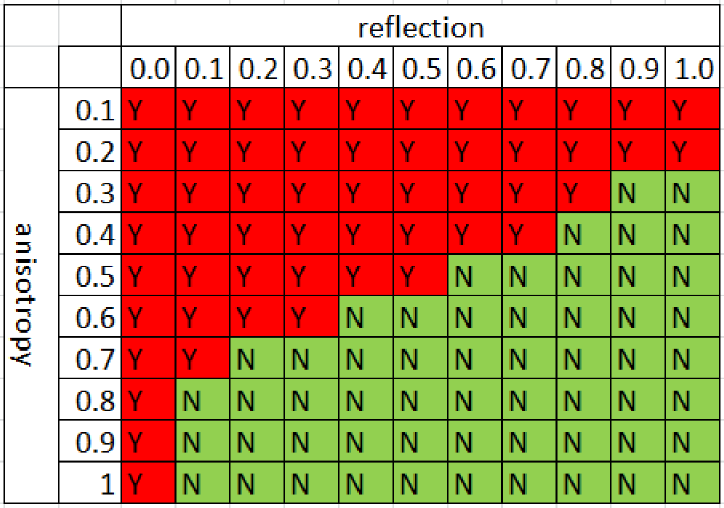


Figure 7. Etch CD bias vs. PR SWA at the conditions of finite ion reflection and finite isotropic flux. The parameter anisotropy = 0.7 means the plasma source is 30% from the isotropic neutrals and 70% from anisotropic ions. The virtual data are fitted by two compact models, however, the compact model #1 (the simple geometrical model) cannot fit the data. The compact model #2 that includes the reflection probability catches the trend of etch CD bias. SWA varies from 65 to 90 degree.

As we can see, model #1 captures the general trend well - without it, an etch model would have a flat or constant response to the varation in SWA. The nonlinear dependency indicates that a higher order model such as model #2 is needed. Model #2, with the inclusion of the probability function as a new term in the etch bias model, fits the data much better.

The detailed Monte Carlo simulations that runs through all parameter space with reflection from 0 to 1 and anisotropy from 0 to 1 are generated to study the SWA dependency at various etch conditions. The data are tested by two compact models at each process condition to check the model form coverage.



		reflection										
		0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
anisotropy	0.1	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
	0.2	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
	0.3	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N
	0.4	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N
	0.5	Y	Y	Y	Y	Y	Y	N	N	N	N	N
	0.6	Y	Y	Y	Y	N	N	N	N	N	N	N
	0.7	Y	Y	N	N	N	N	N	N	N	N	N
	0.8	Y	N	N	N	N	N	N	N	N	N	N
	0.9	Y	N	N	N	N	N	N	N	N	N	N
	1	Y	N	N	N	N	N	N	N	N	N	N

Y: can be fitted with ideal 1/tan() model

N: cannot be fitted with ideal 1/tan() model

Figure 8. Test for compact model form coverage. The virtual data set of etch CD bias vs. PR SWA is generated at each process condition (reflection, anisotropy) and fitted by two compact models. Compact model #1, the simple geometrical model, only works at the condition of small reflection or anisotropy. With increasing the reflection probability and anisotropy, compact model #1 is no longer correct. Compact model #2 that contains an additional reflection probability term can fit all process conditions without changing the model form.

The result of model form coverage is shown in figure 8. For each etch condition (anisotropy, reflection), a set of etch CD bias vs. PR SWA data is generated and fitted by two compact models. It can be seen that compact model #1 covers etch conditions of small ion reflection or anisotropy. As increasing the reflection and anisotropy, the geometrical model is failed to explain the CD bias. However, it needs to be pointed out that (not shown in here) using the compact model #2, all of etch process conditions can be fitted well without changing the model form.

5. CONCLUSION

A mask correction model that targets to etch CD is in demand for years for advanced nodes. In previous empirical approaches, etch CD bias is modeled by pattern density and visibility. However, it is not sufficient anymore for the advanced nodes. Because the resist profile after lithography process is no longer perfect in the advanced 2X nm node, it is found that the effect of photoresist (PR) erosion during etch process comes into play. The effect of PR lateral erosion depends on its sidewall angle (SWA) and plasma ion distribution and it cannot be modeled by pattern density and visibility. We studied the etch CD bias vs. PR SWA in the RIE system under various etch process conditions characterized by anisotropy and ion reflection parameters. Monte Carlo simulation is used to generate etch CD virtual data for a given input structure. The virtual data are fitted by compact models for a study of their accuracy and model form coverage. Two model terms are introduced in this etch bias model to account for the geometrical dependence and ion reflection effect. The result shows that the etch CD bias related to PR lateral erosion in RIE system can be modeled well with compact model #2. It improves the prediction accuracy of etch CD bias model and provides a potential tool for more accurate etch hotspot detection or mask correction using not only resist CD but also resist profile and etch CD.

REFERENCES

[1] T. Mizuno et al., “Analytical model for oblique ion reflection at the Si surface,” IEEE Transactions on Electron Devices, vol. 35, no. 12, 2323, (1988)

[2] Sentaurus Topography 3D, Synopsys Inc.

[3] Internal documents, Synopsys Inc.