Design specific variation in pattern transfer by via/contact etch process: full-chip analysis

Agenda

- Introduction
- Pattern density variation in die-scale modeling
- Microloading and aspect ratio (AR) induced etch rate variation – Physics behind
- Calibration
- Use models



Etch Step in Pattern Transfer Simulation Flow

Etch step is important part of the pattern transfer technology in chip manufacturing

• While the existing capabilities of the predictions of post-illumination and post-photoresist development contours are in line with the current requirements, predictions of the post-etch contours are not so good.

Etch process is characterized by strong pattern density dependency



Pattern Transfer in the Case of Contact Hole Etch





Phot 0 BARC **BARC/ME BARC/ME/OE** Full Etch NCCAVS PAG, Sunnyvale, CA. 2005 By D. Farber, B. Dostalik, B.

It would be quite beneficial for both the design and process development communities to have a design automation tool capable of analyzing the design quality regarding the shape distortions (etch bias) caused by the employed etch recipe and, visa verse, the ability of the developed recipe to handle pattern density variation of a design to be manufactured.



Plasma-assisted etch

- Plasma-assisted etch is a sequence of chemical reactions between etched material and plasmagenerated chemical species resulting generation of volatile products
- In order to initiate and sustain etch process the etchant species should be continuously generated and delivered to those surface segments where the material removal takes place – the bottoms of etched features.
- In order to have a uniform across-chip etch rate, the combination of fluxes of neutrals and ions impinged the etched surface should be a constant.







Effects of Aspect Ratio & Microloading

Etch rate variation across layout caused

- by: Across-layout variation in concentration of neutrals in the above-wafer plasma region - Microloading
 - Variation in resistance to the interfeature transport of neutrals - AR
 - Variation in plasma visibility AR

- AR variations are responsible for the distortion in etch rate, sidewall slope and etch depth developed in neighboring features
- Microloading is responsible for those distortions developed in the identical features located in different neighborhoods characterized by different pattern densities

Layout and averaged patter density











PD Dependency in Etch Processing - Microloading



C. Hedlund, H. O. Blom, and S. Berg, "Microloading effect in reactive ion etching," J. Vac. Sci. Technol. A 12, 1962–1965 (1994)



- Effect of the pattern density on etch is characterized by a specific correlation length depending on a particular process recipe
- The correlation length provides the size of layout area which effects etching of a particular feature
- Correlation length is in order of magnitude of the mean free path of the gas species λ



Main Factors of Microloading



- Consumption/reflection
- Non-uniform concentration
- Diffusion



Flux Boundary Condition Surface



Mass-balance

Differential equation for radical distribution at the flux-BC surface

- averaging the diffusion equations along the plasma thickness (L),
- using the flux BC
- and assuming that diffusion is much faster than the gas flow

Flux BC:

Radical fluxes Γ_0^i coming from plasma impinges a wafer surface. Fluxes impinged a PR surface and an etched feature are consumed with different probabilities: χ_{PR}^{i} and χ^{i} (χ^{i} is AR dependent parameter).

Density of consumed flux of neutrals, which is the difference of the densities of incoming and reflected fluxes depends on the PD:

$$\Gamma_{dS2}^{C} = \frac{N_{i}(\vec{r})c_{i}}{4} \frac{h^{2}}{\pi} \int_{0}^{2\pi R} \int_{0}^{2\pi R} \left(\chi_{PR}^{i}(1-\rho(r_{1},\phi_{1})) + \chi^{i}(AR)\rho(r_{1},\phi_{1})\right) \frac{r_{1}dr_{1}d\phi_{1}}{\left(h^{2}+\left|\vec{r}_{1}-\vec{r}\right|^{2}\right)^{2}} = \frac{N_{i}(\vec{r})c_{i}}{4} \frac{h^{2}}{\pi} \int_{0}^{2\pi R} \left(\chi_{PR}^{i}(1-\rho(r_{1},\phi_{1})) + \chi^{i}(AR)\rho(r_{1},\phi_{1})\right) \frac{r_{1}dr_{1}d\phi_{1}}{\left(h^{2}+\left|\vec{r}_{1}-\vec{r}\right|^{2}\right)^{2}} = \frac{N_{i}(\vec{r})c_{i}}{4} \frac{h^{2}}{\pi} \int_{0}^{2\pi R} \left(\chi_{PR}^{i}(1-\rho(r_{1},\phi_{1})) + \chi^{i}(AR)\rho(r_{1},\phi_{1})\right) \frac{r_{1}dr_{1}d\phi_{1}}{\left(h^{2}+\left|\vec{r}_{1}-\vec{r}\right|^{2}\right)^{2}} = \frac{N_{i}(\vec{r})c_{i}}{4} \frac{h^{2}}{\pi} \int_{0}^{2\pi R} \left(\chi_{PR}^{i}(1-\rho(r_{1},\phi_{1})) + \chi^{i}(AR)\rho(r_{1},\phi_{1})\right) \frac{r_{1}dr_{1}d\phi_{1}}{\left(h^{2}+\left|\vec{r}_{1}-\vec{r}\right|^{2}\right)^{2}} = \frac{N_{i}(r_{1},\phi_{1})}{4} \frac{h^{2}}{\pi} \int_{0}^{2\pi R} \left(\chi_{PR}^{i}(1-\rho(r_{1},\phi_{1})) + \chi^{i}(AR)\rho(r_{1},\phi_{1})\right) \frac{h^{2}}{\left(h^{2}+\left|\vec{r}_{1}-\vec{r}\right|^{2}\right)^{2}} = \frac{N_{i}(r_{1},\phi_{1})}{4} \frac{h^{2}}{\pi} \int_{0}^{2\pi R} \left(\chi_{PR}^{i}(1-\rho(r_{1},\phi_{1})) + \chi^{i}(AR)\rho(r_{1},\phi_{1})\right) \frac{h^{2}}{\pi} \frac{h^{2}}{\pi} \int_{0}^{2\pi R} \left(\chi_{PR}^{i}(1-\rho(r_{1},\phi_{1})) + \chi^{i}(AR)\rho(r_{1},\phi_{1})\right) \frac{h^{2}}{\pi} \frac{h$$

$$=\frac{\Gamma_{i}(\vec{r})}{\pi h^{2}}\int_{R}\chi(\vec{r}+\vec{r}_{1})\rho(r_{1},\phi_{1})\frac{dr_{1}^{2}}{\left[1+\left(\frac{\vec{r}_{1}}{h}\right)^{2}\right]^{2}}$$



$$0 = D\left\{ \left[\frac{\partial^2 \overline{n}_i}{\partial r^2} + \frac{1}{r^2} \cdot \frac{\partial^2 \overline{n}_i}{\partial \phi^2} + \frac{1}{r} \cdot \frac{\partial \overline{n}_i}{\partial r} \right] \right\} - \frac{\overline{n}_i \overline{c} F(r, \phi)}{4L} + \gamma - k_v \overline{n}_i$$

$$F(r, \phi) = \int \hat{\chi}(\vec{r}' + \vec{r}) \rho(\vec{r}' + \vec{r}) \frac{d^2 \vec{r}'}{\left(1 + \frac{\vec{r}'^2}{h^2}\right)^2}$$

$$\hat{\chi}(\vec{r}') = \begin{cases} \chi \\ \chi \end{cases}$$
Stenger AIChE Journal 33 1187-1190 (1987)

 χ_{PR}

Surface "2" \vec{r}_2 dS $\delta\Omega = \sin\Theta\delta\Theta\delta\varphi$ $= |\vec{r_1} - \vec{r_2}|$ Surface "1'

Stenger, AIChE Journal, 33, 1187-1190 (1987)



Mass-balance

Differential equation for across-die distribution of the radicals

Due to complex character of dependency of the introduced parameters on the plasma recipe as well as the difference in generation rates of different radicals it is reasonable to introduce a dimensionless form for radical concentration:

This transformation leads to the dimensionless form of the mass balance equation: $(\alpha \partial^2) = \overline{\alpha} \partial^2$

Here:

$$n_0 = \frac{\gamma}{k_V} \text{ and } \theta_0 = n_0 \left(\frac{\gamma \lambda^2}{D}\right) = \frac{\overline{c} n_0}{3\gamma \lambda}$$

Solution of these mass balance equations generates across-die distributions of concentrations of all radicals participating in etch reactions. Gas-kinetic properties of radicals (D, λ , c) are calculated based on Chapman-Enskog kinetic theory.

Approximate solution of the mass-balance equation clearly demonstrates that an across-die distribution of radicals is characterized by a complex PD dependency, more complicated than the "traditional" reverse PD: 1/PD.



$$1 - \theta(\vec{r}) \left[\frac{1}{\theta_0} + \frac{3}{4} \frac{\lambda}{L} F(\vec{r}) \right] + \lambda^2 \Delta \theta(\vec{r}) = 0$$

Approximate solution

$$\theta(\vec{r}) \approx \frac{1 - \lambda^2 \Delta \left[\frac{1}{\theta_0} + \frac{3}{4} \frac{\lambda}{L} F(\vec{r})\right]}{\left[\frac{1}{\theta_0} + \frac{3}{4} \frac{\lambda}{L} F(\vec{r})\right]}$$

$$F(r, \phi) = \int \hat{\chi}(\vec{r}' + \vec{r}) \rho(\vec{r}' + \vec{r}) \frac{d^2 \vec{r}'}{\left(1 + \frac{\vec{r}'^2}{h^2}\right)^2}$$
Sticking PD-GDSII (1+ $\frac{\vec{r}'^2}{h^2}$)
Visibility factor

Radical Flux to the Feature

• When a radical distribution across "effective reactive" surface is known we can determine a flux coming to the feature from a small area of the "effective reactive" surface and to integrate it through the all area of visibility.



Schematic for determination of the consumed radical flux

Output of the Microloading Analysis







Intra-Feature Radical Transport Resistance





Etch Modeling Backbone



Etch Model

Etch model, representing mathematical formulation of etch mechanism, provides a relation between fluxes of all etch-important species coming to any point at the etched surface and the etch rate at this point.

Example of modeling SiO₂ Etch by Fluorocarbon Plasmas

 CF_x radical fluxes result in SiO₂ etch and C_xF_y polymer deposition

O-atom flux is a major cause of the polymer removal

Precursors for the etch reactions are formed at the polymer-SiO₂ interface by ion-induced energy reactions: "-Si-O-" + E = "Si-" + "O-". Energy flux reaching the interface is controlled by the polymer thickness.

Radical reactions between Si- and O- from SiO_2 and F and C from gas phase and polymer layer are responsible for the silicon oxide etch





Reaction Kinetics

$$\begin{aligned} \frac{\partial x_C}{\partial t} &= k_D \Gamma_{CF_2} - k_R x_C \Gamma_O - k_{etch}^C x_C \theta \\ \frac{\partial x_F}{\partial t} &= k_D \Gamma_{CF_2} - k_{etch}^F x_F \theta \\ \frac{\partial \theta}{\partial t} &= \eta F(H)(1-\theta) - k_{etch}^C x_C \theta \\ F(H) &= \Gamma_i E_0 \left(1 - \frac{M_C}{\rho_S H^*} x_C \right) \\ H &= \frac{x_C M_C}{\rho_S} \end{aligned}$$

 x_{c} is the carbon fraction in $C_{x}F_{y}$ polymer layer; θ is the fraction of precursors formed at the SiO₂ polymer interface

 $\mathbf{H}_{\mathsf{CxFy}}$ is the thickness of polymer layer.

Thin & Thick Polymer Regimes

T. Tatsumi, M. Matsui, M. Okigawa, and M. Sekine, J. Vac. Sci. Technol. B 18, 1897-1902 (2000)



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Ion Energy Loss in Polymer Layer



Sci. Technol. B 18, 1897-1902 (2000)



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(b)

Approximation of "Thin Polymer" Layer

- Rate of generation of active precursors on SiO₂ surface by ions penetrated the adsorbed layer is much higher than the rate of their disappearance by means of etch reactions
- Rate of the reaction between silicon and fluorine atoms is faster than the rate of reactions of polymer formation.

$$H \approx \frac{M_{C}}{\rho_{S}} \frac{k_{D}' \Gamma_{CF_{2}}}{k_{R} \Gamma_{O} + k_{etch}^{C}}$$
$$ER \approx K_{etch} k_{D} \Gamma_{CF_{2}} \left(1 - \frac{k_{etch}^{C} k_{D}' \Gamma_{CF_{2}}}{\eta \Gamma_{i} E_{0} \left(k_{R} \Gamma_{O} + k_{etch}^{C} \right)} \right)$$



Tatsumi, T., Hikosaka, Y., Morishita, S., Matsui, M., and Sekine, M., "Etch rate control in a 27 MHz reactive ion etching system for ultralarge scale integrated circuit processing," J. Vac. Sci. Technol. A 17, 1562-1569 (1999).



"Thick Polymer" Approximation

Ion-energy transfer through polymer layer is a limiting step in SiO₂ etch rate





Matsui, M., Tatsumi, T. and Sekine, M., "Relationship of etch reaction and reactive species flux in C4F8/Ar/O2 plasma for SiO2 selective etching over Si and Si3N4," J. Vac. Sci. Technol. A 19, 2089-2096 (2001).



Etch Stop Condition

Etch stops when ions lose all their energy while penetrating the C-F layer. A condition for the etch stop is follows:

$$\frac{k_D'(\Gamma_i^{LE})\Gamma_{CF_2}}{k_R\Gamma_O} = \frac{\rho_S}{M_C} \frac{E_0^{\frac{1}{3}}}{\mu}$$

Knowledge of distributions of ion-neutrals fluxes along the etched surface:

 $\Gamma_i(x, y), \Gamma_{CF_2}(x, y), \Gamma_O(x, y)$

allows to determine a regions where etch is completely stopped



VEB+ - based correlations









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VCE Input/Output



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Input/output to VCE tool - I

VCE





Calculation of Gas Kinetic Parameters

- Calculation of binary diffusivities

$$D_{ij} = 0.0018583 \frac{\sqrt{T^{3} \left(\frac{1}{M_{i}} + \frac{1}{M_{j}}\right)}}{P \sigma_{ij}^{2} \Omega_{ij}}$$

Here
$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$
, $\Omega_{ij} = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}$ and $T^* = \frac{T}{\varepsilon_{ij}}$, $\frac{\varepsilon_{ij}}{k_B} = \sqrt{\frac{\varepsilon_i}{k_B} \frac{\varepsilon_j}{k_B}}$

A = 1.06036, B = 0.15610, C = 0.193, D = 0.47635, E = 1.03587, F = 1.52996, G = 1.76474, H = 3.89411. Total gas pressure P in [atm], temperature T in [K] and cross-section σ_{ii} in [A]. Parameters T* and Ω_{ij} are dimensionless. The resulting binary diffusivities D_{ij} are in [cm²s⁻¹]. Effective diffusivity of i-th radical in the gas mixture: $D_i = \frac{(1-x_i)}{x_k} x_k$ is the mole fraction of

the k-th component Calculation of binary velocities $c_{ij} = 100 \sqrt{\frac{8RT}{\pi} \left(\frac{1}{M_i} + \frac{1}{M_j}\right)}$. Velocities are in [cm/s]. $c_i = \frac{\left(1 - x_i\right)}{\sum_{k \in \mathcal{K}} \frac{x_k}{C_k}}$

Effective velocities:

$$\lambda_i = 3 \frac{D_i}{c_i}$$





Calibration Methodology

- The major difference between the fully-coupled multi-scale simulations and the approach proposed in this paper is in a calibration-based nature of predictability of the latter one.
- All unknown parameters of the employed model, such as plasma generation-recombination rates, chemical reaction rates, sticking coefficients, interaction radiuses, etc, are calibrated/optimized based on measured post-etch geometries of the different features characterized by a variety of AR and PD.
- This calibration confines our model with the particular type of the reactor and process. While it is
 perfectly well with the process-aware design optimization, however, the calibration-based approach
 introduces some restrictions on the use-model for the design-aware process optimization. Calibrated
 model can be used mostly for exploring the effect of small variation in process parameters on the PDinduced variability by means of the proper link with a reactor-scale model.

	Hole/Pitch=0.135/0.220um	Hole/Pitch=0.140/0.600um	Hole/Pitch=0.138/0.600um
	W/N23 CENTER (1)	W/N23 CENTER (2)	W/N23 CENTER (3)
5	1 A A A A		
cente			
	123368 10.0kV X100K 300nm	123369 10.0kV X100k'''300'nm	123370 10.0kV X100K'''300nm



Calibration Methodology

Allocate a number of vias/contacts not less than the number of model parameters. The best practice is to pick the features from the regions characterized by different pattern densities

- Measure either etch rates, post-etch via depth, or CD for these features
- Run the VCE and extract from the data-base the relative fluxes of all radicals coming to the measured features: γ_{ij}
- Run a optimization module to extract parameters values providing the best fit between calculated and measured characteristics.





Correlation of 92% was achieved for process node: 55 nm; test chip size of 25.2x30.7 mm Measured values (plotted by triangles) and calculated values (squares) of vias (a) with top diameter 110 nm, and (b) with top diameter 67 nm.



VCE Capability

Based on accurate calculation of an across-die flux variation of radicals participating in etch reactions we can predict:

Across-die etch rate variation



VCE Capability

Effect of dummy fill on across-die CD variation

No dummy fill



With dummy fill





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VCE Capability

Across-die etch hot-spots distribution





VCE/LE Capabilities

Post-etch contours





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APPLICATIONS of VCE



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Hot-spot check: Bottom CD variation

 VCE calibrates the bottom CD model based on the customer provided measurements of postlitho top CD and post-etch bottom CD for a number of features

VCE predicts bottom CD variation through the entire chip



Measured values (plotted by diamonds) and calculated values (squares) of vias with top diameter of 67 nm (as-designed)







Process-Aware Design Optimization vs. Design-Aware Process Optimization

Upon completion of the hot spot check the following correction actions can be undertaken:

DESIGN

PROCESS

- Intelligent dummy-fill
- Mask correction at the MDP stage

- Tuning the process parameters
- Modification of the processing gas composition



Design optimization by means of dummy via insertion



Process optimization

• VCE predicts bottom CD variation through the entire chip for different process recipes

- Two cases characterized by the identical etch process recipes are considered. The only difference between these two cases is that some amount of CHF3 was added to the inlet gas flow in the Case 2.
- Addition of CHF3 dramatically reduces the fluorine atom concentration in the plasma bulk.
- The later causes an excessive polymer deposition at the etched feature sidewalls and bottom that results in a bigger etch CD bias.





F Concentration, mass fraction







Summary of Reactor-scale simulation

Case 1

Molar Fractions

С	CF	CF2	CF3	CF4	F	F2	
0.0006693	0.0099706	0.0107488	0.0139769	0.8800164	0.0837992	0.0008187	
Radical Fluxes (#/cm2/sec)							

CF	CF2	CF3	F
5.418E+15	9.415E+15	1.579E+15	9.474E+16
Ion Fluxes (#/cm2/sec)		
CF+	CF2+	CF3+	Sum
1.430E+15	2.760E+15	1.310E+16	1.729E+16

Max. Ion Current: 4.85 mA, Vrf_b=181V Plasma Potential =+178.8V Aver. RFpotential -147.2 Vb/-314.1Vt E_o = 326 V

Case 2

Molar Fractions

С	CF	CF2	CF3	CF4	F	F2	CHF3	HF
0.0002971	0.0065974	0.0101139	0.0177320	0.8162692	0.0457770	0.0005838	0.0914919	0.0111377

Radical Fluxes (#/cm2/sec)						
CF	CF2	CF3	F			
2.835E+15	8.031E+15	2.713E+15	4.879E+16			
Ion Fluxes (
CF+	CF2+	CF3+	Sum			
5.870E+14	1.690E+15	8.070E+15	1.035E+16			
			-			

Max. Ion Current: 2.26 mA, Vrf_b=271V Plasma Potential =+95.5V Aver. RFpotential -388 Vb/-253 Vt E_o = 484 V



Neutral flux maps





CD variation maps: case1 vs case2



OBSERVATION: FIB inspection of 0.26 um via after etching. (a) dense vias; (b) isolated via. Dense vias etch faster than isolated via, i.e. *inverse micro-loading effect*.



Pattern Density & Radical Fluxes Maps





Flux Distributions





Across-Die Distribution of Etch Stop Threshold



- SEMbar1 and SEMbar2, which are identical regarding the local pattern density, are characterized by different radical flux distribution, that transfers into different post-etch feature profiles.
- Radical flux variation in SEMbar is determined by the global pattern density distribution rather than the local one inside this segment of layout.
- Calculated full-chip radical flux distributions suggest that the etch stop is more probable at the iso-via location than in SEMbar.
 - An accurate design/process optimization could be achieved only by analyzing test-chip design with Mentor-VCE tool.



Calibration/Prediction – Resist Model

- CM1(Compact Model 1) is a Mentor Graphics resist model. It provides a dense simulation by considering acid and base neutralization, diffusion length during the exposure, baking, and resist development phases.
- The output of the model is a resist contour obtained from the exposure threshold *T* :

$$M = \left(\left(\nabla^k I_{\pm b} \right)^n \otimes G_{s,p} \right)^{1/n}$$

 $\sum c_i M_i(I) = T$

$$G_{s,p}(r) = \frac{1}{\pi s^2} \exp\left(-\frac{r^2}{s^2}\right) L_p\left(2\frac{r^2}{s^2}\right)$$

• Each term $M_i(I)$ is of the form:

+/-*b* is the neutralization operator (+ for acid, - for base concentration),





 Model is calibrated on BARC opening CD.

Result : R2 = 0.81



Calibration/Prediction – ARC Etch

- Correction for Microloading nature of BARC etcing is added: $\frac{CD_{BARC.o} - CD_{Litho}}{CD_{Litho}} = \delta' + \alpha \gamma_0 [1 - \beta (1 - \kappa D)]$ $CD_{BARC,o} = CD_{Litho} \cdot \{\delta + \alpha \gamma_{O}[1 - \beta(1 - \kappa D)]\}$ $\alpha, \beta, \delta, \kappa$: calibration parameters. : Simulated BARC CD opening prior to main CD_{BARC.0} etching. : Simulated resist opening CD using CM1 resist CD_{Litho} model (calibrated on BARC opening CD measurements) : Normalized flux of néutral i. γ_i : Density of resist opening. • D(Fine term $\beta(1 - \kappa D)$) is introduced to explain carbon assisted polymer formation. Carbon in resist film is considered to be the source.
 - CDSEM measurement error of 3nm is taken into account. TRS 2001 eds. Metrology, p.8
 - Result : R² = 0.82







Calibration/Prediction - Main Etch

BARC CD widening due to PR loss during main etching is considered:

$$\frac{CD_{BARC} - CD_{BARC.o}}{CD_{BARC.o}} = \alpha_0' + \alpha_1 \gamma_F [1 - \alpha_2 (1 - \alpha_3 D)] \ge 0$$

$$\frac{CD_{Bott} - CD_{BARC}}{CD_{BARC}} = \beta_0' + \beta_1 \frac{\gamma_{CF}}{\gamma_F} + \beta_2 (\frac{\gamma_{CF}}{\gamma_F})^2 + \beta_3 (\frac{\gamma_{CF}}{\gamma_F})^3 \le 0$$

$$CD_{Bott} = CD_{BARC} \cdot [\beta_0 + \beta_1 (\frac{\gamma_{CF}}{\gamma_F}) + \beta_2 (\frac{\gamma_{CF}}{\gamma_F})^2 + \beta_3 (\frac{\gamma_{CF}}{\gamma_F})^3]$$

$$= CD_{BARC.o} \cdot \{\alpha_0 + \alpha_1 \gamma_F [1 - \alpha_2 (1 - \alpha_3 D)]\} [\beta_0 + \beta_1 (\frac{\gamma_{CF}}{\gamma_F}) + \beta_2 (\frac{\gamma_{CF}}{\gamma_F})^2 + \beta_3 (\frac{\gamma_{CF}}{\gamma_F})^3]$$

$$\begin{cases} \beta_0 = \beta_0' + 1 \\ \alpha_0 = \alpha_0' + 1 \end{cases}$$

 $\begin{array}{l} \alpha_0,\,\alpha_1,\,\alpha_2,\,\alpha_3,\,\beta_0,\,\beta_1,\,\beta_2,\,\beta_3 \text{ : calibration parameters.} \\ \text{CD}_{\text{bott}} \text{ : simulated Bottom CD after main etching.} \end{array}$





Etch CD Bias Prediction



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