Stochastic Approach to Modeling Line Edge Roughness in Photolithography

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Outline:
There’s a lot going on in LER

• Photon and acid shot noise
• Reaction-diffusion kinetics
• Development and dynamical scaling
• Overall model for LER
• What’s missing – future work
Continuum Approximation

• The real world is discrete (photons, atoms, etc.), but most macroscopic models (e.g., litho simulation) make the **continuum approximation**
  – Matter and energy are described with continuous mathematical functions
  – Ex: aerial image intensity, acid concentration after exposure, resist dissolution

• What are the implications of making the continuum approximation?
  – Line-edge roughness cannot be predicted
Continuum Approximation Example: Chemical Concentration

• Concentration: The number of atoms or molecules of a certain type per unit volume
  – By necessity, an average over a volume

• What is the meaning of \( H(x,y,z) \) – the concentration of acid at a specific point in space?
Stochastic View of Chemical Concentration

- Model atom/molecule as a point located at its center of mass
- Consider a volume $V$ – is the molecule in the volume or not?
  - This is a binary proposition, governed by the binomial distribution:
    $P(n) = \text{probability of finding } n \text{ molecules in } V$
  - The binomial probability distribution can be well approximated by a Poisson distribution with average concentration $C$

$$P(n) = \frac{(CV)^n}{n!} e^{-CV} \quad \langle n \rangle = CV \quad \sigma_n^2 = CV$$

$$\frac{\sigma_n}{\langle n \rangle} = \frac{1}{\sqrt{\langle n \rangle}} = \frac{1}{\sqrt{CV}}$$

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Stochastic View of Chemical Concentration

• Example: for a typical 193nm resist formulation, $G_0 N_A = 0.042 /\text{nm}^3$ ($G_0$ = the initial concentration of PAG, $N_A$ = Avogadro's number)

  For $V = (3 \text{ nm})^3$ \[ \langle n \rangle = 1.13 \quad \sigma_n / \langle n \rangle = 94\% \]

  For $V = (6 \text{ nm})^3$ \[ \langle n \rangle = 9 \quad \sigma_n / \langle n \rangle = 33\% \]

  For $V = (10 \text{ nm})^3$ \[ \langle n \rangle = 42 \quad \sigma_n / \langle n \rangle = 15\% \]
Photon Shot Noise
(Also a Poisson Distribution)

• Example: for a typical 193nm resist with 10 mJ/cm² dose to clear,
  \[
  \langle n \rangle = 97 \quad \sigma_n / \langle n \rangle = 10\%
  \]
  For \( A = (1 \text{ nm})^2 \)

  \[
  \langle n \rangle = 9700 \quad \sigma_n / \langle n \rangle = 1\%
  \]
  For \( A = (10 \text{ nm})^2 \)

• Example: for an EUV resist with 5 mJ/cm² dose to clear,
  \[
  \langle n \rangle = 3 \quad \sigma_n / \langle n \rangle = 58\%
  \]
  For \( A = (1 \text{ nm})^2 \)

  \[
  \langle n \rangle = 300 \quad \sigma_n / \langle n \rangle = 6\%
  \]
  For \( A = (10 \text{ nm})^2 \)

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EUV Resists

• High energy EUV photons (92 eV) produce secondary electrons, which then travel ~few nanometers to expose PAG
  – How far is an important unanswered question
  – Quantum efficiency can be greater than 1

• Simple approach to account for this blur is to convolve aerial image with the secondary electron position probability density function
  – Result is a decrease in image log-slope (ILS)
Stochastic View of Exposure Reaction

• Including photon shot noise, acid uncertainty is

\[ \sigma_h^2 = \frac{\langle h \rangle}{\langle n_{0-PAG} \rangle} + \frac{\left[(1 - \langle h \rangle) \ln(1 - \langle h \rangle)\right]^2}{\langle n_{photon} \rangle} \]

• When \( h = 0 \), \( \sigma_h = 0 \). When \( h = 1 \), max \( \sigma_h^2 = \frac{1}{\langle n_{0-PAG} \rangle} \)

• Max value of \( \left[(1 - \langle h \rangle) \ln(1 - \langle h \rangle)\right]^2 = 0.135 \)

• The pure photon shot noise contribution is very small, even for EUV
Reaction-Diffusion

\[
h_{\text{eff}}(x) = \frac{1}{t_{\text{PEB}}} \int_0^{t_{\text{PEB}}} h(x, t = 0) \otimes \text{DPSF} \, dt
\]

Relative concentration of blocked polymer sites

\[
m(x) = e^{-K_{\text{amp}} t_{\text{PEB}}} h_{\text{eff}}(x)
\]

Deblocking responds to the time-average of the acid latent image
Stochastic View of Reaction-Diffusion

• Is reaction-diffusion different from just diffusion? Yes, if the reaction is catalyzed by the diffusing species.

von Smoluchowski Trap:

Reaction can occur once acid approaches the blocking group within its capture radius, $a$.

$Rate \propto a$
Stochastic View of Reaction-Diffusion

• If an acid passes through the capture zone and a reaction doesn’t occur, that acid is more likely to pass through that zone again because it is close by (correlation)

• Probability of reaction is governed by the time average of the acid concentration as it diffuses around

\[
 h_{\text{eff}}(x) = \frac{1}{t_{\text{PEB}}} \int_{0}^{t_{\text{PEB}}} h(x, t = 0) \otimes \text{DPSF} \, dt
\]

\[
 \text{RDP}SF = \frac{1}{t_{\text{PEB}}} \int_{0}^{t_{\text{PEB}}} \text{DPSF} \, dt
\]

(Reaction-Diffusion Point Spread Function)
Stochastic View of Reaction-Diffusion


\[
\langle h_{\text{eff}} \rangle = \langle h \rangle \otimes \text{RDPoSF}
\]

Derivation of this is approximate – more work is needed

\[
\sigma_{h_{\text{eff}}} \approx \left( \frac{2a}{\sigma_D} \right) \sigma_h
\]
Stochastic View of Deprotection

• Statistical uncertainty in the blocked polymer site concentration comes from the Poisson distribution of the initial blocked sites, plus the stochastics of deblocking

\[
\sigma_m^2 \approx \frac{\langle m \rangle}{\langle n_{0\text{-blocked}} \rangle} + \langle m \rangle^2 \left( K_{amp}t_{PEB} \sigma_{heff} \right)^2 = \frac{\langle m \rangle}{\langle n_{0\text{-blocked}} \rangle} + \left( \langle m \rangle \ln \langle m \rangle \right)^2 \left( \frac{\sigma_{heff}}{\langle h_{eff} \rangle} \right)^2
\]

• Combining with our previous expressions for \( \sigma_{heff} \) and \( \sigma_h \) gives the final result
Stochastic View of Exposure + Reaction-Diffusion

- Final expression for the uncertainty in deblocked polymer concentration:

\[
\left( \frac{\sigma_m}{\langle m \rangle} \right)^2 = \frac{1}{\langle n_{0\text{-blocked}} \rangle} \left( K_{\text{amp}} t_{\text{PEB}} \right)^2 \left( \frac{2a}{\sigma_D} \right)^2 \left( \frac{\langle h \rangle}{\langle n_{0-PAG} \rangle} \right) + \left[ 1 - \langle h \rangle \right] \ln \left[ 1 - \langle h \rangle \right]^2
\]

- Deblocking reaction
- Reaction-diffusion
- Acid concentration, exposure
- Photon shot noise
Correlation and Acid-Catalyzed Reaction-Diffusion

- As one acid diffuses and catalyzes several deprotection reactions, those deprotections are correlated

\[
R(\tau) = \frac{\text{RDP SF} \otimes \text{RDP SF}}{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\text{RDP SF})^2}
\]

- Perform integrations numerically, examine the results
- Results can be almost perfectly fit with the standard exponential correlation function:

\[
R(\tau) = e^{-\left(\frac{\tau}{\xi}\right)^2}\alpha
\]
Correlation and Acid-Catalyzed Reaction-Diffusion

3-D Case

\[ \xi = 1.53 \sigma_D, \quad \alpha = 0.90 \]
Development and Dynamical Scaling

(a 1+1 dimension simulation)

Roughness grows with time during development, and becomes correlated.
Dynamical Scaling (1+1)

\[ \langle r \rangle = 10 \text{ nm} / \text{s}, \quad \sigma_r = 2 \text{ nm} / \text{s} \]

Data collapses to a single curve for the right values of the scaling exponents

\[ \frac{\sigma_w}{L^\alpha} \propto f \left( \frac{t}{L^z} \right) \]

- \( \alpha = 1/2 \)
- \( \beta = 1/3 \)
- \( z = \alpha / \beta \)
Line-Edge Roughness (Tying it all Together)

- Consider a small deviation in resist development rate. The resulting change in resist edge position will be approximately

$$\Delta x = \frac{d x}{d R} \Delta R$$

- For some variation in development rate $\sigma_R$,

$$\sigma_{LER} = \frac{\sigma_R}{d R / d x} = \left( \frac{\sigma_R}{R} \right) \left( \frac{d \ln R}{d x} \right)^{-1}$$
Line-Edge Roughness
(Tying it all Together)

• The Lithographic Imaging Equation

\[
\frac{d \ln R}{dx} = \gamma \frac{d \ln I}{dx} = \gamma (ILS)
\]

• Thus,

\[
\sigma_{LER} = \left( \frac{\sigma_R}{R} \right) \left( \frac{1}{\gamma ILS} \right) \quad \text{or} \quad \frac{\sigma_{LER}}{CD} = \left( \frac{\sigma_R}{R} \right) \left( \frac{1}{\gamma NILS} \right)
\]

Note: \( \gamma \) is not a bulk resist property, but the value at the line edge (see Chapter 9 of Fundamental Principles of Optical Lithography)
Line-Edge Roughness
(Tying it all Together)

• How to improve LER:
  – Increase $ILS$
  – Increase $\gamma$
  – Decrease $\sigma_R/R$

• These terms sometimes work against each other

• The product $\gamma NILS$ controls exposure latitude for a given feature, and thus lithographers already work to maximize this term
Line-Edge Roughness and Acid Diffusion

\[ \sigma_{LER} \propto \frac{\sigma_m}{dm/dx} \]
Line-Edge Roughness and Acid Diffusion

![Graph showing LER (Arb. Units) vs. Acid Diffusion Length (nm) for two different values of a: 0.5 nm and 1.5 nm.](Image)

- $a = 0.5 \text{ nm}$
- $a = 1.5 \text{ nm}$
Future Work (What’s Missing)

• Base quencher has been ignored (by me) to date
  – Quencher will always be at lower concentrations than acid, adding an extra term to the final uncertainty in blocked polymer that could be significant
  – Quencher can dramatically improve the latent image gradient, thus quencher concentration and diffusion will be important levers for optimizing LER (there has to be an optimum quencher concentration)

• Development rate uncertainty
  – Examine impact of correlations of development rate noise
  – How does a development rate gradient affect things?
  – What happens as the dissolution rate becomes very slow – will we move into the directed percolation depinning (DPD) universality class?