Simulating resist stochastics and performance optimization with PROLITH X4.1

John J. Biafore, Mark D. Smith
SEMATECH Resist TWG, EUVL Brussels, 2012
Application of PROLITH to resist optimization problems

• Motivation: At any wavelength, modifying specific resist properties or isolating a particular resist response can be difficult or impossible in experiments. At EUV, photons are expensive and tool time is limited, limiting access to experiment. Computer modeling helps mitigate these difficulties, allowing researchers to reduce or better focus actual experiments.

• In this work:

  • We apply simulation to study noise effects produced by the electron dissociation exposure mechanism

  • We attempt offer an example of resist optimization at EUV by simulation, using data published by Higgins as a starting point.

  • We study the theoretical effects of photo-decomposable quencher upon performance
Possible resist exposure mechanisms

1. Direct photolysis
Photon absorption by the generating molecule produces an electronically-excited state favorable for conversion.


2. Electronic excitation
Absorption of an EUV photon results in ionization and a cascade of secondary electrons. Scattering electrons induce a time-dependent electric field whose individual Fourier components are thought of as virtual photons. If a resonating system (the generating molecule) is within the field, it may interact with the passing charge, producing conversion.

*G. Han, F. Cerrina, J. Vac. Sci. Technology. B18(6), 2000 3297*
*J.D. Jackson, ‘Classical Electrodynamics’, Wiley, 1975*

3. Electron dissociation
Absorption of an EUV photon results in ionization and a cascade of secondary electrons. Scattering electrons which have decelerated sufficiently are trapped by the generating molecule, producing conversion.

Origin of roughness in chemically-amplified resists is the exposure step
Acid centers-of-mass image vs. dose, 13.5 nm, 22 nm hp lines, top-down view through resist

22 nm hp lines, 40nm FT, k = 0.0068, $\alpha = 6.3/\mu m$
Effect of exposure dose upon LER, LWR
13.5 nm, 0.25 NA, 0.5 sigma, 30 nm lines, Esizie adjusted by modification of quencher loading

- Lowering dose degrades LWR

\[
\begin{align*}
E_{\text{SIZE}} &= 7.25 \text{ mJ} \\
CD &= 30.2 \text{ nm} \\
LWR &= 7.4 \text{ nm} \\
\hline
E_{\text{SIZE}} &= 15 \text{ mJ} \\
CD &= 30.1 \text{ nm} \\
LWR &= 5.4 \text{ nm} \\
\hline
E_{\text{SIZE}} &= 30 \text{ mJ} \\
CD &= 29.6 \text{ nm} \\
LWR &= 4.5 \text{ nm} \\
\hline
E_{\text{SIZE}} &= 60 \text{ mJ} \\
CD &= 30.4 \text{ nm} \\
LWR &= 3.8 \text{ nm}
\end{align*}
\]
Effect of exposure dose upon hole uniformity
13.5 nm, 0.25 NA, 0.5 sigma, 40 nm holes, 90 nm pitch

- Lowering exposure dose degrades hole uniformity

\[ \overline{CD} = 40.1 \text{nm} \]
\[ E_{SIZE} = 7.25 \text{mJ} / \text{cm}^2 \]
\[ 3\sigma \text{ CDU} = 3.5 \text{nm} \]

\[ \overline{CD} = 40.1 \text{nm} \]
\[ E_{SIZE} = 15 \text{mJ} / \text{cm}^2 \]
\[ 3\sigma \text{ CDU} = 2.6 \text{nm} \]

\[ \overline{CD} = 40.1 \text{nm} \]
\[ E_{SIZE} = 30 \text{mJ} / \text{cm}^2 \]
\[ 3\sigma \text{ CDU} = 1.9 \text{nm} \]

\[ \overline{CD} = 40.2 \text{nm} \]
\[ E_{SIZE} = 60 \text{mJ} / \text{cm}^2 \]
\[ 3\sigma \text{ CDU} = 1.3 \text{nm} \]
Simulation of photon, electron and acid counting w/ electron dissociation mechanism
13.5 nm, $\alpha = 6.3/\mu m$, FT = 40 nm, 100 nm x 100 nm open frame

- Electron trapping exposure mechanism means acid yield < electron yield
- Theoretical maximum acid production is observed
Simulation of photon, electron and acid counting w/ electron dissociation mechanism
13.5 nm, $\alpha = 6.3/\mu$m, FT = 40 nm, 100 nm x 100 nm open frame

- Model suggests that if electron trapping is the sole exposure mechanism, electron shot is the upper bound for acid shot noise, while photon shot noise is the lower bound
Modeling quantum yield vs. loading for different PAGs
13.5 nm, 0.30 NA, open frame

Data from C. Higgins 2011

Calibration of exposure parameters produces a reasonable match of the yield vs. loading trend observed for three PAG systems

Modeling EL, LER, quantum yield and Esize vs. loading of the DTBPI-nf PAG system
13.5 nm, 0.30 NA, annular, 60 nm hp lines

- Using optimized exposure parameters for DTBPI-nf PAG, further parameter calibration produces a reasonable match to the experimental data
Definition of RLS triangle axes in the following slides

**R** = Aerial image NILS / Resist exposure latitude
- Aerial image NILS at 60 nm half-pitch line
- EUV, 0.30 NA, 0.55 / 0.35 annular
- max( R ) == 1

**L** = Average line-edge roughness, nm
- 60 nm half-pitch line, 500 nm line length, 2 nm step-size
- <LER> = Average of left and right line edges

**S** = Sizing dose, mJ/cm²
- 60 nm half-pitch line at best focus
RLS triangles of Higgins data vs. calibrated PROLITH model, 5% DTBPI PAG
13.5 nm, 0.30 NA, annular, 60 nm hp lines

- Experimental vs. simulated RLS triangles
RLS triangles of Higgins data vs. calibrated PROLITH model, 7.5% DTBPI PAG 13.5 nm, 0.30 NA, annular, 60 nm hp lines

- Experimental vs. simulated RLS triangles
RLS triangles of Higgins data vs. calibrated PROLITH model, 15% DTBPI PAG
13.5 nm, 0.30 NA, annular, 60 nm hp lines

- Experimental vs. simulated RLS triangles
RLS triangles of Higgins data vs. calibrated PROLITH model, 20% DTBPI PAG
13.5 nm, 0.30 NA, annular, 60 nm hp lines

- Experimental vs. simulated RLS triangles
- Additional PAG observed to degrade EL
RLS triangles of Higgins data vs. calibrated PROLITH model, 30% DTBPI PAG
13.5 nm, 0.30 NA, annular, 60 nm hp lines

- Experimental vs. simulated RLS triangles
- Additional PAG observed to degrade EL
RLS performance of initial condition: attempt to improve performance using model

\[ EL = 18\% \]
\[ \langle LER \rangle = 4.6 \text{nm} \]
\[ E_{size} = 6 \text{mJ/cm}^2 \]
\[ \Phi = 3.8 \text{acids/photon} \]

- Attempt to improve performance using modeling
  - Use parameters calibrated for 15% PAG loading as initial condition
RLS performance improvement with reduced acid diffusivity and quencher addition

\[ E_{\text{size}} = 10 \text{mJ/cm}^2 \]
\[ \Phi = 3.4 \text{ acids/photon} \]

\[ EL = 22\% \]
\[ \langle LER \rangle = 4.3 \text{nm} \]

• Reduction of acid diffusivity improves exposure latitude
• Conventional quencher addition increases Esize to 10mJ/cm², reducing PSN effects

Reduce acid diffusivity
Add quencher
15% PAG
\[ <\text{nPAGs}>/\text{nm}^3 = 0.145 \]
\[ <\text{nQs}>/\text{nm}^3 = 0.04 \]
\[ \text{Dacid} = 1.5 \text{nm}^2/\text{s} \]
RLS performance improvement with reduced acid diffusivity and PDB addition

\[ EL = 21.5\% \]
\[ \langle LER \rangle = 4 \text{nm} \]
\[ E_{\text{size}} = 10 \text{mJ/cm}^2 \]
\[ \Phi = 2.9 \text{ acids/photons} \]
\[ \Phi_q = 0.9 \text{ PDB/photons} \]

- Reduction of acid diffusivity improves exposure latitude
- PDB addition further reduces LER, even though acid yield decreases
RLS performance comparison with improved formulation

PROLITH

Initial condition
15% PAG
\(<\text{nPAGs}/\text{nm}^3 = 0.145\)
\(<\text{nQs}/\text{nm}^3 = 0.027\)
\(\text{Dacid} = 3.6 \text{ nm}^2/\text{s}\)

PROLITH

Reduce acid diffusivity
Replace Q with PDB
15% PAG
\(<\text{nPAGs}/\text{nm}^3 = 0.145\)
\(<\text{nPDBs}/\text{nm}^3 = 0.045\)
\(\text{Dacid} = 1.5 \text{ nm}^2/\text{s}\)

\[ EL = 18\%, \langle LER \rangle = 4.6 \text{ nm}, \ E_{\text{size}} = 6 \text{ mJ/cm}^2 \]  
\[ EL = 21\%, \langle LER \rangle = 4 \text{ nm}, \ E_{\text{size}} = 10 \text{ mJ/cm}^2 \]

• Net is 17% increase in EL, 13% reduction in LER
Photodecomposable bases, PDBs

- First proposed for use in KrF resists by Funato et al.\textsuperscript{3} at Hoechst 1996 to reduce t-topping and improve latent image stability, PDBs are radiation-sensitive basic compounds such as TPS-OH.
- Are decomposed upon expose into neutral fragments which don’t act as acid quenchers.
- Remain active as quencher in unexposed region.

\textsuperscript{3} “Application of photodecomposable base concept to two-component deep-UV chemically amplified resists” Funato et al, Proc. SPIE 2724, 186 (1996)
Simulation of photodecomposable bases, PDBs

- First proposed for use in KrF resists by Funato et al.\textsuperscript{3} at Hoechst 1996 to reduce t-topping and improve latent image stability, PDBs are radiation-sensitive basic compounds such as TPS-OH.
- Are decomposed upon expose into neutral fragments which don’t act as acid quenchers.
- Remain active as quencher in unexposed region.

\begin{equation}
\frac{\partial q}{\partial t} = -C_q I q
\end{equation}

\begin{equation}
q(t) = q_0 \exp(-C_q E)
\end{equation}

Simulated effect of PDBs on EUV relief image
27 nm hp, 0.25NA, 0.5 partial coherence, 50 nm resist on Si

$E = 12.8\, mJ / cm^2$
$\langle LER \rangle = 5.1\, nm$
$\langle LWR \rangle = 7.3\, nm$
$\alpha = 6.33 / \mu m$
$\langle nPAGs \rangle / nm^3 = 0.35$
$\langle nQs \rangle / nm^3 = 0.094$

$E = 12.8\, mJ / cm^2$
$\langle LER \rangle = 4.5\, nm$
$\langle LWR \rangle = 6.2\, nm$
$\alpha = 6.33 / \mu m$
$\langle nPAGs \rangle / nm^3 = 0.35$
$\langle nPDBs \rangle / nm^3 = 0.112$

• In this experiment, PDB shows a 12-15% reduction in LER & LWR
• PDB loaded at a higher density than conventional quencher
• Acid yield required with conventional quencher can be relaxed by 9.5%
Simulated EUV exposed latent image with PDB
27 nm hp lines, 0.25NA, 0.5 partial coherence, 50 nm resist on Si

\[
\langle \text{abs. photons} \rangle / \text{nm}^3
\]

\[
\langle \text{acids} \rangle / \text{nm}^3
\]

\[
\langle \text{PDB} \rangle / \text{nm}^3
\]

\[
\langle n\text{PAGs} \rangle / \text{nm}^3 = 0.35
\]

\[
\langle n\text{PDBs} \rangle / \text{nm}^3 = 0.112
\]

Exposure neutralizes quencher
Simulated effect of PDBs on EUV PEB latent image
27 nm hp, 0.25NA, 0.5 partial coherence, 50 nm resist on Si

- Blocked polymer conc. $[M]$ and gradient $[\nabla M]$ after PEB for conventional quencher vs. PDB
- System containing PDB has steeper chemical gradient
- Less acid titration in highly exposed regions = more deprotection = steeper gradient
Simulated effect of PDBs on power spectral density

- Simulated PSD of resist with PDB suggests reduction of roughness at all frequencies
Acknowledgements

The PROLITH team:
Pat Lee
Trey Graves
Stewart Robertson
David Blankenship
Dan Grubbs
Chris Walker
Heather Spears
Greg Floyd

Thanks for your attention