KLA-Tencor
Accelerating Yield

Simulating resist stochastics and performance optimization with PROLITH X4.1

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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.

N. Turro, 'Modern Molecular Photochemistry', Univ. Sci. Books, 1991

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.

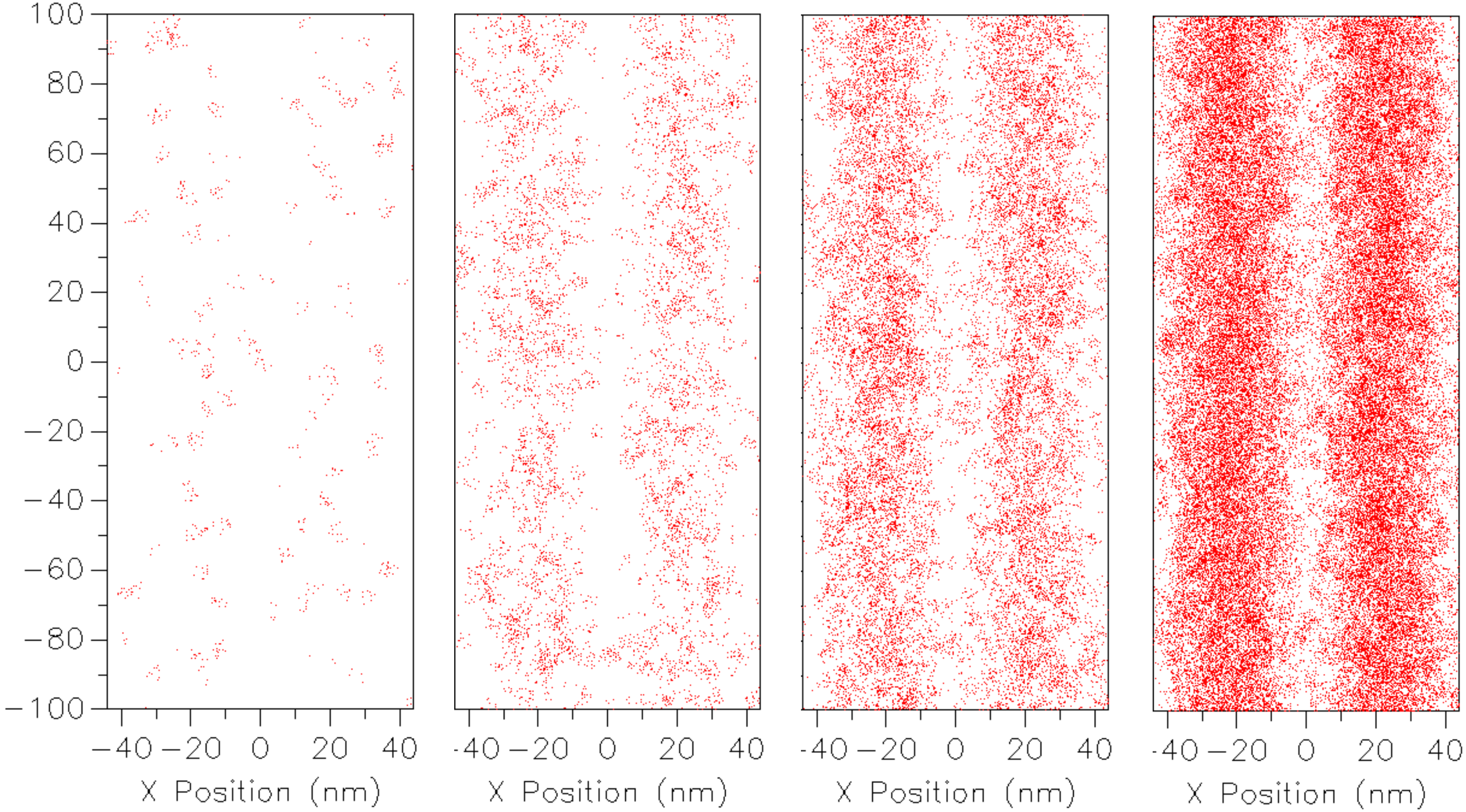
Scattering electrons which have decelerated sufficiently are trapped by the generating molecule, producing conversion.

T. Kozawa et al, J. Vac. Sci. Technology. B22, 2004 3489

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

$22\,nm\ hp\ lines,\ 40nm\,FT, k = 0.0068,\ \ \alpha = 6.3/um$



$0.1mJ/cm^2$ $1mJ/cm^2$ $3mJ/cm^2$ $10mJ/cm^2$

Effect of exposure dose upon LER, LWR

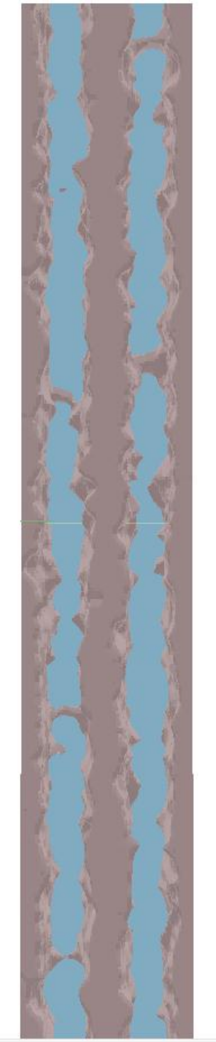
13.5 nm, 0.25 NA, 0.5 sigma, 30 nm lines, Esize adjusted by modification of quencher loading

- Lowering dose degrades LWR

$E_{SIZE} = 7.25\ mJ$

$\overline{CD} = 30.2\,nm$

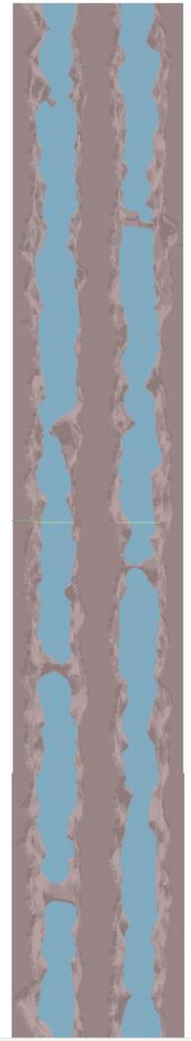
$LWR = 7.4\,nm$



$E_{SIZE} = 15\ mJ$

$\overline{CD} = 30.1\,nm$

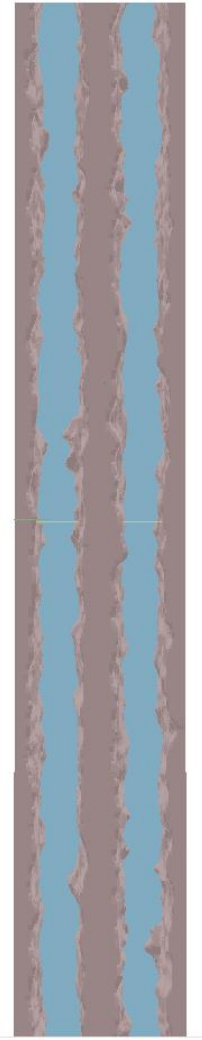
$LWR = 5.4\,nm$



$E_{SIZE} = 30\ mJ$

$\overline{CD} = 29.6\,nm$

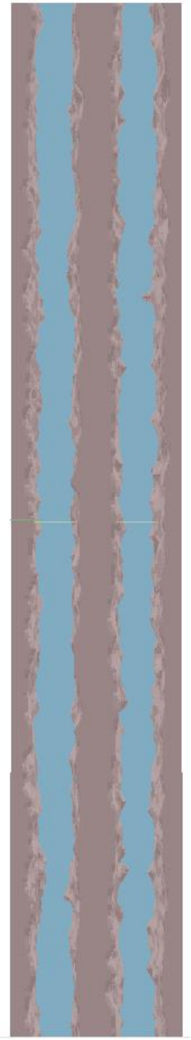
$LWR = 4.5\,nm$



$E_{SIZE} = 60\ mJ$

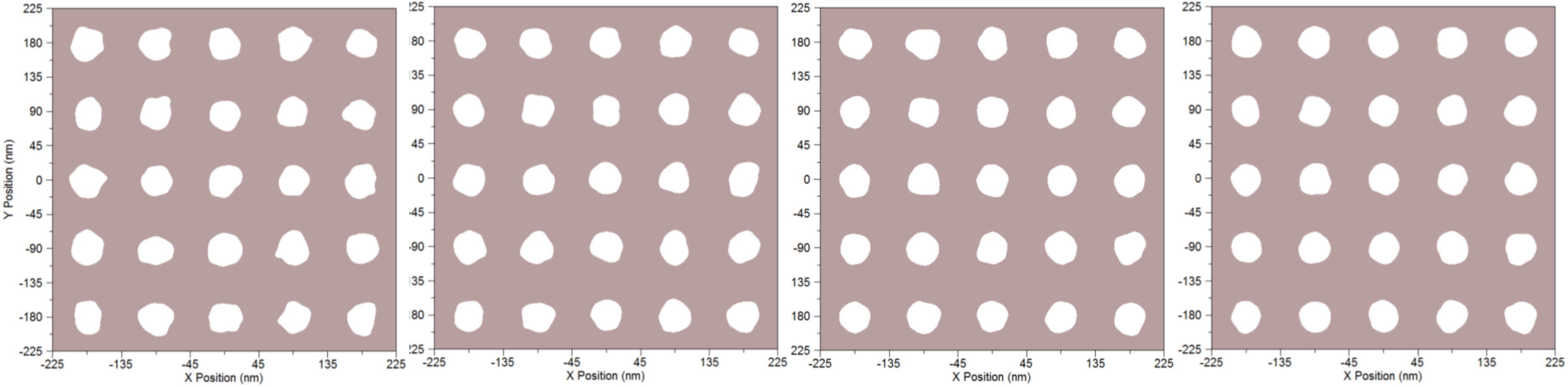
$\overline{CD} = 30.4\,nm$

$LWR = 3.8\,nm$



Effect of exposure dose upon hole uniformity

13.5 nm, 0.25 NA, 0.5 sigma, 40 nm holes, 90 nm pitch



$\overline{CD} = 40.1nm$

$E_{SIZE} = 7.25mJ / cm^2$

$3\sigma\ CDU = 3.5nm$

$\overline{CD} = 40.1nm$

$E_{SIZE} = 15mJ / cm^2$

$3\sigma\ CDU = 2.6nm$

$\overline{CD} = 40.1nm$

$E_{SIZE} = 30mJ / cm^2$

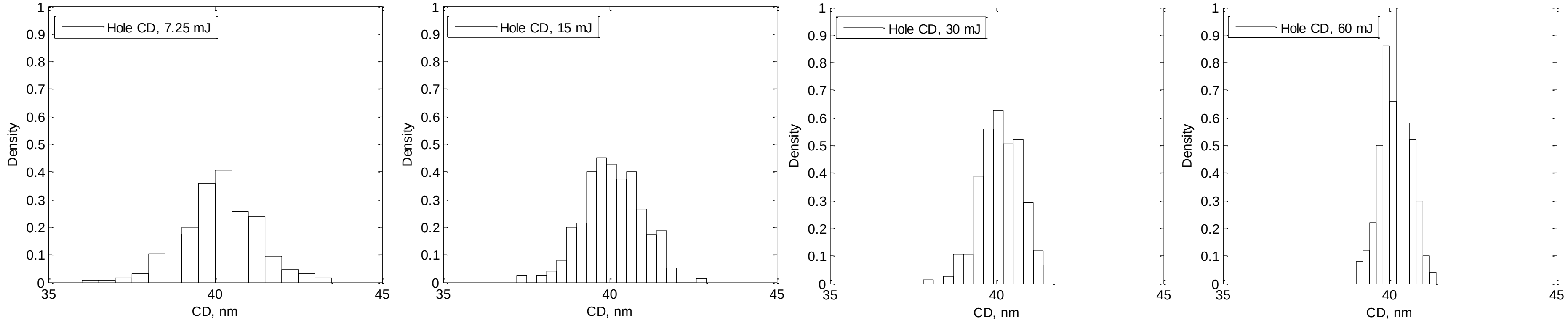
$3\sigma\ CDU = 1.9nm$

$\overline{CD} = 40.2nm$

$E_{SIZE} = 60mJ / cm^2$

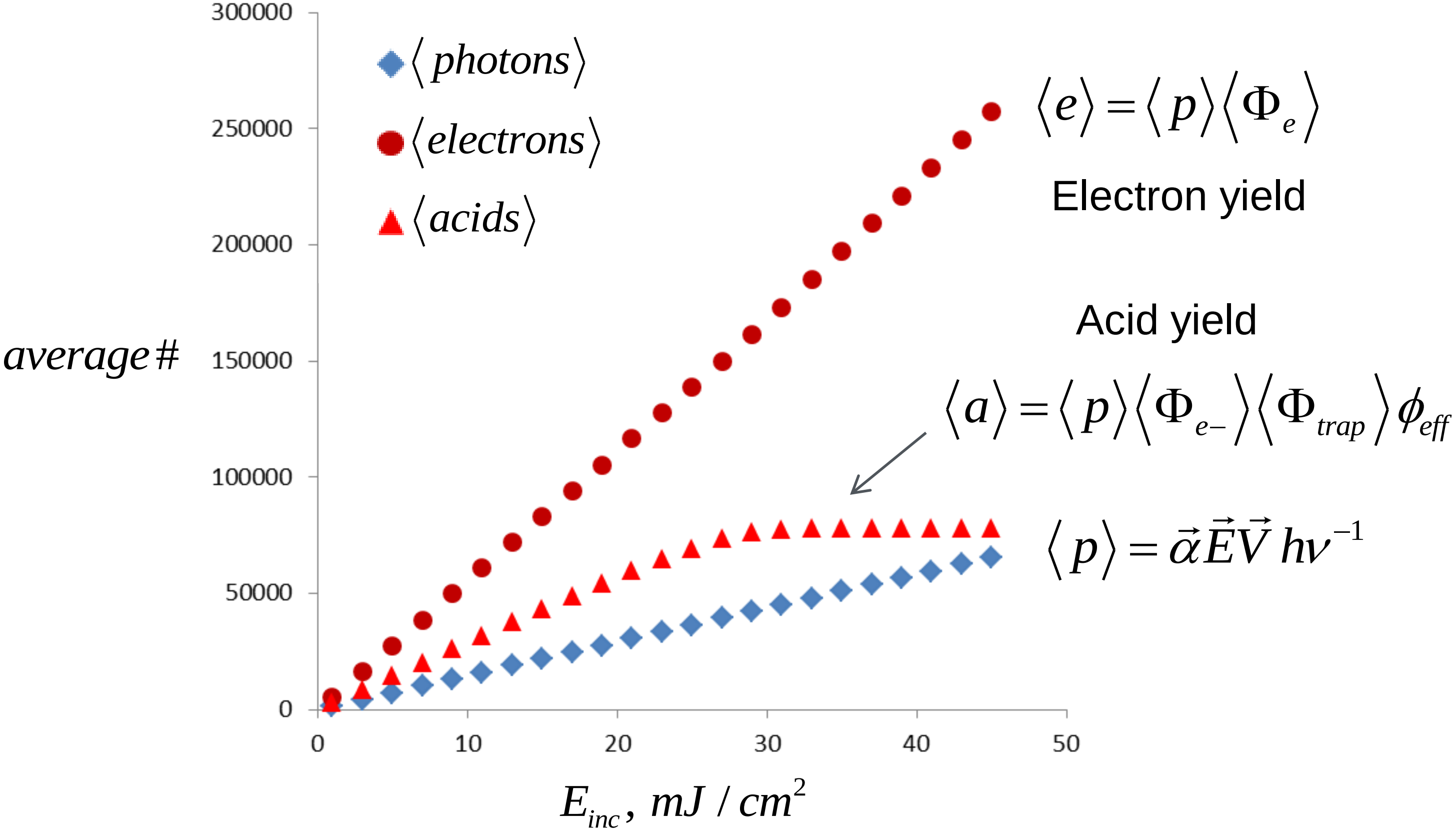
$3\sigma\ CDU = 1.3nm$

- Lowering exposure dose degrades hole uniformity



Simulation of photon, electron and acid counting w/ electron dissociation mechanism

13.5 nm, α = 6.3/um, FT = 40 nm, 100 nm x 100 nm open frame



$$\langle e \rangle = \langle p \rangle \langle \Phi_e \rangle$$

Electron yield

Acid yield

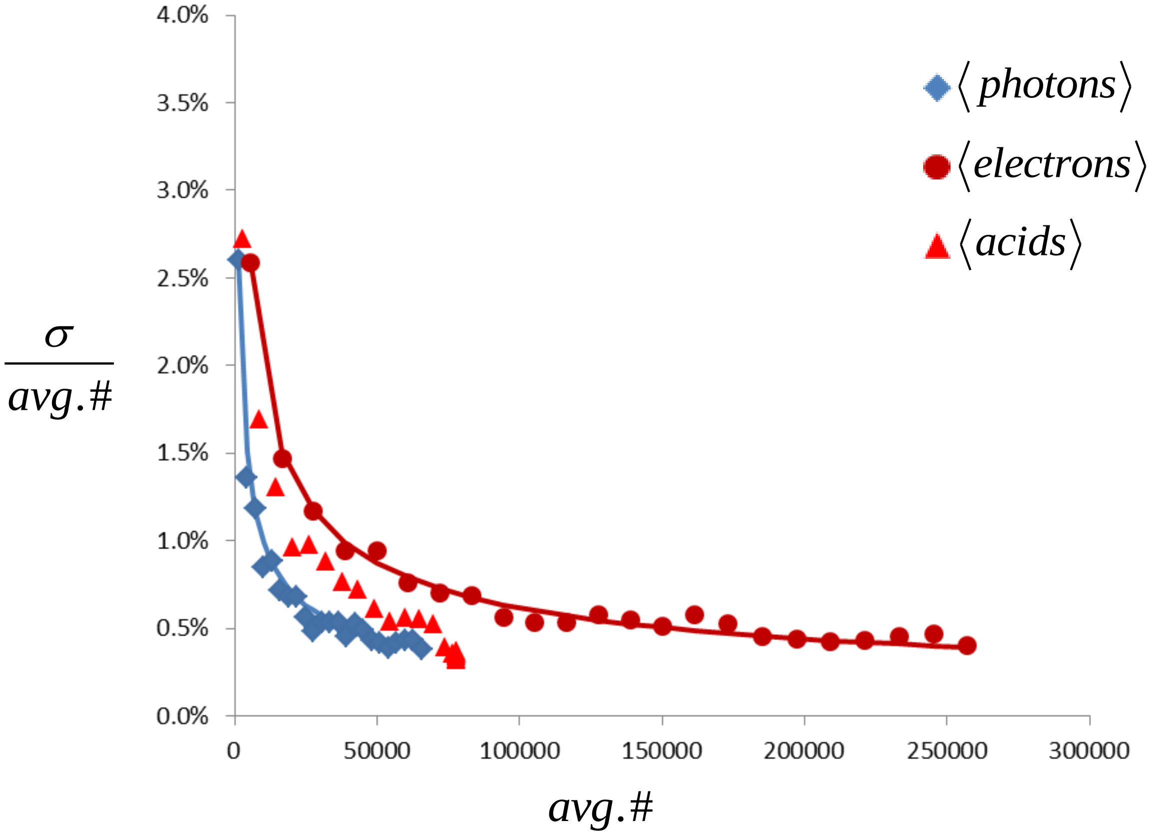
$$\langle a \rangle = \langle p \rangle \langle \Phi_{e-} \rangle \langle \Phi_{trap} \rangle \phi_{eff}$$

$$\langle p \rangle = \vec{\alpha} \vec{E} \vec{V} \, h\nu^{-1}$$

- 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, α = 6.3/um, FT = 40 nm, 100 nm x 100 nm open frame

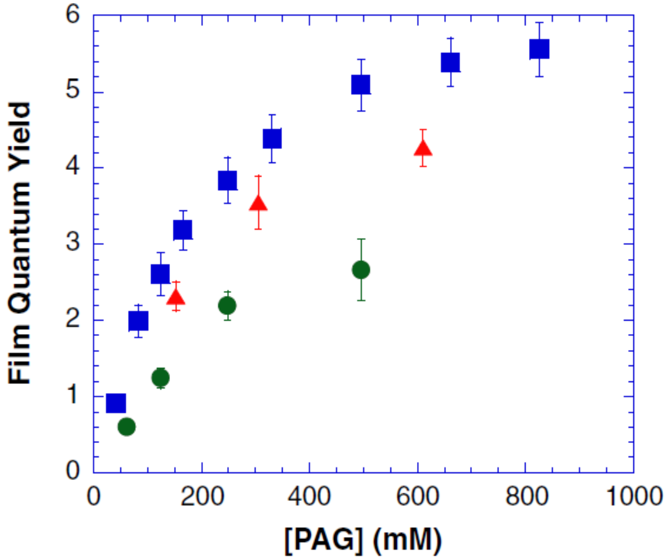


- Model suggests that if electron trapping is the sole exposure mechanism, electron shot is the upper bound for acid shot noise, while photon shot noise is the lower bound

Modeling quantum yield vs. loading for different PAGs

13.5 nm, 0.30 NA, open frame

Data from C. Higgins [2] 2011



PROLITH = lines, data = points

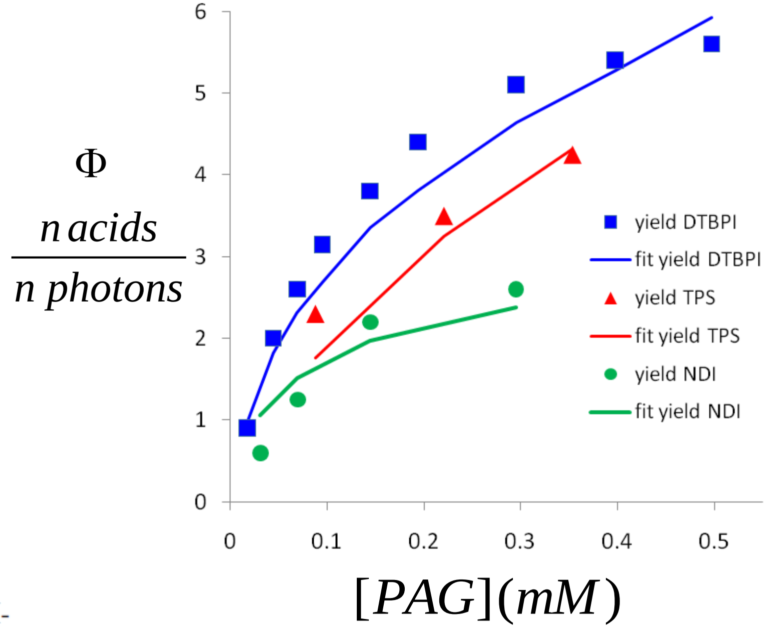
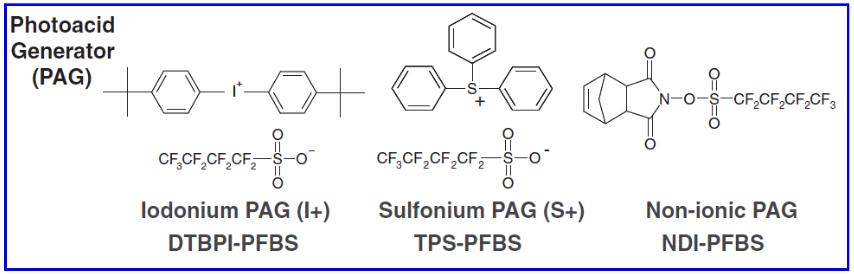


Fig. 5. (Color online) Film quantum yield vs PAG loading for DTBPI-PFBS and NDI-PFBS PAGs determined by dye indicator method and TPS-PFBS PAG determined by base titration method.



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

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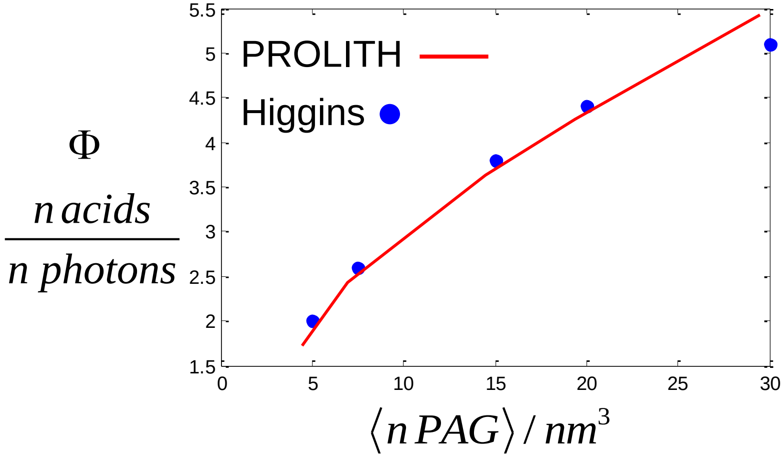
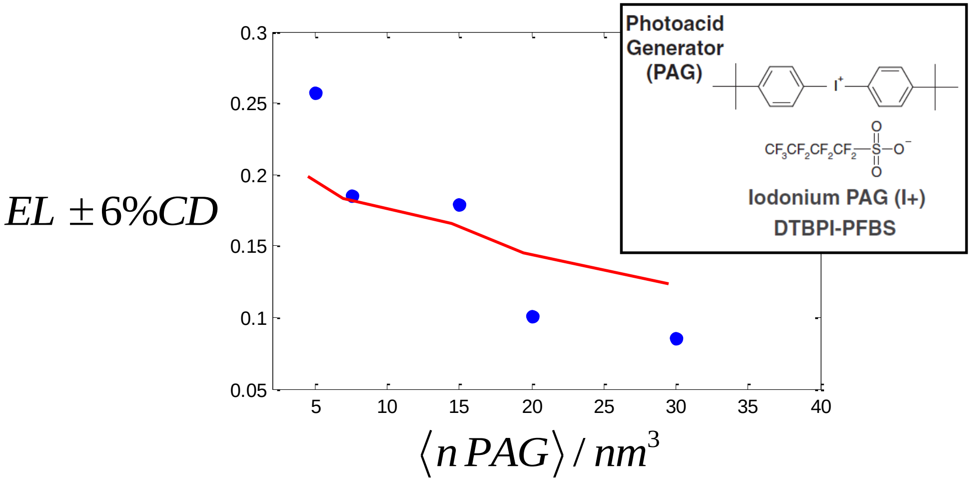
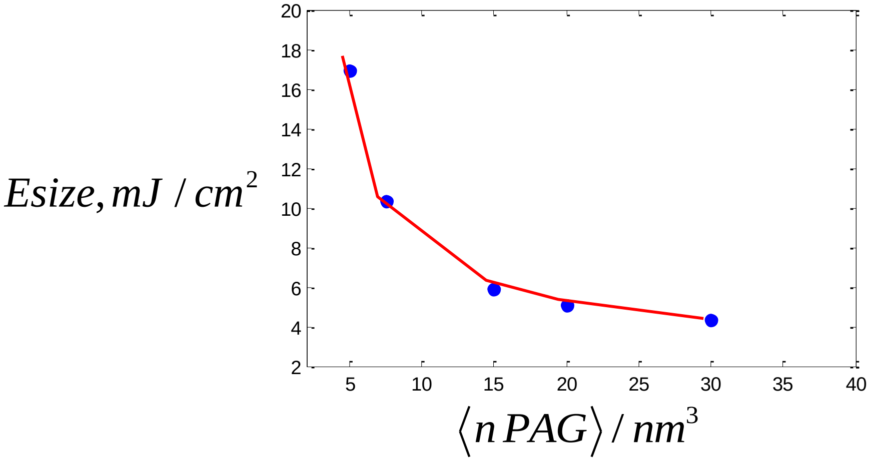
2. *"EUV Photoresists: Film Quantum Yield and LER of Thin Film Resists"*, C. Higgins, dissertation, Univ. Albany, NY, CNSE, 2011

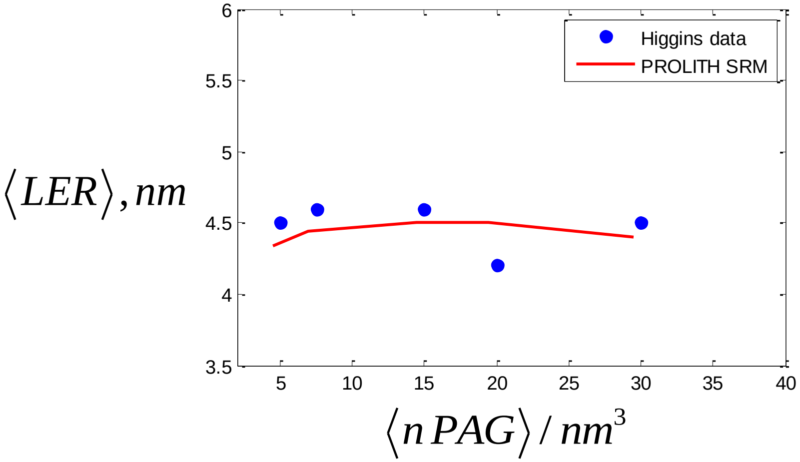
Modeling EL, LER, quantum yield and Esize vs. loading of the DTBPI-nf PAG system

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

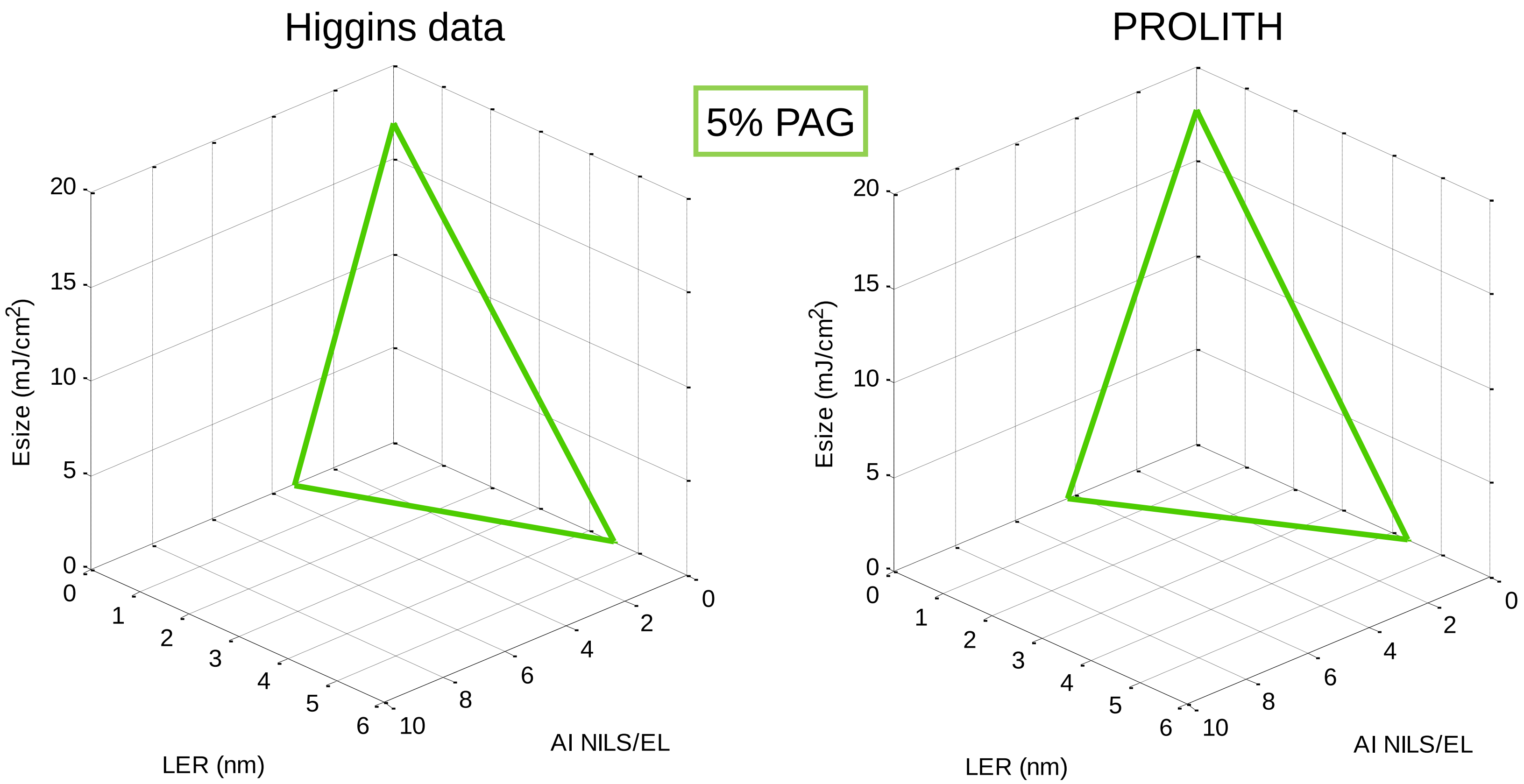
- 60 nm half-pitch line, 500 nm line length, 2 nm step-size
- <LER> = Average of left and right line edges

S = Sizing dose, mJ/cm^2

- 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


Higgins data

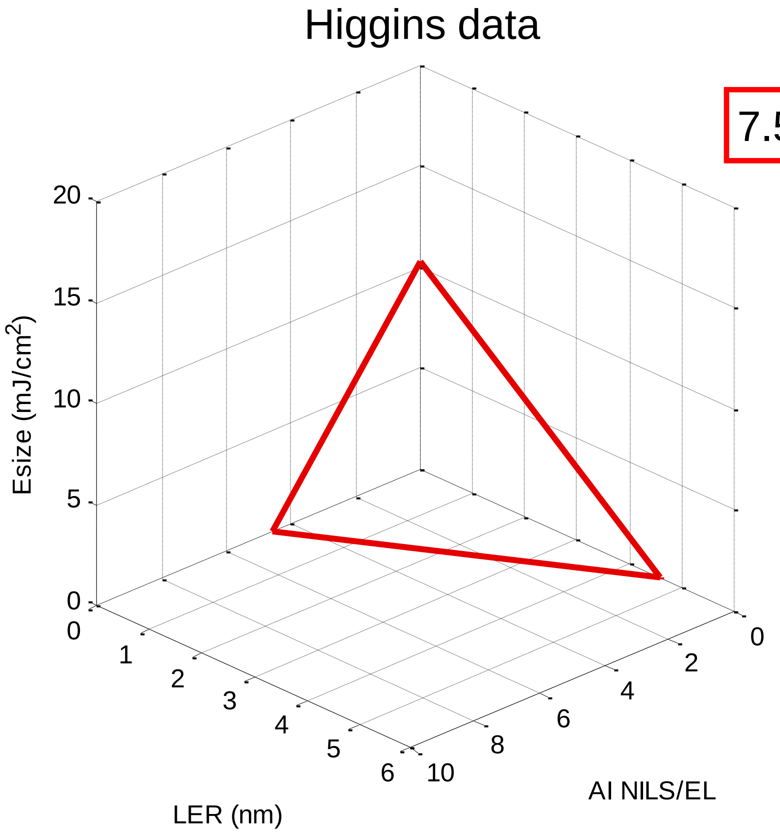
PROLITH

5% PAG

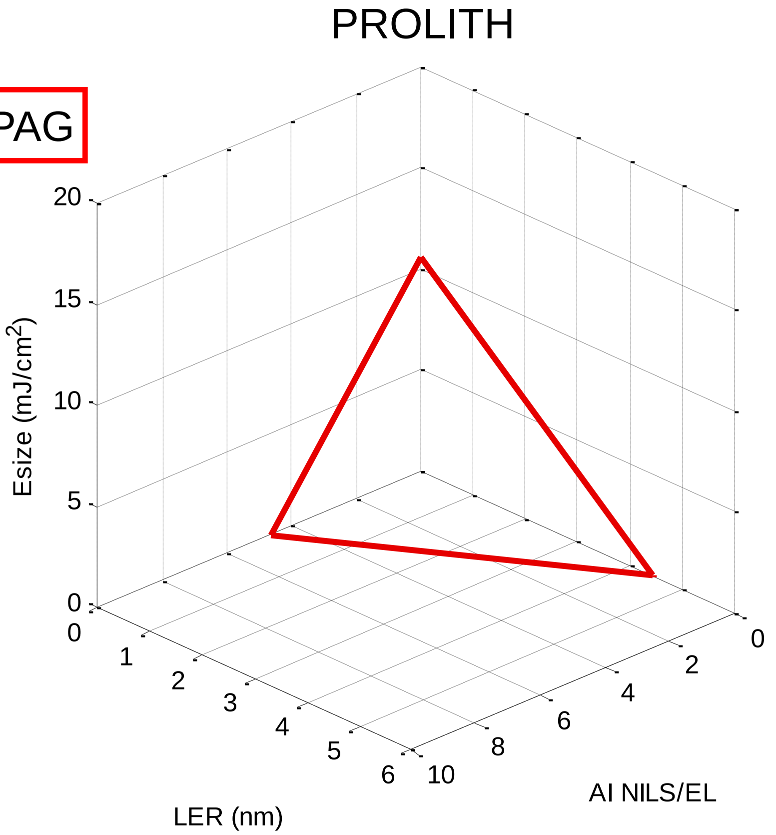
- Experimental vs. simulated RLS triangles

RLS triangles of Higgins data vs. calibrated PROLITH model, 7.5% DTBPI PAG

13.5 nm, 0.30 NA, annular, 60 nm hp lines


Higgins data

7.5% PAG


PROLITH

- Experimental vs. simulated RLS triangles

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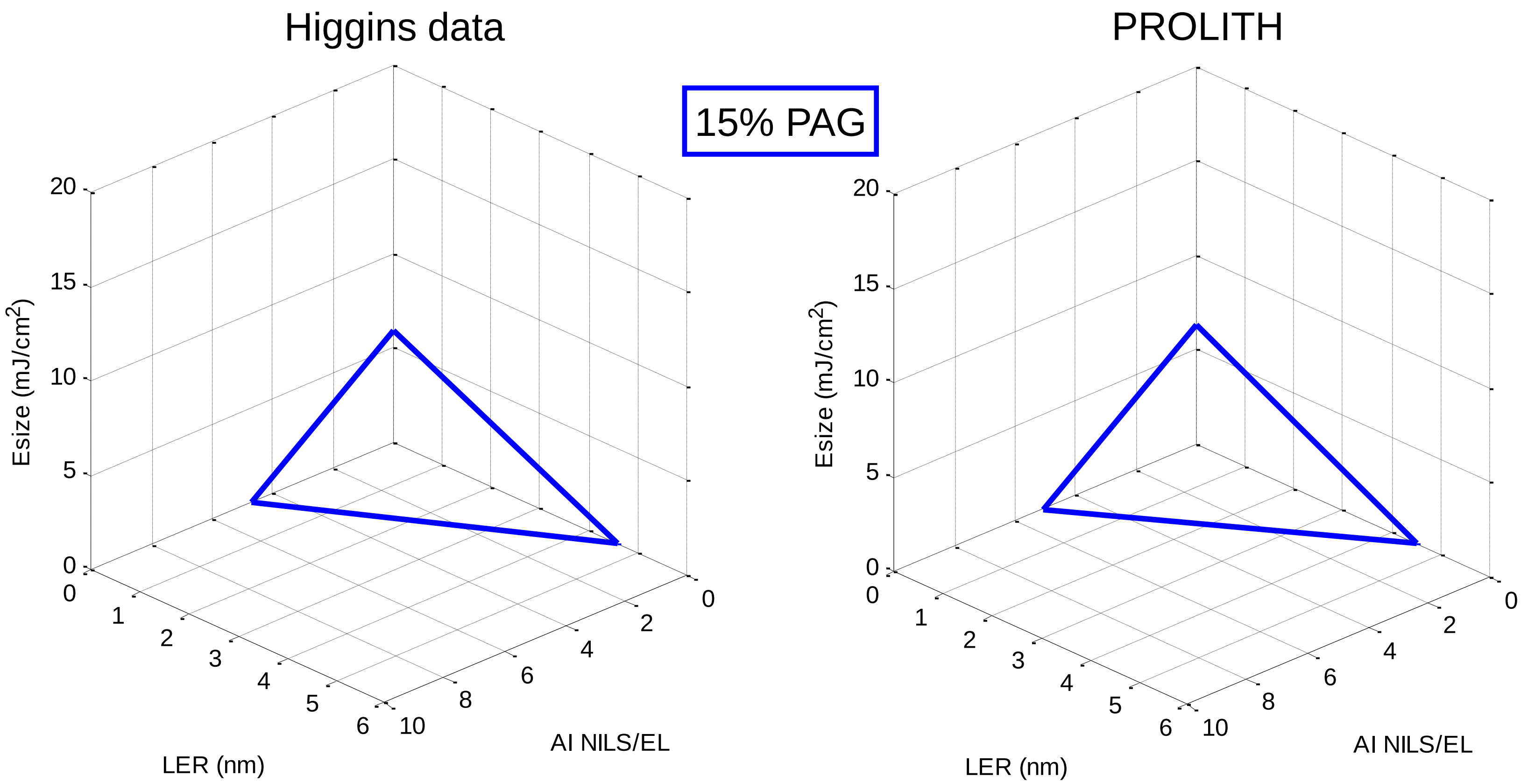
RLS triangles of Higgins data vs. calibrated PROLITH model, 15% DTBPI PAG

13.5 nm, 0.30 NA, annular, 60 nm hp lines

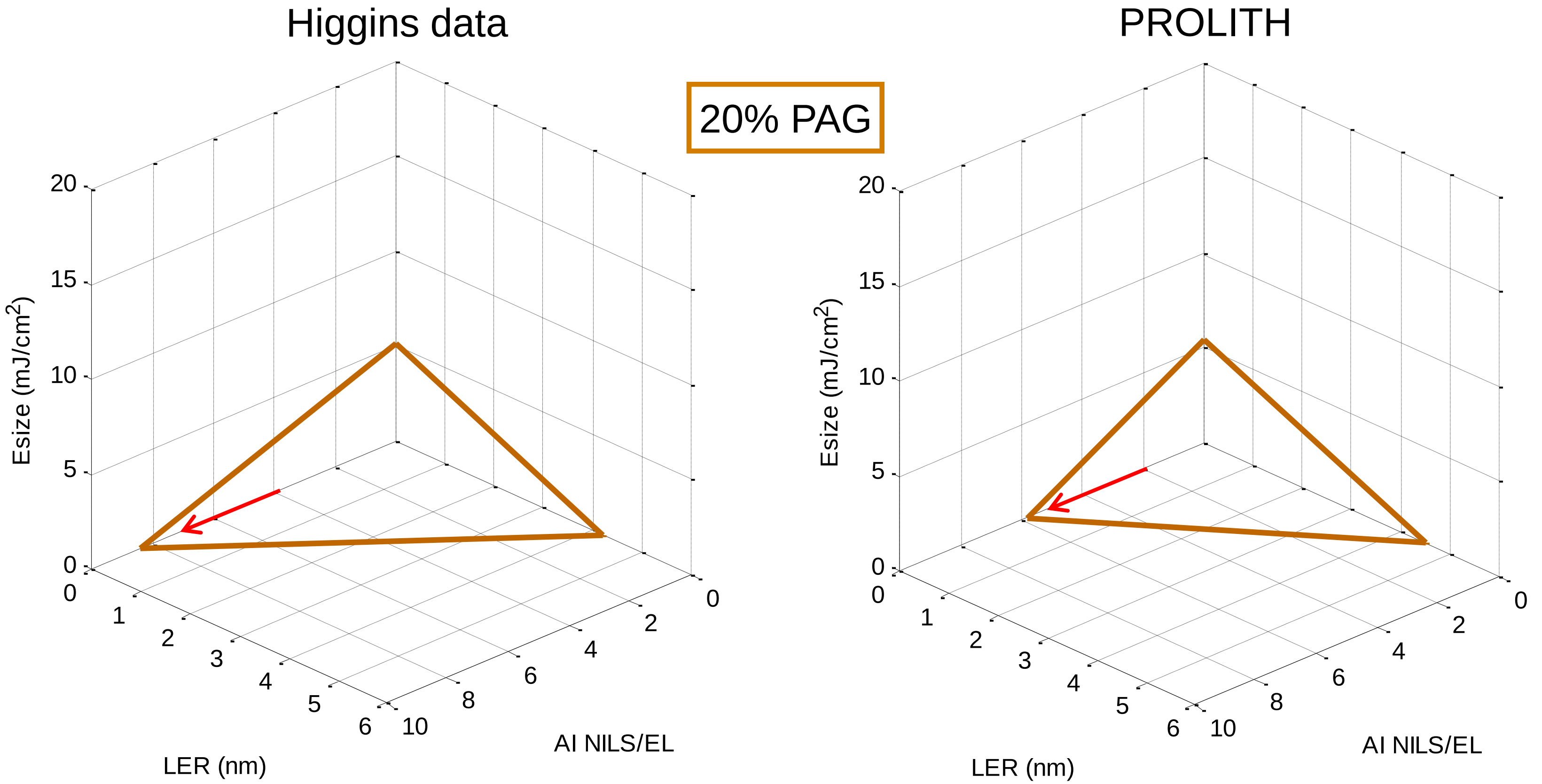


15% PAG

- Experimental vs. simulated RLS triangles

RLS triangles of Higgins data vs. calibrated PROLITH model, 20% DTBPI PAG

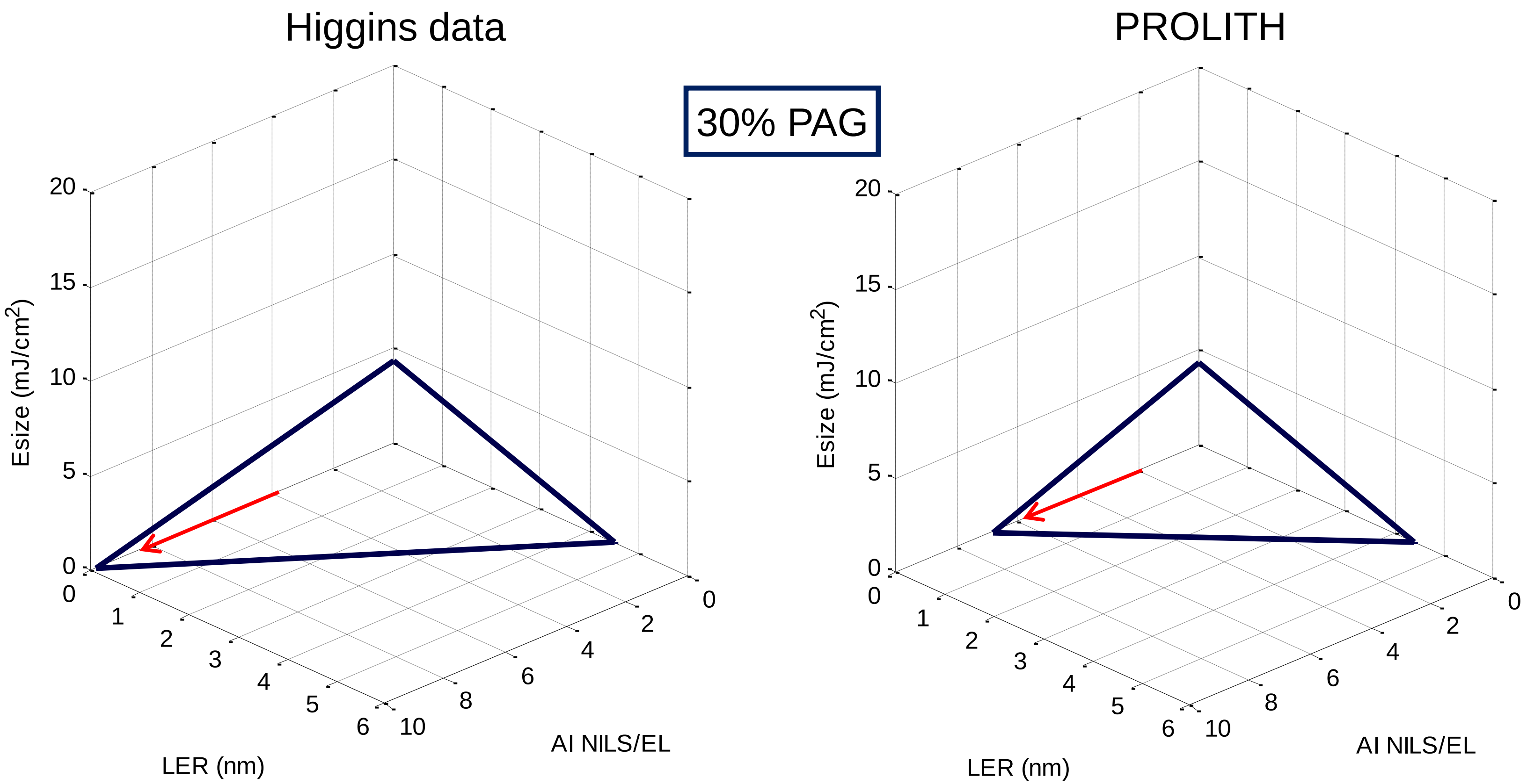
13.5 nm, 0.30 NA, annular, 60 nm hp lines



- 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

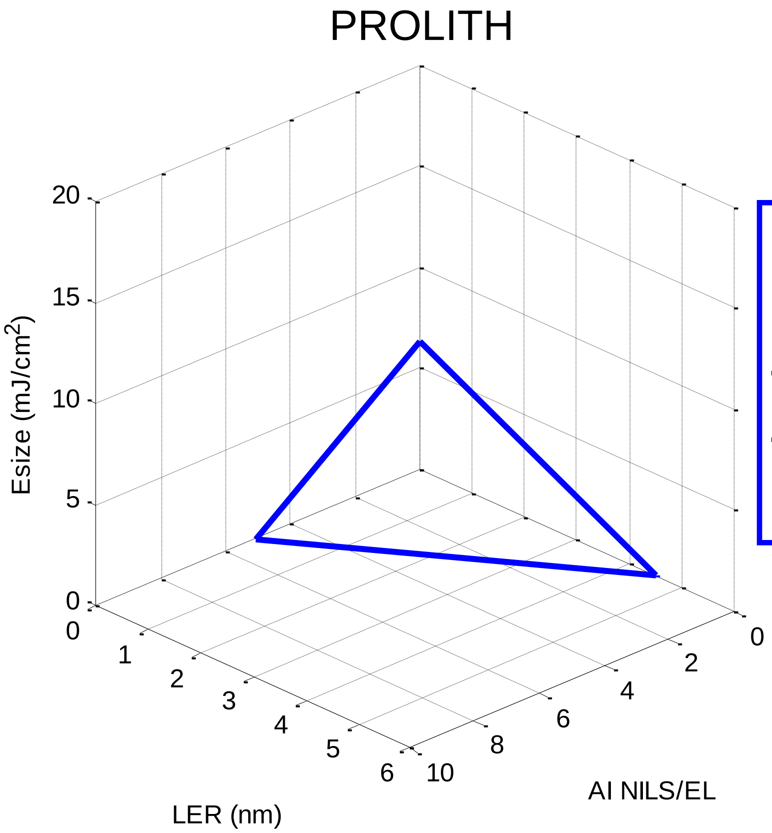
RLS performance of initial condition: attempt to improve performance using model

$$EL = 18\%$$

$$\langle LER \rangle = 4.6\,nm$$

$$E_{size} = 6\,mJ\,/\,cm^2$$

$$\Phi = 3.8\ acids\,/\ photon$$



Initial condition

15% PAG

<nPAGs>/nm^3 = 0.145

<nQs>/nm^3 = 0.027

Dacid = 3.6 nm^2/s

- Attempt to improve performance using modeling
- Use parameters calibrated for 15% PAG loading as initial condition

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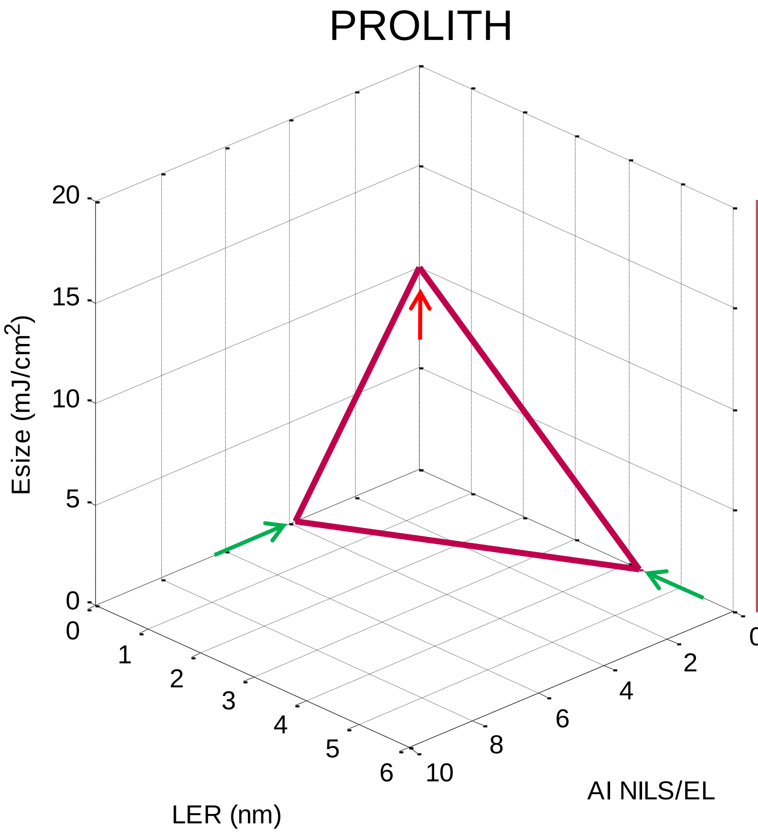
RLS performance improvement with reduced acid diffusivity and quencher addition

$$EL = 22\% \uparrow$$

$$\langle LER \rangle = 4.3\,nm \downarrow$$

$$E_{size} = 10\,mJ/cm^2 \uparrow$$

$$\Phi = 3.4\ acids/photon$$



Reduce acid diffusivity

Add quencher

15% PAG

$\langle nPAGs \rangle/nm^3 = 0.145$

$\langle nQs \rangle/nm^3 = 0.04$

Dacid = 1.5 nm^2/s

- Reduction of acid diffusivity improves exposure latitude
- Conventional quencher addition increases Esize to 10mJ/cm^2 , reducing PSN effects

RLS performance improvement with reduced acid diffusivity and PDB addition

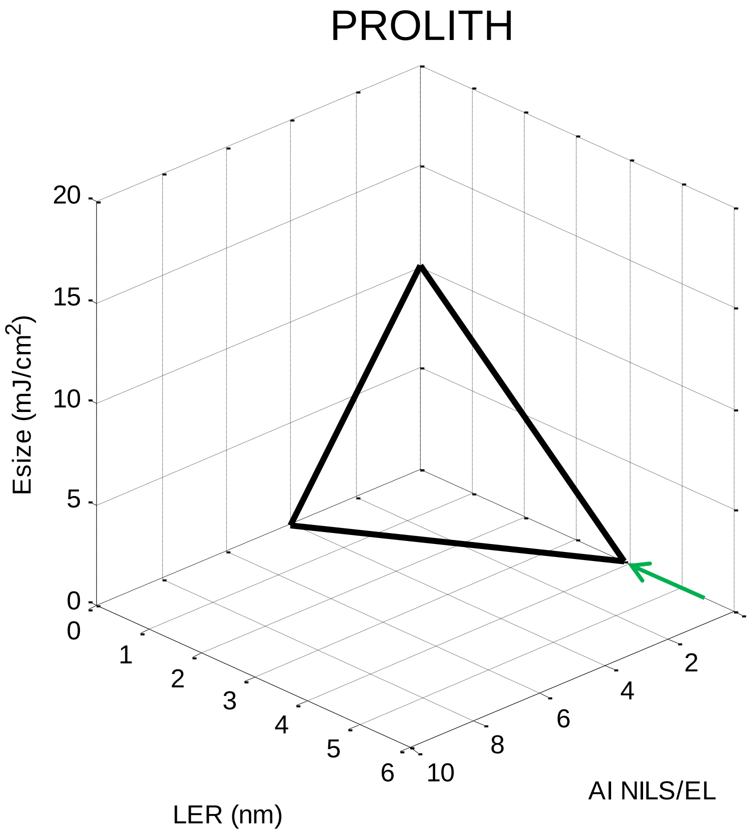
$EL = 21.5\%$

$\langle LER \rangle = 4\,nm$ ↓

$E_{size} = 10\,mJ/cm^2$

$\Phi = 2.9\ acids/photon$

$\Phi_q = 0.9\ PDB/photon$



Reduce acid diffusivity

Replace Q with PDB

15% PAG

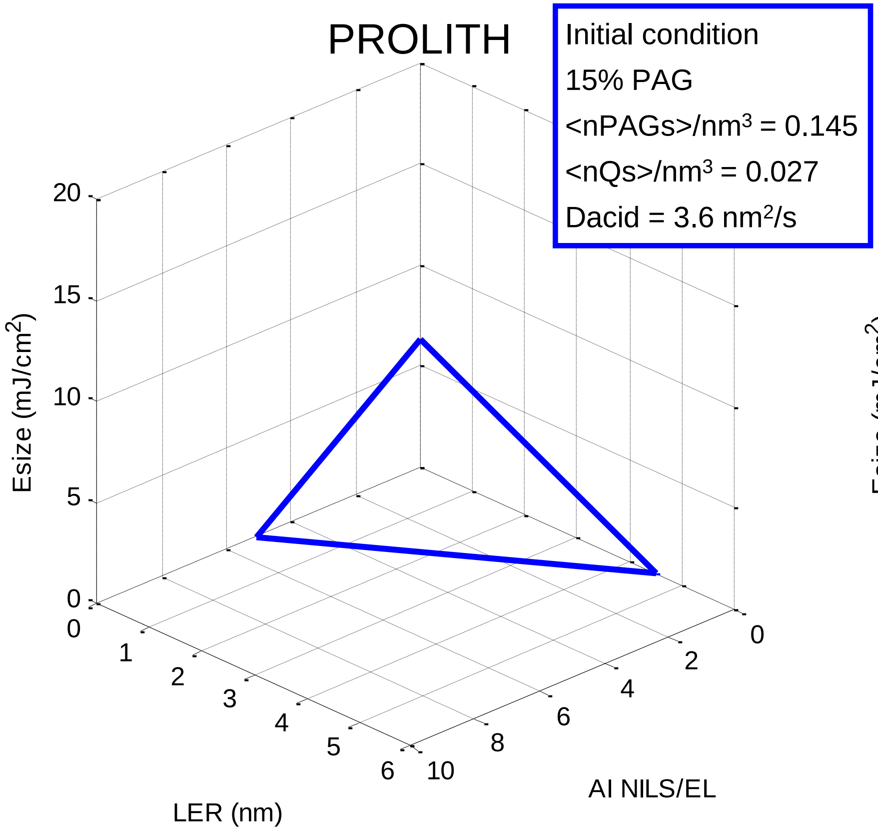
$\langle nPAGs\rangle/nm^3 = 0.145$

$\langle nPDQs\rangle/nm^3 = 0.045$

Dacid = 1.5 nm^2/s

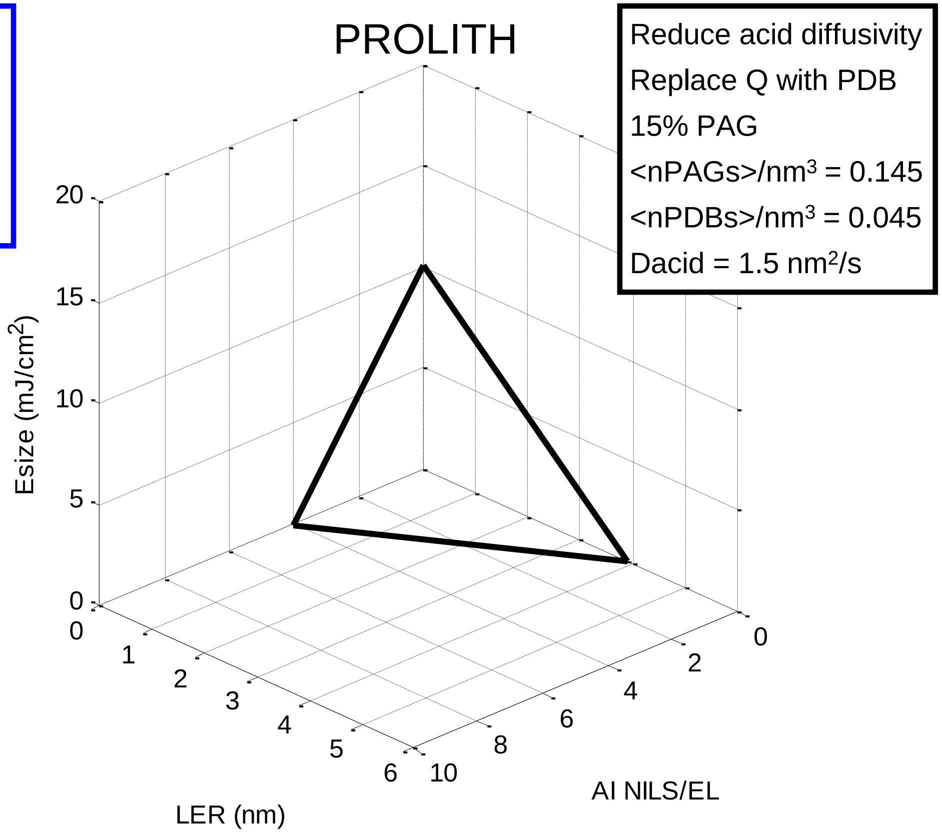
- Reduction of acid diffusivity improves exposure latitude
- PDB addition further reduces LER, even though acid yield decreases

RLS performance comparison with improved formulation



Initial condition
15% PAG
<nPAGs>/nm^3 = 0.145
<nQs>/nm^3 = 0.027
Dacid = 3.6 nm^2/s

$$EL = 18\%, \langle LER \rangle = 4.6\,nm,\ E_{size} = 6\,mJ / cm^2$$



Reduce acid diffusivity
Replace Q with PDB
15% PAG
<nPAGs>/nm^3 = 0.145
<nPDBs>/nm^3 = 0.045
Dacid = 1.5 nm^2/s

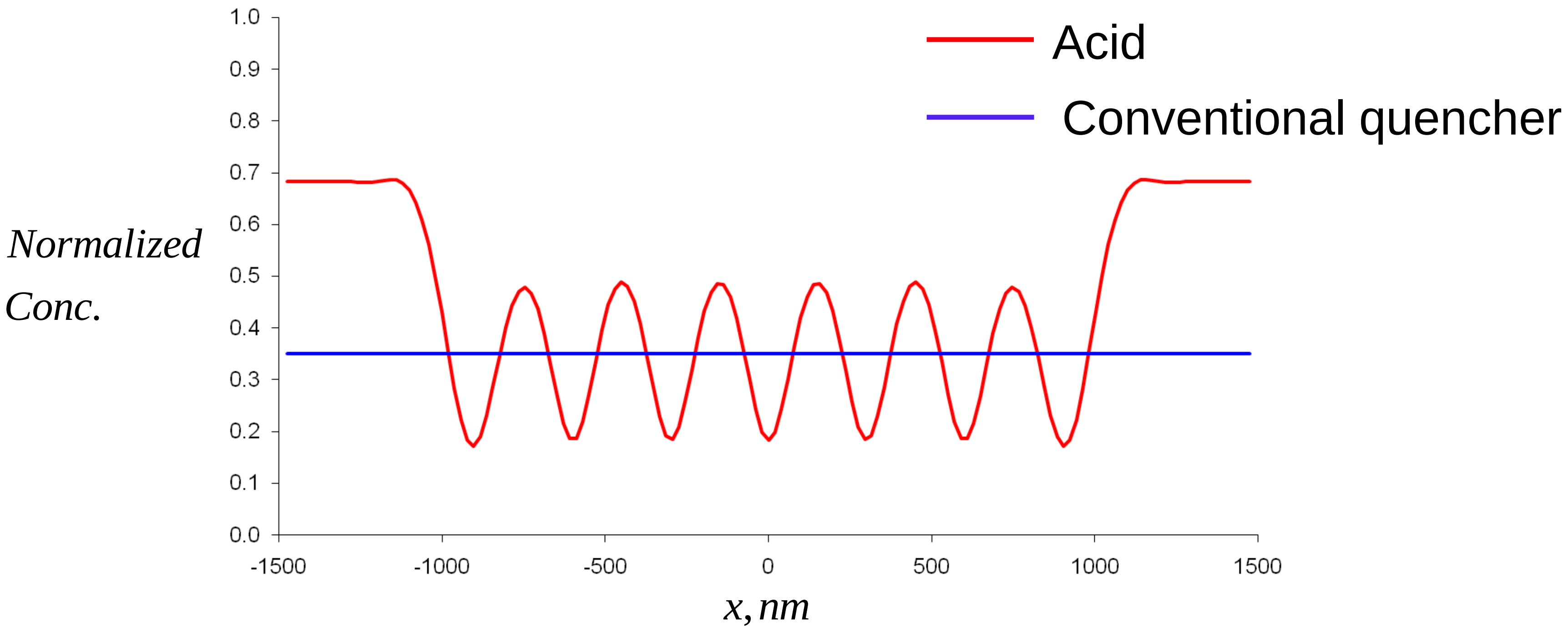
$$EL = 21\%, \langle LER \rangle = 4\,nm,\ E_{size} = 10\,mJ / cm^2$$

- Net is 17% increase in EL, 13% reduction in LER

Photodecomposable bases, PDBs

- First proposed for use in KrF resists by Funato et al [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

Acid and conventional quencher conc. vs. *x* , post-expose, 120 nm lines, ArF

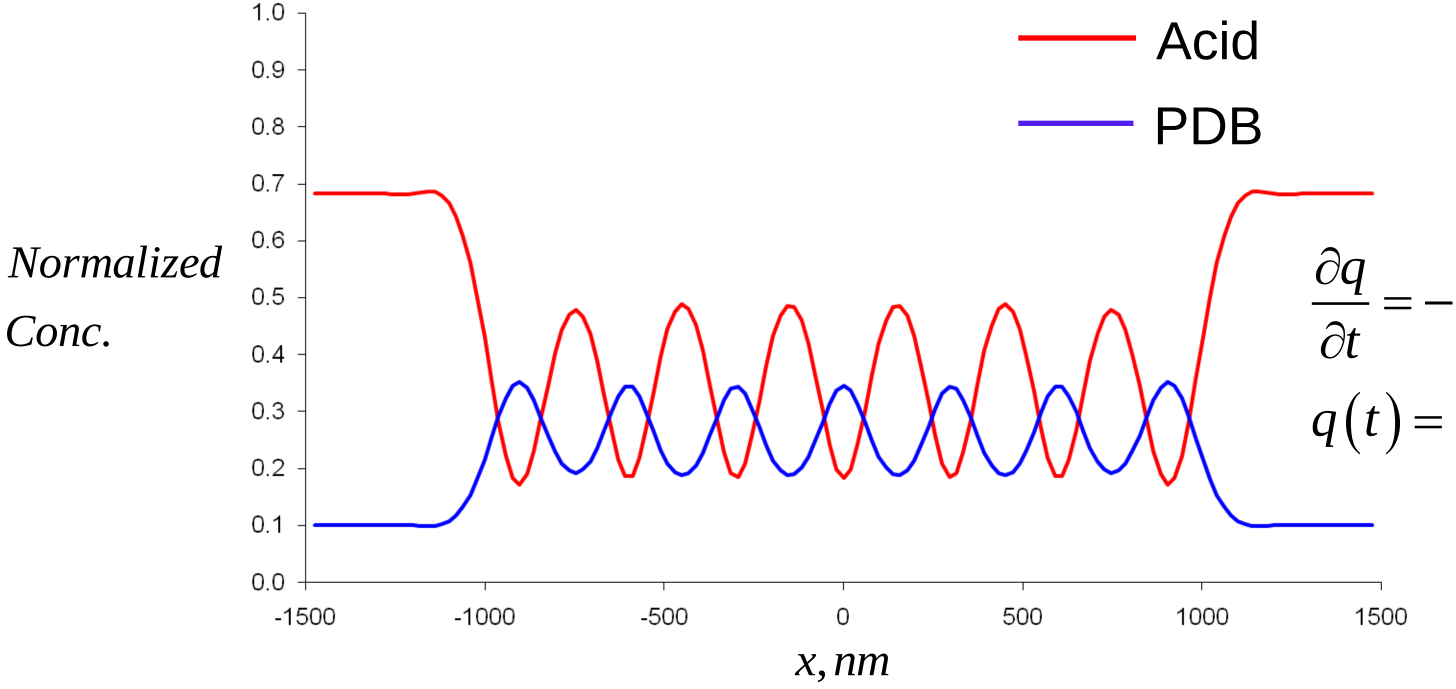


3. *“Application of photodecomposable base concept to two-component deep-UV chemically amplified resists”* Funato et al, Proc. SPIE 2724, 186 (1996)

Simulation of photodecomposable bases, PDBs

- First proposed for use in KrF resists by Funato et al [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

Acid and PDB conc. vs. *x* , post-expose, 120 nm lines, ArF



$$\frac{\partial q}{\partial t} = -C_q I\, q$$

$$q(t) = q_0 \exp\left(-C_q E\right)$$

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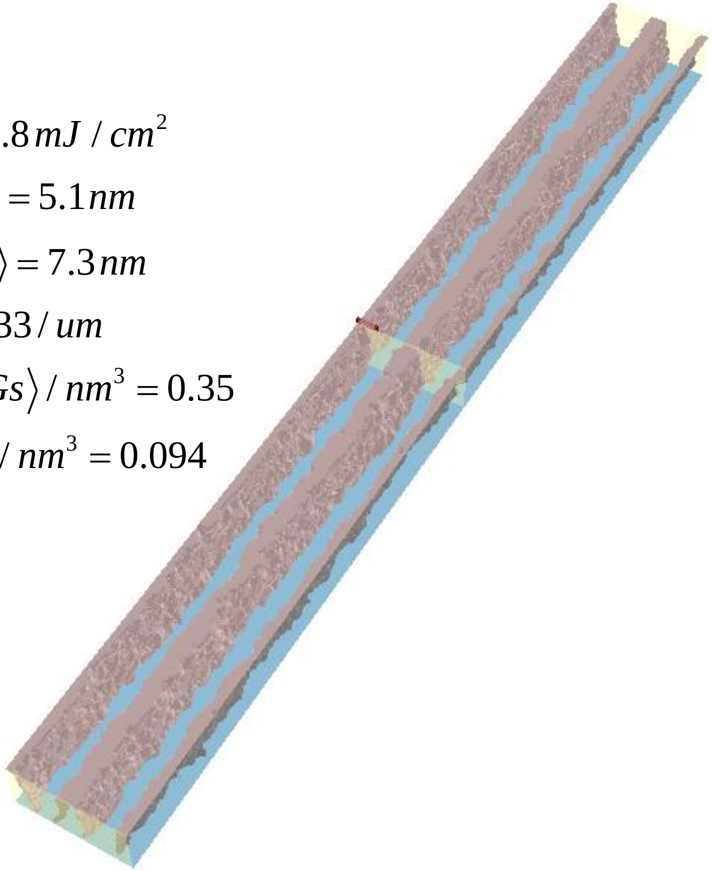
3. *"Application of photodecomposable base concept to two-component deep-UV chemically amplified resists"* Funato et al, Proc. SPIE 2724, 186 (1996)

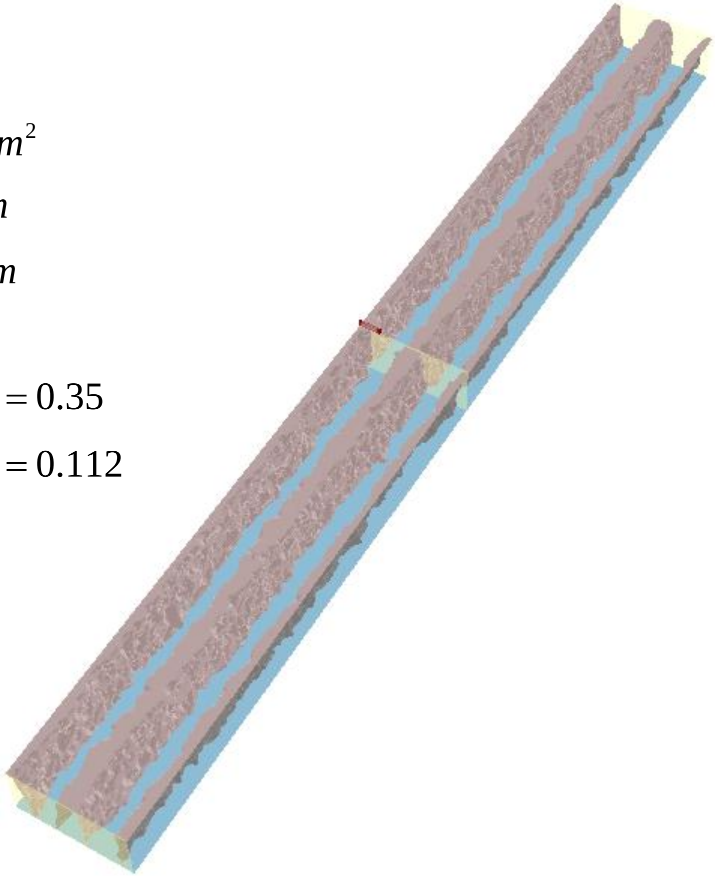
Simulated effect of PDBs on EUV relief image

27 nm hp, 0.25NA, 0.5 partial coherence, 50 nm resist on Si

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



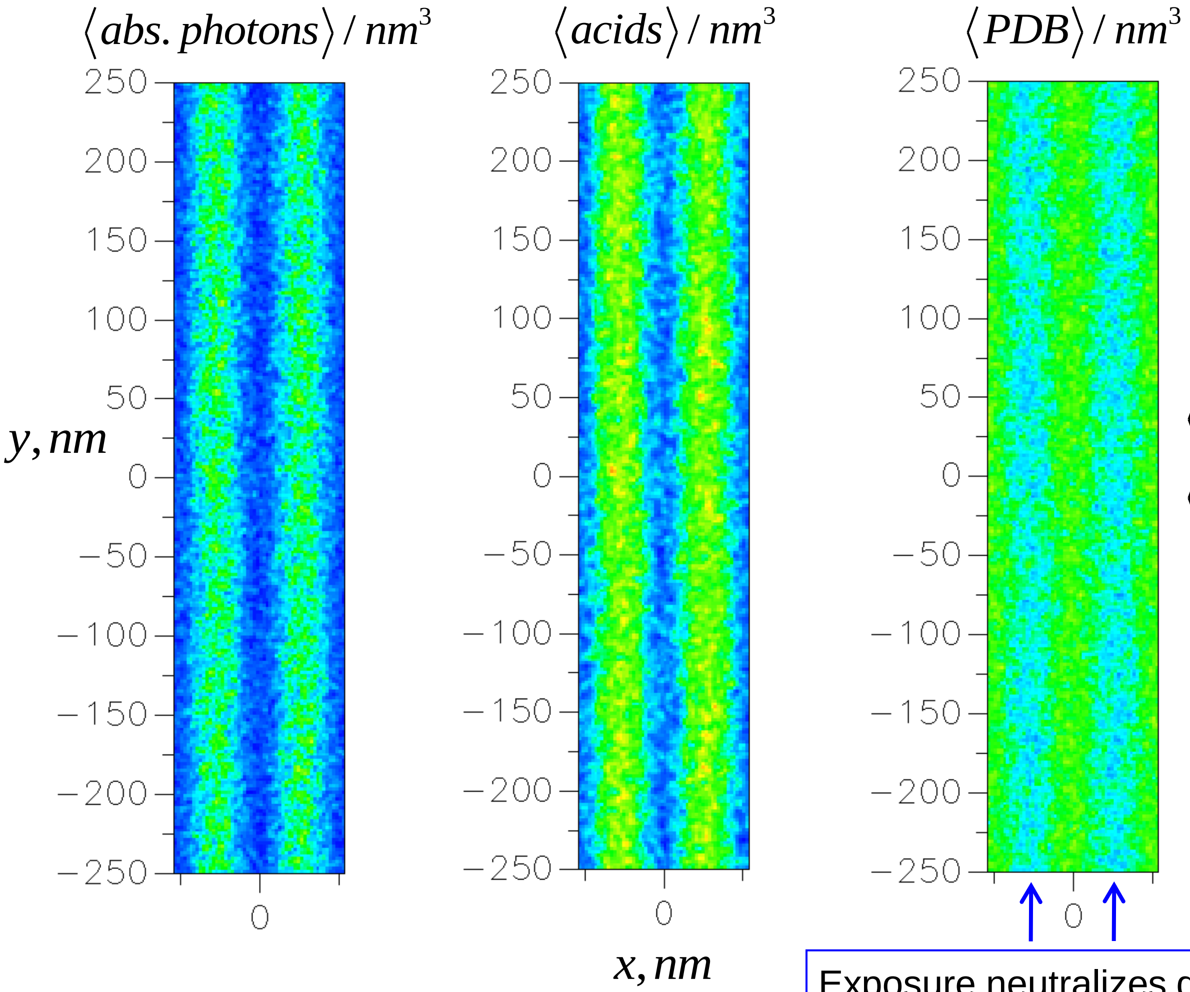
$$E = 12.8\,mJ/cm^2$$
$$\langle LER \rangle = 4.5\,nm$$
$$\langle LWR \rangle = 6.2\,nm$$
$$\alpha = 6.33/um$$
$$\langle nPAGs \rangle / nm^3 = 0.35$$
$$\langle nPDBs \rangle / nm^3 = 0.112$$



- 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



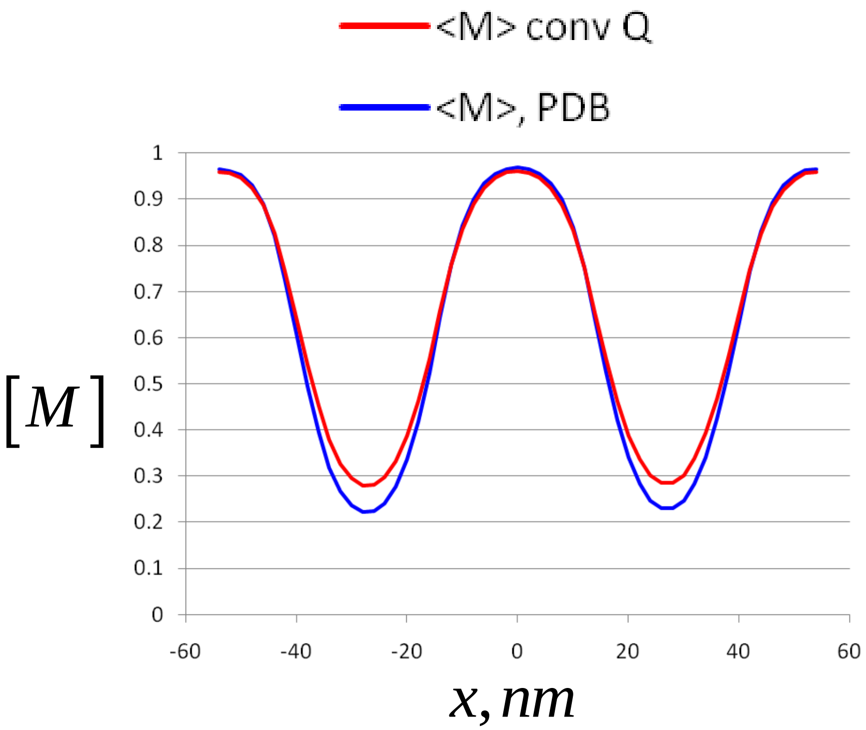
$$\langle nPAGs \rangle / nm^3 = 0.35$$

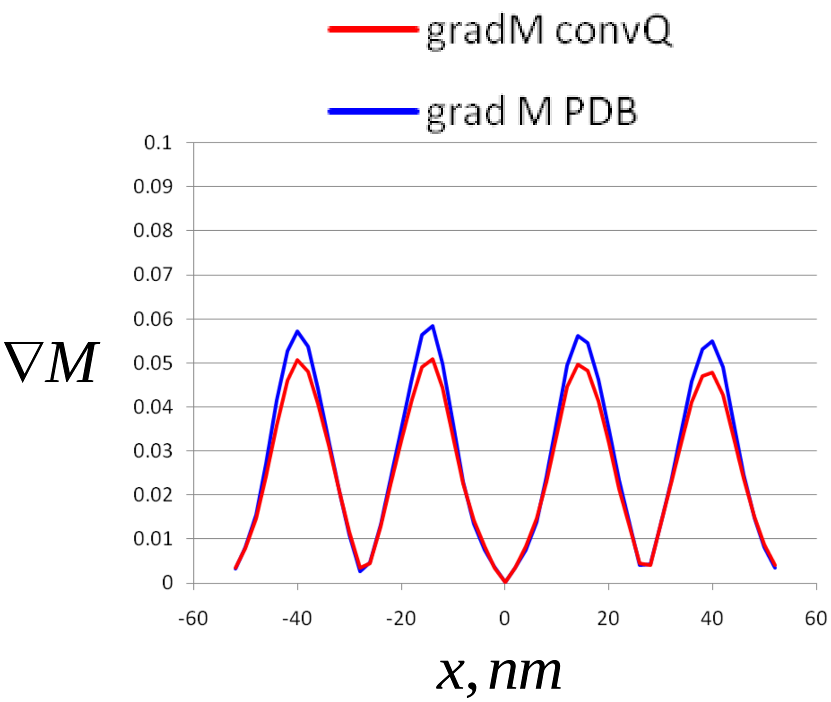
$$\langle nPDBs \rangle / nm^3 = 0.112$$

Exposure neutralizes quencher

Simulated effect of PDBs on EUV PEB latent image

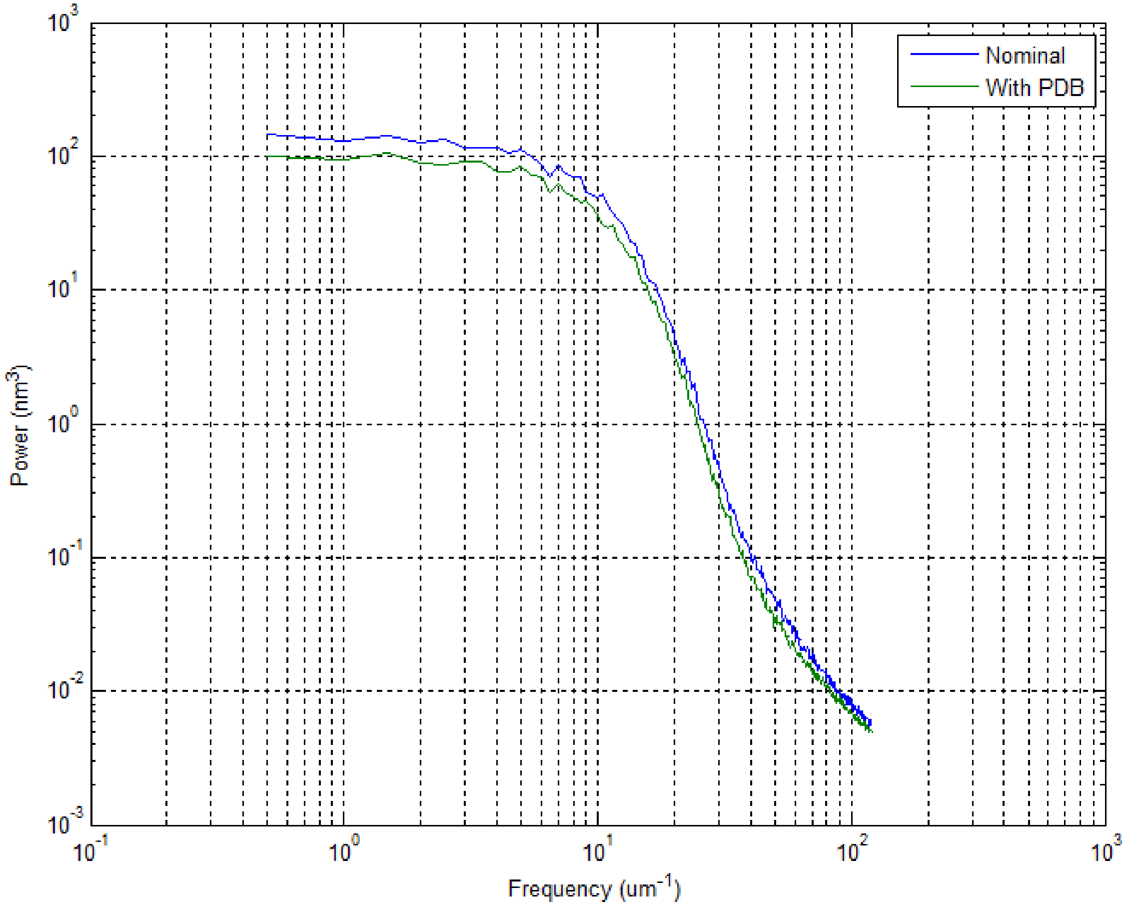
27 nm hp, 0.25NA, 0.5 partial coherence, 50 nm resist on Si





- Blocked polymer conc. [*M*] and gradient [*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

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Pat Lee

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David Blankenship

Dan Grubbs

Chris Walker

Heather Spears

Greg Floyd

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