

Line Edge Roughness, part 2

In the last edition of this column [1], I began the difficult process of trying to understand the fundamental mechanisms behind the formation of line edge roughness (LER). The approach I've taken is called *stochastic modeling*, and involves the use of random variables and probability density functions to describe the statistical fluctuations that are expected. We began with photon shot noise, which follows Poisson statistics, then looked at the initial distribution of photoacid generator (PAG) in the resist, which also follows Poisson statistics. The exposure reaction itself is probabilistic, with the probability that any particular PAG will be exposed given by the solution to the continuum kinetic equation of exposure. The results so far are summarized in the following table:

Name	Formula
Exposure shot noise coefficient	$\psi = \left(\frac{hc}{\lambda}\right) \frac{C}{A} = \frac{\Phi a_M}{N_A A} = \frac{\Phi \sigma_{M-abs}}{A}$
Mean number of photons	$\langle n \rangle = \frac{C \langle I \rangle t}{\psi}$
Standard deviation of number of photons	$\sigma_n = \sqrt{\langle n \rangle}$
Mean initial number of PAGs	$\langle n_0 \rangle = \langle G_0 \rangle N_A V$
Mean relative acid concentration	$\langle h \rangle = 1 - e^{-\langle n \rangle (1 - e^{-\psi})}$
Standard deviation of relative acid concentration	$\sigma_h = \sqrt{\frac{\langle h \rangle}{\langle n_0 \rangle}}$

Here, A is the cross-sectional area and V is the volume of the resist under consideration. As A and V increase, the mean values of the quantities approach their continuum limits and the variances of the quantities go to zero. C is the familiar Dill exposure parameter and hc/λ is the photon energy [1].

The results show two interesting aspects to the variability of acid concentration after exposure as a function of the volume of resist you are looking at. Both the mean value of the concentration of acid in a volume and the standard deviation of the concentration change as the volume changes. The second result, that the standard deviation of acid concentration is higher if the number of PAGs originally in the volume is lower, is intuitively obvious from standard counting statistics of concentration. Less obvious is that photon shot noise causes the mean concentration of acid to vary systematically with the volume under consideration. As Figure 1

shows, however, for a typical 193 nm resist the length scale must be appreciably less than 1 nm before any shot noise effects can be noticed.

Diffusion

How does diffusion affect the uncertainty in acid concentration? Does diffusion ‘smooth out’ the roughness in acid concentration, or does it add an extra uncertainty since diffusion itself is a stochastic process? In a previous issue of this column (*MLW*, May 2006), diffusion was treated using a Gaussian diffusion point spread function (*DPSF*) – the latent image after diffusion is the initial latent image convolved with a Gaussian, whose standard deviation σ is called the diffusion length. From a stochastic modeling perspective, the Gaussian represents a probability distribution: for a particle initially at some position, the Gaussian *DPSF* represents the probability density of finding that particle some distance r from its original location. This probability distribution is itself derived from a stochastic look at the possible motions of the particle during the bake. Given that the particle can randomly move in any possible direction at a particular speed determined by its diffusivity, and can change directions randomly, the resulting path of the particle is called a *random walk*. Averaging over all possible random walk paths produces the Gaussian probability distribution (when the diffusivity is constant).

Consider first the diffusion of a single acid molecule. Defining a binary random variable y to represent whether that molecule is found in some small volume dV located a distance r from its original location ($y=1$ implies that it is present, $y=0$ means it’s absent),

$$P(y=1) = \left(2\pi\sigma^2\right)^{-3/2} e^{-r^2/2\sigma^2} dV \quad (1)$$

This binary random variable will follow all of the properties of binary variables derived in the last edition of this column. If, instead of one acid molecule at a certain location which then diffuses, there are n acid molecules at this location that then diffuse, the total number of acid molecules in that volume dV will be Y , again with the properties derived before. Adding up the contributions from all of the locations that could possibly contribute acid molecules into the volume dV produces the convolution result below, giving the after-bake acid concentration h^* and its standard deviation:

$$\langle h^* \rangle = \langle h \rangle * DPSF, \quad \sigma_{h^*} = \sqrt{\frac{\langle h^* \rangle}{\langle n_0 \rangle}} \quad (2)$$

Thus, diffusion does not intrinsically increase the uncertainty in acid concentration due to the extra stochastic process of the random walk, nor does it intrinsically ‘smooth out’ any uncertainties through the process of diffusion. Only through a change in the mean concentration does diffusion affect the uncertainty in the concentration. For a typical conventional resist, the concentration of exposure products near the edge of the resist feature does not change appreciably due to diffusion during PEB. Thus, it is unlikely that diffusion will have a significant impact on the concentration statistics near the resist line edge.

Reaction-Diffusion

Of course, for a chemically amplified resist acid diffusion is accompanied by one or more reactions. Here, we'll consider only the polymer deblocking reaction (acid-quencher neutralization will be ignored). In the continuum limit, the amount of blocked polymer left after the PEB, M , was described in a previous edition of this column (*MLW*, August 2006) using an effective acid concentration (the convolution of the acid latent image with the reaction-diffusion point spread function, *RDPSF*):

$$M = M_0 e^{-K_{amp} t_{PEB} h_{eff}}, \quad h_{eff}(x, y, z) = h(x, y, z, t=0) * RDPSF \quad (3)$$

Where M_0 is the initial concentration of blocked polymer, K_{amp} is the amplification rate constant and t_{PEB} is the PEB time. As before, the latent image of acid after exposure, $h(x, y, z, t=0)$, used in the continuum approximation is actually the mean acid concentration $\langle h \rangle$, with a standard deviation as given above. The effective acid concentration, however, has a very specific interpretation: it is the time average of the acid concentration at a given point. The interesting question to be answered, then, is whether this time-averaging effect of diffusion coupled with the acid-catalyzed reaction affects the uncertainty in the effective acid concentration compared to the original acid concentration uncertainty.

While a detailed derivation is beyond the scope of this article, the final result is somewhat intuitive. Letting a be the deblocking reaction capture distance (that is, it represents the how close the acid must come to a blocked site before it can potentially participate in a deblocking reaction), for a problem of dimensionality p ($p = 1, 2, \text{ or } 3$),

$$\sigma_{h_{eff}} \approx \left(\frac{a}{\sigma_D} \right)^{\frac{p}{2}} \sigma_h \quad (4)$$

where σ_D is the diffusion length of the acid. In other words, if the acid diffuses a distance less than the reaction capture range, the catalytic nature of the amplification reaction actually increases the stochastic variation in the effective acid concentration, and thus the blocked polymer concentration. If, however, the diffusion length is greater than this capture range, the time-averaging effect of the catalytic reaction will smooth out stochastic roughness. It is not diffusion, *per se*, that reduces stochastic uncertainty, but rather the diffusion of a reaction catalyst that does so. Since in real resist systems the diffusion length will invariably be greater than the reaction capture distance, the net affect will always be a reduction in the effective acid concentration standard deviation.

At this point, it will be useful to apply a linear propagation of uncertainty approach. By assuming that uncertainties are small and independent, a Taylor series expansion of a function about its mean value leads to the standard textbook approach to error propagation: given some function $z = f(x, y)$,

$$\sigma_z^2 = \left(\frac{\partial f}{\partial x} \right)^2 \sigma_x^2 + \left(\frac{\partial f}{\partial y} \right)^2 \sigma_y^2 \quad (5)$$

where the partial derivatives are evaluated at the means of the function inputs. Applying this equation to the deblocking kinetics of equation (3) gives

$$\sigma_M^2 = \left(\frac{\partial M}{\partial h_{\text{eff}}} \right)^2 \sigma_{h_{\text{eff}}}^2 + \left(\frac{\partial M}{\partial M_0} \right)^2 \sigma_{M_0}^2 = (K_{\text{amp}} t_{\text{PEB}})^2 \langle M \rangle^2 \left(\frac{a}{\sigma_D} \right)^p \sigma_h^2 + \frac{\langle M \rangle^2}{\langle M_0 \rangle^2} \sigma_{M_0}^2 \quad (6)$$

Since both the acid concentration h and the initial blocked concentration M_0 will follow Poisson statistics,

$$\sigma_h^2 = \frac{\langle h \rangle}{\langle n_0 \rangle}, \quad \text{and} \quad \sigma_{M_0}^2 = \frac{\langle M_0 \rangle^2}{\langle n_0 - \text{blocked} \rangle} \quad (7)$$

where $\langle n_0 - \text{blocked} \rangle$ is the mean initial number of blocked polymers in the volume of interest. Letting the relative blocked polymer concentration m be given by

$$m = \frac{M}{\langle M_0 \rangle} \quad (8)$$

we can arrive at our final result for the relative uncertainty in m :

$$\frac{\sigma_m}{m} = \left[- (K_{\text{amp}} t_{\text{PEB}}) \ln \langle m \rangle \left(\frac{a}{\sigma_D} \right)^p \frac{1}{\langle n_0 \rangle} + \frac{1}{\langle n_0 - \text{blocked} \rangle} \right]^{\frac{1}{2}} \quad (9)$$

Putting some typical values into this equation, $- (K_{\text{amp}} t_{\text{PEB}}) \ln \langle m \rangle$ will be in the range of about 1 – 3, the value of $\langle n_0 - \text{blocked} \rangle / V$ is on the order of 1 blocked polymer per cubic nanometer, and $\langle n_0 \rangle / V$ is typically near 0.04 / nm³. The reaction capture distance, a , is not easy to determine, but should be on the order of 1 nm.

Figure 2 shows how the relative uncertainty in the relative blocked concentration varies with amount of diffusion for two different volumes of interest, $V = (3 \text{ nm})^3$ and $V = (5 \text{ nm})^3$, for a two-dimensional problem. For this example, acid fluctuations dominate when $\sigma_D / a < 7$, whereas the Poisson distribution of blocked polymer sites becomes the most significant factor for diffusion lengths greater than this amount.

So far we have looked at the statistics of photons, chemical concentration, PAG exposure, diffusion, and reaction-diffusion (deblocking only) to give a concentration of blocked polymer after PEB. [Acid-base quenching, though ignored here due to its complexity, is expected to significantly affect LER.] To understand how these statistics will impact line edge roughness, a stochastic model of dissolution will be developed in the next edition of this column.

Reference

1. C. A. Mack, The Lithography Expert: Line Edge Roughness, Part 1, Microlithography World 16.1, p. 13 (Feb. 2007) or http://sst.pennnet.com/display_article/284620/28/ARTCL/none/none/The-Lithography-Expert:-Line-edge-roughness,-Part-1/

Figure Captions

- Figure 1. Systematic dependence of the mean value of photo acid concentration after exposure resulting from the quantization of light into photons as a function of the area (= length squared) being exposed. Typical 193 nm resist values were used: $\psi A = 0.005 \text{ nm}^2$, mean number of photons = $100 / \text{nm}^2$.
- Figure 2. Variation of the relative uncertainty in the relative blocked concentration with amount of diffusion for two different volumes of interest, $V = (3 \text{ nm})^3$ and $V = (5 \text{ nm})^3$ ($\rho = 2$, $-\ln\langle m \rangle K_{\text{amp}} t_{\text{PEB}} = 2$).

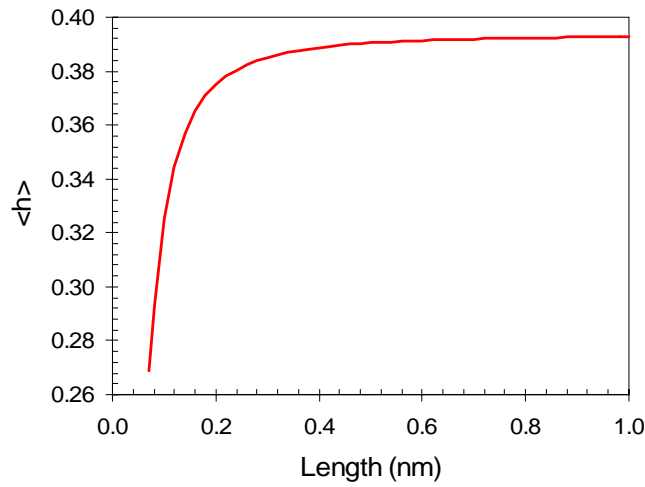


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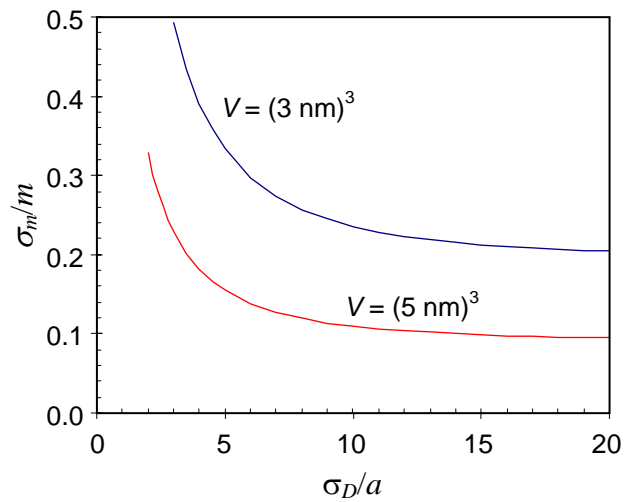


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