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JM^3 Letters

Uncertainty in roughness measurements: putting error bars on line-edge roughness

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Abstract. Measurement of line-edge or linewidth roughness involves uncertainty, like all measurements, and an estimate of that uncertainty should be reported whenever a roughness measurement is reported. However, roughness measurement uncertainty estimates are complicated by the correlations along the length of the rough feature. As a result, roughness measurements are often not accompanied by uncertainty estimates or error bars on graphs. Here, both theoretical considerations and simulations of random rough features will be used to derive a simple formula to estimate the uncertainty of a roughness measurement using the standard parameters describing that roughness: standard deviation, correlation length, and roughness exponent. Additionally, a more accurate formula to estimate the systematic bias in roughness standard deviation is provided. [DOI: 10.1117/1.JMM.16.1.010501]

Keywords: line-edge roughness; linewidth roughness; measurement uncertainty; power spectral density.

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1 Introduction

As everyone learns early in their education in science and engineering, all measurements should be accompanied by an estimate of the uncertainty of that measurement. Unfortunately, measurements of the standard deviation of a rough surface or edge are often not accompanied by an estimate of the uncertainty of those measurements. This is especially true in the measurement of line-edge roughness (LER) or linewidth roughness (LWR) of lithographically patterned features, where presentation of error estimates (or the use of error bars on graphs) by metrology users is almost universally absent. One reason for this lack of scientific rigor is the complicated nature of the statistics involved: we are calculating the standard deviation of a set of correlated measurement values.[1–4] Understanding the uncertainty of such a measurement is complicated by the correlations, and standard textbook treatments are generally not useful.

In this letter, both the uncertainty and the bias of LER/LWR measurements will be derived for the case of an exponential autocovariance function (equivalent to a roughness exponent of 0.5). Using simulations, those results will be extended to other roughness exponents, so a general expression will be obtained. Given estimates of the correlation length and the roughness exponent, these expressions will allow uncertainty estimates to be made for any measurement of LER/LWR. While important in its own right, these error estimates will also allow better prediction of the impact of LER on other lithography metrics such as local critical dimension uniformity.[3]

2 Derivation of the Uncertainty of LER Measurement

The typical estimate of standard deviation of a rough feature is given by the well-known equation

$$s = \sqrt{\frac{\sum_{i=0}^{N-1} (w_i - \bar{w})^2}{N-1}}, \tag{1}$$

where s is the sample estimate of the true value σ, w_i is the linewidth (for the case of LWR) measured at a position $i\Delta y$ up from the 0th measurement position, and $\bar{w}$ is the mean of the N measurements made over a line of length $L = N\Delta y$. The sample estimate of the variance is, of course, the square of s. Assuming a stationary stochastic process, the expected value of the sample variance can be found as

$$E[s^2] = \sigma^2 - \frac{2}{N-1}\sum_{m=1}^{N-1}\left(1 - \frac{m}{N}\right) R_d(m\Delta y), \tag{2}$$

where R_d is the discrete autocovariance function (ACF), describing the correlation between points a distance $m\Delta y$ apart along the feature. Note that for finite N, the sample estimate of the variance is biased lower by the correlation behavior of the roughness. The expected value of the standard deviation is given by

$$E[s] = \sqrt{E[s^2] - \mathrm{var}(s)}. \tag{3}$$

Thus, to find the bias in our measured LER (i.e., in s), we need an expression for the variance of the standard deviation estimate, which is needed in any case to provide an estimate of the uncertainty in our measurement.

We will begin by finding an expression for $\mathrm{var}(s^2)$. Recently, expressions were derived for the variance of the discrete ACF.[4] Consider the case of an exponential ACF

$$\mathrm{ACF}(\tau = m\Delta y) = \sigma^2 e^{-\tau/\xi} = \sigma^2 \rho^m \quad \rho = e^{-\Delta y/\xi}, \quad m \geq 0, \tag{4}$$

where ξ is the correlation length. For this particular ACF

$$\begin{aligned} \mathrm{var}(s^2) &= \left(\frac{N}{N-1}\right)^2 \mathrm{var}[R_d(m=0)], \\ \frac{\mathrm{var}[R_d(m=0)]}{\sigma^4} &\approx \frac{2}{N}\left(\frac{1+\rho^2}{1-\rho^2}\right)\left[1 - \frac{2\rho^2}{N(1-\rho^4)}\right] \\ &= \frac{2}{N\tanh(\Delta y/\xi)}\left[1 - \frac{1}{N\sinh(2\Delta y/\xi)}\right]. \end{aligned} \tag{5}$$

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For typical parameters such that $\Delta y < \xi < L$, the hyperbolic functions of can be approximated by the first few terms of their Taylor series, giving

$$\frac{\mathrm{var}[R_d(m=0)]}{\sigma^4} \approx \left(\frac{2\xi}{L}\right)\left(1-\frac{\xi}{2L}\right)\left[1+\frac{1}{3}\left(\frac{\Delta y}{\xi}\right)^2\right]. \tag{6}$$

Equation (5) was derived assuming the mean of the distribution was known *a priori*. In reality, the ACF is estimated using the sample mean. Such mean detrending will cause a reduction in the ACF and its variance.[2,4] For $\Delta y \ll \xi$,

$$\mathrm{var}[R_{d\text{-mean}}(m=0)] = \mathrm{var}[R_d(m=0)]\left[1-\frac{2\xi}{L}\left(1-\frac{\xi}{L}\right)\right]^2. \tag{7}$$

The var(s) can be approximated from the var(s^2) by

$$\mathrm{var}(s^2) \approx 4\sigma^2 \mathrm{var}(s). \tag{8}$$

The standard error (SE) of our roughness estimate s is simply the square root of var(s)

$$\mathrm{SE}(s) \approx \sigma\sqrt{\frac{\mathrm{var}[R_{d\text{-mean}}(m=0)]}{4\sigma^4}}. \tag{9}$$

Combining Eqs. (6), (7), and (9),

$$\frac{\mathrm{var}[R_{d\text{-mean}}(m=0)]}{\sigma^4} \approx \left(\frac{2\xi}{L}\right)\left(1-\frac{9\xi}{2L}\right)\left[1+\frac{1}{3}\left(\frac{\Delta y}{\xi}\right)^2\right],$$

$$\mathrm{SE}(s) \approx \sigma\sqrt{\frac{\xi}{2L}}\left(1-\frac{9\xi}{4L}\right)\left[1+\frac{1}{6}\left(\frac{\Delta y}{\xi}\right)^2\right] \approx \sigma\sqrt{\frac{\xi}{2L}}. \tag{10}$$

Equation (10) is our first desired result: an estimate of the random uncertainty of our LWR measurement (i.e., the uncertainty in the standard deviation of the linewidth of the rough feature). As an example, consider the measurement of a 1-μm-long line whose roughness has a correlation length of 20 nm. The SE of the LER or LWR measurement will be 10%, so the 95% confidence interval will be $\sim\pm 20\%$.

This estimate of the SE allows us to complete Eq. (3) and determine the bias in our roughness estimate for the case of an exponential ACF. For typical values of parameters,

$$\begin{aligned} E[s^2] &= \sigma^2\left[1-\frac{2}{N-1}\left(\frac{\rho}{1-\rho}\right)\left(1-\frac{1}{N(1-\rho)}\right)\right] \\ &\approx \sigma^2\left[1-\frac{2\xi}{L}\left(1-\frac{\xi}{L}\right)\right], \end{aligned} \tag{11}$$

$$(E[s])^2 = E[s^2] - \mathrm{var}(s) \approx \sigma^2\left[1-\left(\frac{5}{2}\right)\frac{\xi}{L}\left(1-\frac{2\xi}{L}\right)\right]. \tag{12}$$

Thus,

$$E[s] \approx \sigma\left[1-\left(\frac{5}{4}\right)\frac{\xi}{L}\left(1-\frac{2\xi}{L}\right)\right] \approx \sigma\left[1-\left(\frac{5}{4}\right)\frac{\xi}{L}\right]. \tag{13}$$

Since $L \gg \xi$, it is clear that the bias in s will be small compared to the SE of s. For example, for the same case as before, with $\xi = 20$ nm and $L = 1000$ nm, the bias is only 2.5% (as compared to the 20% confidence interval due to the SE).

Our final estimate for the SE of the roughness s can now be given by replacing the true standard deviation σ in Eq. (10) with its estimate from Eq. (13).

$$\mathrm{SE}(s) \approx s\sqrt{\frac{\xi}{2L}}\left(1-\frac{\xi}{L}\right)\left[1+\frac{1}{6}\left(\frac{\Delta y}{\xi}\right)^2\right] \approx s\sqrt{\frac{\xi}{2L}}. \tag{14}$$

This result is intuitive when compared to the case of uncorrelated measurements. For n independent and identically distributed measurements, the SE of the standard deviation is generally estimated as $s/\sqrt{2n}$. For a rough line of length L and a correlation of length ξ, the number of statistically "independent" pieces along the line is L/ξ, so the approximate form of Eq. (14) becomes the textbook result.

The results presented so far assume the measurement of a single feature. Often, multiple features are measured and the results averaged together. It seems reasonable to assume that each feature is independent of the others, so if M features are measured the SE of the resulting averaged LER standard deviation will be reduced by $\sqrt{M}$. From the perspective of SE(s), this is equivalent to measuring one feature of length ML. The bias, on the other hand, is not affected by the measurement of multiple features since the bias is the same for each one.

3 Comparison to Simulation

To validate the above expressions, simulated rough features with a predetermined autocovariance behavior were generated and virtually measured to obtain the standard deviation of the roughness.[5] By repeating these simulations on the order of 10^6 times, both the mean and standard deviation of the measured roughness standard deviation were obtained. The correlation length was varied over a range of 5 to 50 nm, the measurement grid size was varied between 1 and 10 nm, and the number of measurement points ranged from 128 to 1024. All simulations used a true 1-sigma LER of 2 nm (an arbitrary choice since the results will scale linearly with this value). The results are shown in Fig. 1.

The results from Fig. 1 show a very good match between simulations and the analytically derived expressions from the previous section. The largest deviation in Fig. 1(a) between simulation and Eq. (13) comes when ξ/L is at its largest (near 0.1). These results can now be extended by simulating features with different correlation behavior. Most LER/LWR data have been found to be well described by the Palasantzas power spectral density (PSD) function[6]

$$\mathrm{PSD}(f) = \frac{\mathrm{PSD}(0)}{[1+(2\pi f\xi)^2]^{H+1/2}}, \tag{15}$$

where H is the Hurst roughness exponent and PSD(0) is found (using the gamma function, Γ) by

$$\mathrm{PSD}(0) = 2\sigma^2\xi\left[\frac{\sqrt{\pi}\,\Gamma(H+\frac{1}{2})}{\Gamma(H)}\right]. \tag{16}$$

The PSD and the ACF form a Fourier transform pair. When $H = 0.5$, the Palasantzas PSD is the Fourier transform of the exponential ACF of Eq. (4). Using this PSD function as an

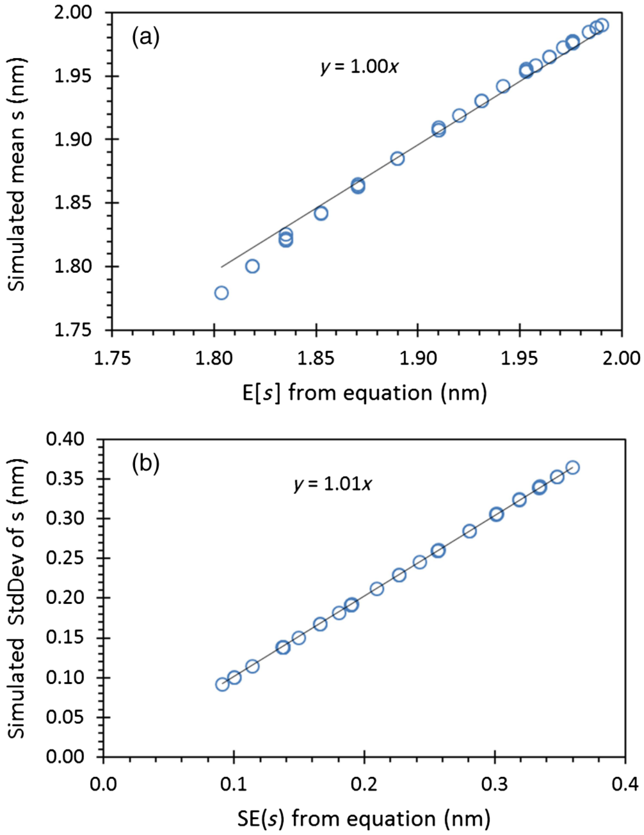

Fig. 1 Comparing simulations to analytical expressions: (a) the mean of the standard deviation of many simulated rough features as compared to Eq. (13) and (b) the standard deviation of the standard deviation of many simulated rough features as compared to Eq. (14).

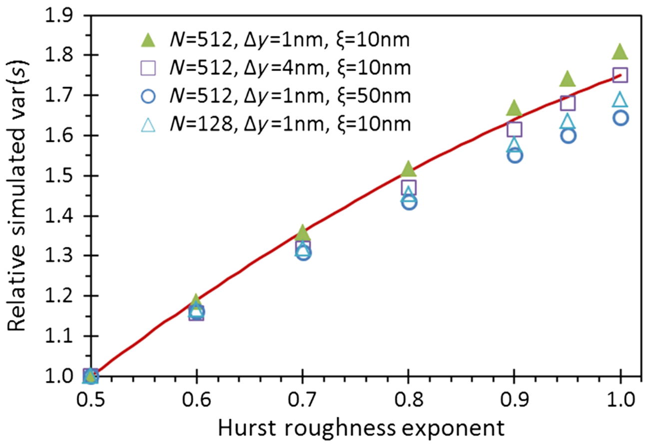

Fig. 2 Varying the Hurst roughness exponent H, the variance of the simulated LER is shown relative to that for $H = 0.5$ (symbols). The line shows a plot of Eq. (17).

input, rough features were generated over a range of roughness exponents. Figure 2 shows the var(s) relative to that obtained for $H = 0.5$. The simulated results can be approximated by

$$\mathrm{SE}(s) \approx s\sqrt{\left(\frac{\xi}{2L}\right)[2H-(H-0.5)^2]}. \tag{17}$$

The analytical and simulation results presented so far assume ideal measurements. Real roughness measurements include noise in the measurements (which add in quadrature to the measured variance of the linewidth or line edge) and a non-zero width metrology probe that averages the roughness over the width of the probe.[1,4] Using simulations to investigate these effects, it was found that metrology noise and metrology probe averaging both have only a very small impact on SE(s) (changing the value by only a few percent for typical parameter values) and so can be neglected.

4 Conclusions

The derivations and simulations presented above have accomplished two goals. First, a general expression that allows error estimates to be made for a measurement of LER or LWR has been developed. By estimating the three parameters of the PSD (σ, ξ, and H), a measurement of σ for a rough feature can be accompanied by its SE using Eq. (17). Typical SEs are likely to be in the 5% to 15% range, so 95% confidence intervals on the measurements will be in the ±10% to ±30% range. Such error estimates are critical, for example, when comparing resists or processes to decide which provides better LER performance. Small differences in measured LER are unlikely to be statistically significant. It should be noted that each of our estimates of σ, ξ, and H for use in Eq. (17) has uncertainties that will propagate into uncertainty in our SE estimate.

The second goal was to develop a better estimate of the bias in the measured LER. Most prior results described the bias in the variance,[7,8] thus leaving out an important term due to var(s) when determining the bias in the standard deviation. Including this term increases the estimated bias by about 25%. It is hoped that the simple results presented here will change the current practice of reporting roughness measurements, so estimates of their uncertainty become commonplace. Further, the approach taken here has a wider application to two-dimensional surface roughness measurements, although a full treatment is outside of the scope of this paper.

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