Theory, Modeling, and Simulation of Line Edge Roughness in Diblock Copolymer Resists

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Diblock copolymer thin films are being considered as potential lithographic masks for next-generation nanomanufacturing. However, in order for block copolymer (BCP) films to function as viable resists, fabrication scientists must have significant control over the long-range order *and* uniformity of the BCP mesophase.[1] Template-directed self-assembly (TDSA) appears to be an attractive method to control long-range order; however, TDSA methods do not guarantee uniformity of the mesophase domains. Thermal fluctuations in the BCP film can cause interfacial fluctuations that can significantly affect device function. Fabrication scientists utilizing TDSA-fabricated BCP resists are primarily concerned with fluctuation wavelengths on the order of and larger than the desired feature size[1] (*i.e.*, the *critical dimension*, the *half-pitch*, or, in our case, half of the *mesophase interdomain spacing* $L_0/2$) because LER/LWR on this length scale can adversely affect the shape, size, and placement of the fabricated pattern(s) and thus have a pronounced negative affect on device function. It remains unclear if intrinsic noise at this length scale will represent a limiting factor in the use of BCP resists.[2] Clearly, fabrication scientists need a complete understanding of the physics of long-wavelength interfacial fluctuations in BCP resists.

We review the various frameworks available for modeling BCP LER/LWR. We note that at and above the $L_0/2$ length scale, phenomenological phase-field models are an attractive alternative to traditional particle-based and field-theoretic BCP modeling frameworks. Accordingly, we use a polymer phase-field model to examine long-wavelength LER and LWR in an AB diblock copolymer melt. We find that the phase-field model is capable of capturing the essential features of LER and LWR in a two-dimensional AB diblock coplymer resist. We show that LER and LWR in our phase-field simulations depend monotonically on the A–B segregation strength (Fig. 1a) and the noise strength (Fig. 1b), and that the spectra of LER and LWR both exhibit a peak at k_0 (Fig. 1c-d)—the characteristic wavenunber of mesophase separation in diblock copolymers. For $k \lessapprox k_0$, we show that the LER spectrum roughly scales like $k^{-1.6}$ (Fig. 1c). This scaling is consistent with recent scanning electron microscope (SEM) measurements of LER in a thin film poly(styrene-*b*-methyl methacrylate) melt.[3] Finally, we demonstrate that an external pinning field—similar to the chemically templated substrates developed by Nealey and coworkers[4]—suppresses long-wavelength LER.

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[1] *International Technology Roadmap for Semiconductors (ITRS), 2007 Edition*, `http://www.itrs.net/Links/2007ITRS/Home2007.htm`, (2007).

[2] A. W. Bosse *et al.*, *Soft Matter* **5**, 4266 (2009).

[3] G. E. Stein *et al.*, *Macrmolecules* **43**, 433 (2010).

[4] S. O. Kim *et al.*, *Nature* **424**, 411 (2003).

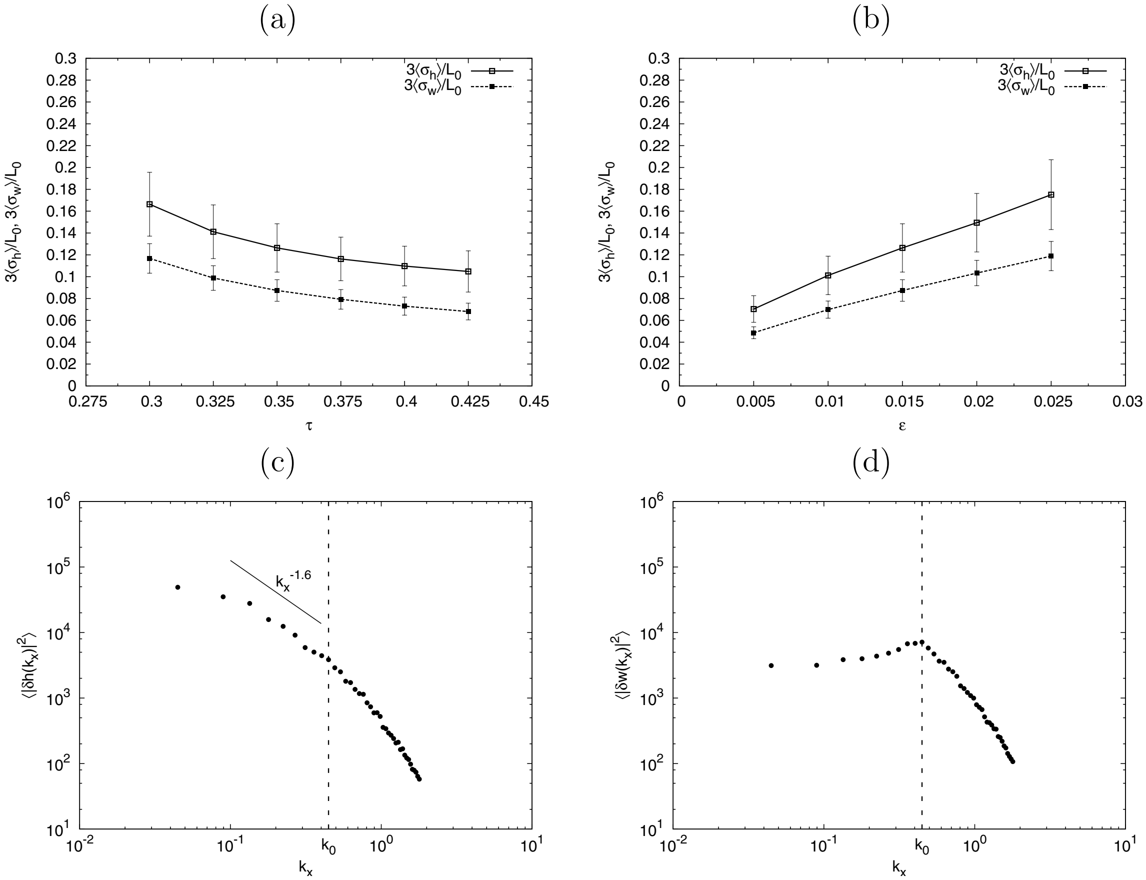

Figure 1: Plots of (a) $3\langle\sigma_h\rangle/L_0$ and $3\langle\sigma_w\rangle/L_0$ vs. τ for $\epsilon = 0.015$, and (b) $3\langle\sigma_h\rangle/L_0$ and $3\langle\sigma_w\rangle/L_0$ vs. ϵ for $\tau = 0.35$, where $3\langle\sigma_h\rangle$ and $3\langle\sigma_w\rangle$ are LER and LWR, respectively, τ is the "quench depth" (proportional to the A–B segregation strength), and ϵ is the noise strength. The error bars in (a) and (b) represent the standard deviation over a stochastic simulation run, and the lines in (a) and (b) are provided as a guide to the eye. We also present plots of (c) $\langle|\delta h(k_x)|^2\rangle$ and (d) $\langle|\delta w(k_x)|^2\rangle$ for $\epsilon = 0.015$ and $\tau = 0.35$, where $|\delta h(k_x)|^2$ and $|\delta w(k_x)|^2$ are the spectra of LER and LWR, respectively. The dotted lines in (c) and (d) correspond to $k_x = k_0 = 2\pi/L_0$—the diblock copolymer characteristic wavenumber—and the solid line in (c) illustrates $k_x^{-1.6}$ scaling.