Fluctuations in Lamellar Diblock Copolymer Resists

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Diblock copolymer thin films are being considered as $\mathcal{O}(10 \text{ nm})$ lithographic masks for next-generation nanomanufacturing. However, in order for block copolymer (BCP) films to function as viable resists, fabrication scientists must have control over the long-range order and uniformity of the BCP mesophase.¹ Directed self-assembly (DSA) appears to be an attractive method to control long-range order; however, DSA 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 DSA-fabricated BCP resists are primarily concerned with fluctuation wavelengths on the order of and larger than the half-pitch because fluctuations 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.

I derive an approximate analytic expression for the long-wavelength composition fluctuation spectrum of a lamellar diblock copolymer melt that is a Lorentzian in k^2 , where **k** is the wavevector. The expression fits appropriate test simulations exactly with zero fitting parameters over a wide range of phase-space (*cf.*, Fig. 1a), and it provides an acceptable approximate fit outside its range of formal applicability. Combining this expression for the composition fluctuation spectrum with an established theory of fluctuating interfaces allows one to construct an analytic function for the spectrum of interfacial fluctuations (*i.e.*, line edge roughness [LER]) in a diblock copolymer resist (*cf.*, Fig. 1b). My preliminary work suggests that this expression can be used to fit the LER spectra in my test simulations with as little as one, but not more than a few fitting parameters. I also examine other functions for fitting the fluctuation spectra,³ and discuss the benefits and drawbacks of each (*cf.*, Fig. 1c).

This framework affords the polymer physicist, resist scientist, and fabrication scientist a simple, easy-to-interpret, approximate analytic expression for the line edge roughness spectrum of a diblock copolymer resist, and as such it could represent an invaluable tool for the rational design and dimensional metrology of BCP resists.

¹E.g., see International Technology Roadmap for Semiconductors (ITRS), 2007 Edition, http://www.itrs.net/Links/2007ITRS/Home2007.htm, (2007).

²A. W. Bosse et al., Soft Matter 5, 4266 (2009); G. E. Stein et al., Macroolecules 43, 433 (2010).

³M. C. Cross and D. I. Meiron, *Physical Review Letters* **75**, 2152 (1995).



Figure 1: (a) Concentration fluctuation spectrum in a diblock copolymer melt extracted from a stochastic simulation [open circles] fit using a Lorentzian analytic expression [dotted line]. Here $\delta \phi$ is the concentration fluctuation and k_0 is the characteristic wavenumber for diblock copolymer mesophase separation. (b) LER spectrum constructed from the Lorentzian function from panel (a) and a capillary wave model for interfacial fluctuations. Here δh is the line edge fluctuation. (c) Concentration fluctuation spectrum from panel (a) [solid line] and a squared Lorentian function [dotted line]. The squared Lorentzian is conjectured to be a more appropriate fitting function for more strongly segregated diblock copolymer melts.