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Removal of non-equilibrium microdomain defects in block copolymer thin film simulations AUGUST BOSSE, University of California, Santa Barbara, SCOTT SIDES, Tech-X Corporation, KIRILL KATSOV, CARLOS GARCIA-CERVERA, GLENN FREDRICKSON, University of California, Santa Barbara —
In recent years, there has been increased interest in using microphase-separated block copolymer thin films as sub-optical lithographic masks in next generation semiconductor and magnetic media fabrication. However, if such techniques are to evolve into a useful and commercially feasible lithographic tool, one must have control over, or at least an understanding of the in-plane ordering of the block copolymer microdomains. In the context of self-consistent field theory (SCFT), we introduce new simulation techniques intended to efficiently remove non-equilibrium microdomain defects in 2D block copolymer simulations, and thus allow further study of equilibrium defect populations associated with 2D systems (cf., KTHNY theory) and/or defects induced by confinement. The first technique, which we call *spectral amplitude filtering*, is used in parallel with a saddle point relaxation algorithm. Spectral amplitude filtering zeros out all Fourier components with amplitude below some fraction of the maximum amplitude. This encourages symmetries associated with the dominant Fourier modes to rapidly set in. The other technique is a variation on a force-biased, Fourier-accelerated Monte Carlo algorithm, which is shown to be efficient in controlled removal of non-equilibrium microdomain defects.

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