Phenomenological and Single Chain in Mean Field Simulations Study of Interface Roughness in Copolymers Assembled on Patterned Substrates

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Directing block copolymer (BCP) assembly with chemically patterned substrates is a promising strategy for creating thin films of perfectly ordered arrays of nanostructures with device oriented shapes. However, locally, the interfaces of BCP structures exhibit an amount of roughness. Factors contributing to this effect include a) local imperfections in the pattern (pattern line edge roughness: LER) directing the assembly and b) thermal fluctuations of the interfaces. Here these issues are addressed theoretically using interface Hamiltonians and Single Chain in Mean Field (SCMF) simulations. We consider BCP melts assembled on patterns with stripes with two generic, single wavelength, types of LER imposed on the stripe-edges: undulation and peristaltic. The effect of local pattern imperfections is highlighted considering the average shape of the BCP interfaces. Both SCMF simulations and the phenomenological theory show that one of the basic factors determining the decay of the roughness, transferred into the assembled morphology, is the characteristic LER wavelength of the pattern: The distance of roughness propagation away from the substrate increases with wavelength. However, the interplay of pattern LER with the other characteristic system length scales is also important: In thin films, the induced deformation of the interfaces decays slower with distance from the patterned surface than in thicker films. The effect of thermal fluctuations is elucidated by calculating the instantaneous shapes of the BCP interfaces from the SCMF snapshots. Results for the deviation of the instantaneous interface position from its average shape and instantaneous-shape autocorrelation functions will be presented. The Fourier spectrum of the later is analyzed and the thermal fluctuations effects are discussed by focusing on the low wave-vector region. The theoretical predictions will be compared against relevant experimental data.