

Abstract Submitted
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String method study of heterogeneous nucleation SARAH DAWSON, AN-CHANG SHI, McMaster Univ — The self-assembly of block copolymers into ordered microphases typically proceeds through nucleation. The free-energy barrier and the nucleation pathway are altered in the presence of a nucleating agent. By exploiting this fact, recent theoretical work has shown that an appropriately designed substrate may be used to fabricate defect-free films of block copolymers in an ordered phase. In this work, we look at a method for quantifying the effect of heterogeneities on the nucleation pathway in a model system. We find the minimum free energy path between the initial, metastable state and the stable state using the string method. We investigate the change in height of the free-energy barrier when the interface is included. The results obtained are compared with those from classical nucleation theory.

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