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Identifying the ODT in simulations of diblock copolymers using thermodynamic integration with a flexible simulation cell PAVANI MEDAPURAM, JENS GLASER, DAVID MORSE, University of Minnesota — The order-disorder transition (ODT) has been precisely identified in several simulation models by using a thermodynamic integration procedure introduced by Mueller and Daoulas (*J. Chem. Phys.*, 128, 024903, 2008). We have applied the method to constant pressure simulations with a flexible tetragonal simulation unit cell to avoid incommensurability effects. The transition is found to be surprisingly weakly first order, even for very short chains, in agreement with recent experiment results on short, strongly-incompatible diblocks. Precise values for the value of χ N at the transition are obtained by combining this free energy method with a fit of the disordered state scattering data to the renormalized one-loop theory, which is found to give an excellent fit for several different models over a wide range of molecular weights. Results from different chain lengths and models are compared to test the degree of universality of the ODT, and to test the accuracy of the Fredrickson-Helfand theory predictions for the ODT.

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