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Free energies and commensurability effects in simulations of three-dimensional ordered phases of diblock copolymers TAHER GHASIMAKBARI, DAVID MORSE, University of Minnesota — We present an approach to the calculation of precise phase boundaries in simulations of diblock copolymer melts that is based on the calculation of free energies by thermodynamic integration. Results of simulations of three dimensionally periodic structures are extremely sensitive to commensurability effects, i.e., to the relationship between the dimensions of the (generally small) periodic simulation cell and the (generally unknown) preferred dimensions of a particular ordered phase. We avoid this by measuring the free energy for each ordered phase of interest using several different simulation sizes to estimate free energies as functions of unit cell size and thereby estimate the optimal cell size and corresponding free energy.

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