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Universality between Experiment and Simulation of a Diblock Copolymer Melt

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The equivalent behavior among analogous block copolymer systems involving chemically distinct molecules or mathematically different models has long hinted at an underlying universality, but only recently has it been rigorously demonstrated by matching results from different simulations. The profound implication of universality is that simple coarse-grained models can be calibrated so as to provide quantitatively accurate predictions to experiment. Here, we provide the first compelling demonstration of this by simulating a polyisoprene-polylactide diblock copolymer melt using a previously calibrated lattice model. The simulation successfully predicts the peak in the disordered-state structure function, the position of the order-disorder transition and the latent heat of the transition in excellent quantitative agreement with experiment. This could mark a new era of precision in the field of block copolymer research.

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