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A Monte Carlo Free Energy Approach to Microphase study and Its Application on the ANNNI Model KAI ZHANG, PATRICK CHARBONNEAU, Duke University — Microphases are complex and interesting patterns that self-assemble in systems with competing short-range ordering and long-range frustrating interactions. They form in certain colloidal suspensions and in diblock copolymers, but controlling the morphology is notoriously difficult. Knowing the equilibrium behavior of model systems would help understand how to tune the modulated phases. But even for these systems, reliable results for the microphase regime are notoriously difficult to obtain, because of the presence of long-lived metastable states. We develop a Monte Carlo simulation method based on thermodynamic integration that resolves this problem. With our method, we determine with high accuracy the phase behavior of the canonical three-dimensional axial next nearest-neighbor Ising (ANNNI) model, which is one of the simplest models to form lamellas. The XY nature of the modulated-disorder phase transition is confirmed and critical exponents are obtained. We discuss how to generalize our simulation approach to particle-based microphase-forming model.

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