A Degenerate Ising Model for Atomistic Simulation of Crystal-melt Interfaces

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We consider an Ising-type model for a solid-liquid interface. While the standard Ising model admits only second-order phase transitions as one increases temperature, making it a poor choice for modeling the solid-liquid phase transition, a simple modification of the model introduces a first-order phase transition. This is accomplished by weighting one of the two ``spin'' states more heavily in the partition function, representing the larger entropy of the liquid phase. This model is combined with micro-canonical Monte-Carlo techniques to simulate systems with solid-liquid phase coexistence. The model will first be illustrated in two dimensions using a simple square lattice before presenting results for the face centered cubic lattice and further generalization to partially melted nano-cluster.