Direct Evaluation of Solid-Fluid Phase Coexistence Using a New Monte Carlo Technique

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The simulation of solid phases presents severe challenges. Difficulty in traversing free energy barriers prevent adequate sampling that is required for evaluating free energy landscapes and acquiring accurate statistics. In an effort to surmount this challenge, we present a novel Monte Carlo technique that permits the 'creation' or 'destruction' of particles in a solid phase while maintaining long ranged order. This is done by altering the periodicity of the boundaries through a technique we call 'Periodic Retiling' (PRMC). We evaluate the efficacy of the new technique, originally described by Tilwani [1], by producing the full phase diagram of Lennard-Jones system through the use of Gibbs ensemble simulations. PRMC is implemented here as an algorithm in the Gibbs ensemble, but it is extensible to any ensemble in which solid particles are added or removed. Its use provides accurate results in a less computationally expensive manner than traditional simulation techniques.

[1] P. Tilwani. Master's thesis, Colorado School of Mines, Department of Chemical Engineering, Golden, CO 80401, 2000.