An efficient way to determine a phase boundary

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Abstract

An orthodox way to determine an equilibrium phase boundary is to look for the thermodynamic conditions under which the free energies of the two phases under consideration equilibrate. However, the evaluation of a free energy is usually not an easy task. The two-phase simulation method [1] has been proposed to avoid such a time-consuming step of free-energy evaluation. Here, we propose a new type of the two-phase simulation method with which to estimate effectively the location of a solid-liquid phase boundary. The modified Lennard-Jones (mLJ) system was chosen because the accurate melting points are known as a function of pressure [2]. One of the methods is to apply the nonequilibrium relaxation (NER) method [3]. A combined system consisting of solid and liquid states was prepared as a proper initial state. On the solid side, 13500 particles with the reduced density 1.0 were located on the face-centered cubic lattice points whereas 14196 particles with the density 0.7 located on the face-centered orthorombic lattice points were taken to the liquid state using the isothermal-isobaric molecular dynamics simulation. The systems were then combined together to be evolved under isothermal and isobaric conditions. The density of the whole system was monitored during the evolution. Whether the thermodynamic condition under consideration is in the solid or liquid state could be judged by observing the density is to increase or decrease. The error of the melting point was less than 1% at the highest pressure condition examined [4]. To our knowledge, this is the first successful realization of applying the NER method to a system other than spin systems. A second method is to trace the phase boundary by slowly varying the pressure or temperature in such a way that the solid-liquid interface within the combined system remains unmoved. The latter method also gave almost the same melting points as those obtained by the NER method. [1] A. B. Belonoshko, Geochim. Cosmochim. Acta, 58, 4039 (1994). [2] Y. Asano and K. Fuchizaki, J. Chem. Phys. 137, 174502 (2012). [3] Y. Ozeki and N. Ito, J. Phys. A: Math. Theor. 40, R149 (2007). [4] Y. Asano and K. Fuchizaki, to be published.

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