Solid-Liquid Coexistence and Triple Points of the Lennard-Jones Family of Potentials

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Molecular simulation algorithms for solid-liquid coexistence commonly encounter difficulties associated with transferring particles between the dense phases, or they are not self-starting. In this work, we report the solid-liquid coexistence and triple points of fluids interacting via a *n-6* Lennard-Jones potential where *n = 7, 8, 9, 10, 11* and *12*. The calculations involved combining equilibrium and nonequilibrium molecular dynamics (NEMD) [1], Gibbs-Duhem [2, 3] and Gibbs Ensemble [4] algorithms. The significance of the NEMD algorithm is that it avoids the problem of particle interchange and it is self-starting. The results indicate that the solid-liquid coexistence shifted towards decreasing density with the increasing value of *n*. The effect of *n* on the triple point is that the triple point density decreases with the increasing *n* and triple point temperature increases with increasing *n*. In addition, high temperature scaling behavior [3], Lindemann melting rule [5] and Simon-Glatzel [6] equation are examined using the simulation data obtained in this work.

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