87d Phase Behavior of Elemental Aluminum Using Monte Carlo Simulations

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Monte Carlo simulations are presented for two different models for aluminum, the embedded-atom and the explicit many-body potentials, that are optimized to reproduce accurate ab-initio binding energies for dimers and small clusters. Vapor/liquid coexistence curves are determined using Gibbs-ensemble Monte Carlo simulations. The normal boiling points for both potentials are somewhat higher (by about 10 %) than the experimental value, but the predicted critical temperatures fall within the rather large experimental uncertainty. Isothermal constant-stress simulations are used to simulate solid Al from 300 K to the triple point. The solid structures are stable in the fcc configuration, and the specific heat is determined to be lower than the experimental value. Gibbs-ensemble simulations for solid slabs show that the solid phase is stable well above the experimental melting point. However, the small difference in enthalpies of boiling and sublimation prevents an accurate determination of the triple point.