

87c Computing Vapor-Liquid Coexistence Curves for Metals

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Vapor-liquid coexistence curves are computed for metallic elements using the Towhee Monte Carlo molecular simulation package. Results are presented for several Embedded-Atom Method models of iron and for some Stillinger-Weber models of silicon. Deviations from the law of rectilinear diameters are observed over a significant temperature range, and a more complex set of equations for fitting coexistence densities is utilized to predict critical points. Finally, the highly non-ideal vapor pressures serve as a good test of the of the thermodynamic and virial methods for computing the pressure, and the relative merits of these two methods are discussed.