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Molecular dynamics of liquid lead near its melting point

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Abstract

The molecular dynamics of liquid lead is simulated at T = 613 K using the following three models of an interparticle interaction potential: the Dzugutov pair potential and two multiparticle potentials (the "glue" potential and the Gupta potential). One of the purposes of this work is to determine the optimal model potential of the interatomic interaction in liquid lead. The calculated structural static and dynamic characteristics are compared with the experimental data on X-ray and neutron scattering. On the whole, all three model potentials adequately reproduce the experimental data. The calculations using the Dzugutov pair potential are found to reproduce the structural properties and dynamics of liquid lead on the nanoscale best of all. The role of a multiparticle contribution to the glue and Gupta potentials is studied, and its effect on the dynamic properties of liquid lead in nanoregions is revealed. In particular, the neglect of this contribution is shown to noticeably decrease the acoustic-mode frequency. © 2009 Pleiades Publishing, Ltd.

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