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Interatomic potential fitted for lead

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ABSTRACT

By using the recently improved generalized-simulated-annealing algorithm and the molecular dynamics method, we numerically fit an interatomic potential for lead. The potential obtained can correctly reproduce many physical properties of lead in crystalline and non-crystalline phases. The surface energy and surface relaxation obtained are in good agreement with the experimental results. The melting point predicted by this potential is very close to the experimental data. The present potential is used to study the surface melting and liquid structure; good agreement with experimental results is observed.

Over the last two decades, computer simulation methods have played an increasingly important role in many areas of condensed-matter physics and material science. While first-principles methods are rapidly improving in speed and accuracy, classical interatomic potentials continue to constitute the only way to perform molecular dynamics (MD) or Monte Carlo computations on systems with a very large size (number of atoms, $N \approx 10^4 - 10^7$) or for a long simulation time (t in nanoseconds). There have been several methods to build empirical interatomic potentials in metallic systems, such as the embedded-atom method (EAM) (Daw and Baskes 1984), the second-moment approximation to the tight-binding model (SM-TBM) (Ducastelle 1970, Tomanek *et al.* 1985, Zhong *et al.* 1991), the glue model (Ercolessi *et al.* 1988, Ercolessi and Adams 1994, C. P. Toh, H. S. Lim, C. K. Ong and F. Ercolessi unpublished), also the Finnis-Sinclair (1984, 1986) potentials and the effective-medium model (Norskov 1990); currently most of them are widely used.

Lead is a very interesting material in the sense that it is the only real fcc metal among all its neighbours in the fourth column of the periodic table. Lead has long acquired an important status in the petrochemical industries. Moreover, it is a metal which shows rich surface properties, for example different surfaces exhibit different melting behaviour, that is non-melting, incomplete and surface melting. Many experiments have been performed on lead; however, only limited theoretical work has been done. To meet the need of heavy simulations, a couple of interatomic potentials for lead were constructed. For example, Karimi and Mostoller (1992) built an EAM potential for lead, which was used to study the physical properties of lead surfaces (Tibbits *et al.* 1991, Karimi and Mostoller 1992, Karimi *et al.* 1993).

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