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An EAM potential for the dynamical simulation of Ni-Al alloys

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Abstract. An embedded atom method potential for Ni-Al alloys is developed. The expression of the embedded function is constructed by analogy with the density function theory. Both the repulsive function and the electron density function here have simple forms. The potential parameters of pure Al and Ni are fitted to the experimental values, including their lattice parameters, cohesive energies, vacancy formation energies and three elastic constants (c_{11},c_{12},c_{13}). The potential for the Ni-Al alloy are then constructed from the Ni and Al potentials. The equation of states and the phonon dispersion calculated by the present potential parameters are in good agreements with first-principles calculations and experimental data, indicating the reliability of the present potential.

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Key words: embedded atom method, potential, Al-Ni alloy.

1 Introduction

In the atomic-scale simulation of materials, the first-principles calculations are restricted to a small number of atoms and short time scale. On the other hand, the empirical and semi-empirical methods are very efficient for larger systems and longer time scale. The embedded-atom method (EAM) [1–3], which was developed by Daw and Baskes over two decades ago, has been widely applied in large molecular dynamic simulations because of its computational simplicity. The predictions using EAM for metals have generally been quite good, both qualitatively and quantitatively superior to the early pair potential calculations.

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In the embedded atom method, the energy required to place an impurity atom in a lattice is taken solely as a function of the electron density at that particular site. Each atomic species therefore has a unique energy function which is in turn a function of just the electron density. However, the theory leads to non-unique EAM potential functions. Different EAM potential functions have been presented [4–13], some with no reference to their physical meaning. In this paper, new EAM potentials for fcc metals Ni, Al and their alloys are constructed. The embedded function in the present work is constructed by analogy with the density function theory and simple forms for the electron density function and the repulsive function are given.

2 Formalism

Under EAM formalism, the total energy is represented as

$$U_{tot}=\frac{1}{2}\sum_{i,j(i\neq j)}\Phi(R_{ij})+\sum_{i}F[\rho_i], \tag{1}$$

where Φ is the pair potential between atoms i and j, $F(\rho_i)$ is the embedded function which is the energy to embed an atom i in an electron density ρ_i. R_{ij} is the separation between atoms i and j, and, ρ_i denotes the host electron density at atom i due to all the other atoms. The host electron density is assumed to be a linear superposition of contributions from individual atoms, and it is given by

$$\rho_i=\sum_{i\neq j}f_i(r_{ij}), \tag{2}$$

where $f_i(r_{ij})$ is the electron density of atom j as a function of distance from its center.

As indicated in the previous section, the EAM potential is not unique. Different forms of $F(\rho_i)$, Φ and $f_i(r_{ij})$ can be presented. Here, we present a new form for the embedded function F by analogy with the density functional theory in order to understand its physical meaning. The density-functional expression for the cohesive energy of a solid is [14]

$$U_{tot}=\frac{1}{2}\sum_{i,j(i\neq j)}\frac{Z_iZ_j}{R_{ij}}+\sum_i\int\frac{\rho(\vec{r})}{|\vec{r}-\vec{R}_i|}d\vec{r}+\frac{1}{2}\iint\frac{\rho(\vec{r})\rho(\vec{r'})}{|\vec{r}-\vec{r'}|}d\vec{r}d\vec{r'}+E_{xc}[\rho]+T_e[\rho] \tag{3}$$

where the first term in the right side of Eq. (3) is the core-core repulsion potential, the second term is the electron-core coulomb interaction, the third term is the electron-electron coulomb interaction, the fourth term is the exchange and correlation energy, and, the fifth term is the electronic kinetic energy. According to Daw [3], the kinetic and exchange-correlation energy density is

$$g(\rho)=t(\rho)+x(\rho)+c(\rho),$$