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A lattice inversion method to construct the alloy pair potential for the embedded-atom method

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Abstract. The lattice inversion method is used to construct the pair potential between a pair of unlike atoms for Cu–Au and Cu–Pd intermetallic compounds within the framework of Johnson's analytical model of the embedded-atom method. Compared with previous treatises, the alloy potential obtained by the present method is based on the $L1_2$ superstructures Cu_3Au and Cu_3Pd as references so that the usual assumption that the pair potential between distinct atoms is a function of monatomic pair potentials is cancelled. The alloy potentials from inversion fall in with those from the average schemes of Foiles *et al* and Johnson in the short range but show deviation in the long range. The present method is used to solve the considerable disagreements of Johnson's calculations for the dilute-limit heats of solution and the phase stabilities of the intermetallic compounds of palladium with noble metals. While the overall degree of agreement is substantially improved, it is not good in some cases, nor is the phonon spectrum of gold.

1. Introduction

The embedded-atom method (EAM), proven to be effective in modelling the interatomic interaction in metals, has gained wide applications in atomistic simulation for the geometrics and energetics of metallic systems [1–3]. The idea of the EAM is to separate the cohesive energy into two contributions: one from the screened electrostatic force between two ionic cores; the other from the overlapping energy, the exchange–correlation energy and so on. The latter is represented by the embedding function, which means the energy needed to immerse an atom into a lattice site with the electron background contributed by the surrounding atoms as environment. The immersion energy is assumed to be a function of local electron density, and this density is supposed to be the rigid superposition of the so-called atomic electron density from all the other atoms on the lattice. The basic equations for the EAM are

$$E_{\text{coh}} = \sum_i F_i(\rho_i) + \sum_i \Phi_i \quad (1)$$

$$\rho_i = \sum_{j \neq i} f_j(R_{ji}) \quad (2)$$

$$\Phi_i = \frac{1}{2} \sum_{j \neq i} V_{ji}(R_{ji}) \quad (3)$$

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where $f_j(r)$ is the electron density centred on site j and $V_{ji}(r)$ is the pair potential related to a specified pair of atoms i and j . ρ_i and Φ_i are the lattice sums on the corresponding sublattices. In a binary alloy system with type-a and type-b atoms, there exist two kinds of density function $f_a(r)$, $f_b(r)$ and three kinds of potential functions $V_{aa}(r)$, $V_{ab}(r)$, $V_{bb}(r)$. As usual, the four functions $f_a(r)$, $f_b(r)$, $V_{aa}(r)$ and $V_{bb}(r)$ are assumed to be transferable from the monatomic systems to the alloy system, so that they can be determined from the properties of the respective pure metals. The remaining function $V_{ab}(r)$ is assumed to be the geometric mean of monatomic pair potentials

$$V_{ab}(r) = \sqrt{V_{aa}(r)V_{bb}(r)} \quad (4)$$

by the model of Foiles, Baskes and Daw (FBD) [4], or alternatively to be a density-weighted combination of monatomic pair potentials

$$V_{ab}(r) = \frac{1}{2} \left[\frac{f_b(r)}{f_a(r)} V_{aa}(r) + \frac{f_a(r)}{f_b(r)} V_{bb}(r) \right] \quad (5)$$

by the model of Johnson [5].

The common assumption that the pair potential between a pair of unlike atoms is a function of monatomic pair potentials has insufficient theoretical evidence, because it is uncertain whether the assumed diatomic pair potential is able to reproduce the crystalline cohesion of alloy phases. Johnson has used equation (5) to study the dilute-limit heats of solution and the phase stabilities of some FCC-based binary intermetallic systems [5, 6] (the same formula was also used to study a BCC based binary intermetallic compound by Zhang and Ouyang [7]). He found particular disagreement with the first-principles results of Takizawa *et al* [8] and Terakura *et al* [9] for the phase stabilities of noble-metal and palladium compounds [6]. The dilute-limit heats of solution of binary alloys containing palladium predicted by Johnson also seriously disagree with experiments [5]. Since the model of Johnson predicted the properties of pure metals fairly well [10, 11], these disagreements may result from the improper construction of the potential $V_{ab}(r)$ as equation (5).

In this paper, we present a method for constructing the pair potential $V_{ab}(r)$ for the Cu–Au and Cu–Pd systems with the use of the lattice inversion method (LIM) developed by Chen *et al* [12–14] and us [15, 16]. The LIM is a generalization of the old famous Möbius inversion formula to the three-dimensional lattice, and thus is concise for its arithmetical feature. The pair potential $V_{ab}(r)$ given by the present method is based on the L_{12} superstructures Cu_3Au and Cu_3Pd as references. Calculation results show that the inverted alloy potentials coincide with those from the FBD scheme and Johnson's scheme at short interatomic distances and gradually deviate when the distance becomes longer. The present method is used to solve the serious disagreement appearing in Johnson's calculations about the dilute-limit heats of solution and the phase stabilities of intermetallic alloys of palladium with noble metals.

2. Model

For a binary superstructure with type-a and type-b atoms, the total cohesive energy can be written as

$$E_{\text{coh}} = \sum_{j^a} [F^a(\rho_j^a) + \Phi_j^a] + \sum_{j^b} [F^b(\rho_j^b) + \Phi_j^b] \quad (6)$$

with

$$\rho_j^a = \sum_{j^a} f_a(R_{ij}) + \sum_{j^b} f_b(R_{ij}) \quad (7)$$

$$\rho_i^b = \sum_{j^a} f_a(R_{ij}) + \sum_{j^b} f_b(R_{ij}) \quad (8)$$

$$\Phi_i^a = \frac{1}{2} \sum_{j^a} V_{aa}(R_{ij}) + \frac{1}{2} \sum_{j^b} V_{ab}(R_{ij}) \quad (9)$$

$$\Phi_i^b = \frac{1}{2} \sum_{j^a} V_{ab}(R_{ij}) + \frac{1}{2} \sum_{j^b} V_{bb}(R_{ij}) \quad (10)$$

where i^a (j^a) and i^b (j^b) are the summation subscripts over sublattices a and b.

Cu_3Au and Cu_3Pd crystallize into $L1_2$ superstructures. The $L1_2$ superstructure A_3B defines four sublattices, with three containing a atoms and one containing b atoms. Each sublattice is a simple cubic structure. Viewed from the site of a b atom, the corner vertices (CVs) are occupied by b atoms and the face centres (FCs) are occupied by a atoms. Therefore one can write the pairwise energy of a b atom as

$$\Phi^b = \frac{1}{2} \sum_i^{\text{CV}} V_{bb}(R_i) + \frac{1}{2} \sum_i^{\text{FC}} V_{ab}(R_i). \quad (11)$$

If viewed from the site of an a atom, the corner vertices are occupied by a atoms while a third of the face centres are occupied by b atoms and the other two-thirds are occupied by a atoms. Therefore one can write the pairwise energy of an a atom as

$$\Phi^a = \frac{1}{2} \sum_i^{\text{CV}} V_{aa}(R_i) + \frac{1}{3} \sum_i^{\text{FC}} V_{aa}(R_i) + \frac{1}{6} \sum_i^{\text{FC}} V_{ab}(R_i). \quad (12)$$

The total pairwise energy of a unit cell then reads

$$\begin{aligned} 3\Phi^a + \Phi^b &= \frac{1}{2} \sum_i^{\text{CV}} [3V_{aa}(R_i) + V_{bb}(R_i)] + \sum_i^{\text{FC}} [V_{aa}(R_i) + V_{ab}(R_i)] \\ &= \frac{1}{2} \sum_{n=1}^{\infty} w(2n) [V_{aa}(\sqrt{2n}R_1) + V_{bb}(\sqrt{2n}R_1)] \\ &\quad + \sum_{n=1}^{\infty} w(n) V_{aa}(\sqrt{n}R_1) + \sum_{n=1}^{\infty} w(2n-1) V_{ab}(\sqrt{2n-1}R_1) \end{aligned} \quad (13)$$

where $w(n)$ is the number of atoms in the shell with radius $\sqrt{n}R_1$ for the FCC structure. If $2n$ cannot be decomposed into a sum of three square non-negative integers then $w(n) = 0$. Throughout this paper, we cut off any lattice summation at $n = 50$, thereby including atoms up to the 47th-nearest neighbours. The total electron densities at the site of an a atom and a b atom are

$$\begin{aligned} \rho^a &= \sum_i^{\text{CV}} f_a(R_i) + \frac{1}{3} \sum_i^{\text{FC}} f_b(R_i) + \frac{2}{3} \sum_i^{\text{FC}} f_a(R_i) \\ &= \sum_{n=1}^{\infty} w(2n) f_a(\sqrt{2n}R_1) + \frac{1}{3} \sum_{n=1}^{\infty} w(2n-1) f_b(\sqrt{2n-1}R_1) \\ &\quad + \frac{2}{3} \sum_{n=1}^{\infty} w(2n-1) f_a(\sqrt{2n-1}R_1) \end{aligned} \quad (14)$$

$$\rho^b = \sum_i^{CV} f_b(R_i) + \sum_i^{FC} f_a(R_i) = \sum_{n=1}^{\infty} w(2n) f_b(\sqrt{2n}R_1) + \sum_{n=1}^{\infty} w(2n-1) f_a(\sqrt{2n-1}R_1). \quad (15)$$

Imposing a homogeneous deformation on the superstructure, the total pairwise energy $3\Phi^a + \Phi^b$ and the total embedding energy $3F^a(\rho^a) + F^b(\rho^b)$ then vary as functions of NN distance R_1 . Here we make a plausible supposition that the cohesive energy of a unit cell with respect to R_1 follows the universal cohesion equation given by Rose, Smith, Guinea and Ferrante (RSGF), which can be constructed from the equilibrium lattice constant, the sublimation energy and the bulk modulus [17]. Our first-principles calculations with the linear-muffin-tin-orbitals (LMTO) method with the atomic-sphere approximation (ASA) underpinned this suggestion. The functions of *ab initio* cohesive energies of Cu_3Au and Cu_3Pd in relation to R_1 follow the functional form of RSGF but the theoretical sublimation energies and bulk moduli of the alloys do not agree with the experimental values [18]. Therefore we have the cohesive energy of a unit cell for the alloy system as

$$E^c(R_1) = -E_s^c \left[1 + \alpha^c \left(\frac{R_1}{R_1^c} - 1 \right) \right] \exp \left[-\alpha^c \left(\frac{R_1}{R_1^c} - 1 \right) \right] \quad (16)$$

where E_s^c is the sublimation energy of a unit cell of the superstructure, $\alpha^c = (9\Omega_e^c B^c / E_s^c)^{1/2}$. The lattice constants a_e^c , the unit cell sublimation energies E_s^c , and the bulk moduli B^c for Cu_3Au and Cu_3Pd are listed in table I. The experimental data for Cu_3Pd are not available, so they are approximately chosen as follows. The lattice constant and the bulk modulus of Cu_3Pd are given by Vegard's law, which will bring minor second-order errors. The sublimation energy per unit cell of Cu_3Pd is obtained by the *ab initio* result of absolute excess heat of enthalpy calculated by Takizawa *et al* [8] plus $3E_s[\text{Cu}] + E_s[\text{Pd}]$.

Therefore we have

$$\sum_{n=1}^{\infty} w(2n-1) V_{ab}(\sqrt{2n-1}R_1) = \Phi_{ab}(R_1) \quad (17)$$

with

$$\begin{aligned} \Phi_{ab}(R_1) &= 3\Phi^a(R_1) + \Phi^b(R_1) - \frac{1}{2} \sum_{n=1}^{\infty} w(2n) [V_{aa}(\sqrt{2n}R_1) + V_{bb}(\sqrt{2n}R_1)] \\ &\quad - \sum_{n=1}^{\infty} w(n) V_{aa}(\sqrt{n}R_1) \end{aligned}$$

and

$$3\Phi^a(R_1) + \Phi^b(R_1) = E^c(R_1) - 3F^a[\rho^a(R_1)] - F^b[\rho^b(R_1)].$$

Johnson's model [6] defines the pair potential and the scaled electron density as follows:

$$V(R) = V_e \left(\frac{R_{1e}}{R} \right)^\gamma \quad (18)$$

$$f(R) = f_e \left(\frac{R_{1e}}{R} \right)^\beta \quad (19)$$

where R_{1e} is the nearest-neighbour (NN) distance, and $V_e = 2\Phi_e/S_\gamma$, $f_e = \rho_e/S_\beta$, $\Phi_e = E_s$, $\rho_e = E_s/\Omega$, with the lattice summation

$$S_k = \sum_{n=1}^{\infty} w(n)/\sqrt{n^k}.$$

Johnson defined the embedding function by using the cohesion equation of RSGF

$$F(\rho) = -E_s[1 + \alpha(x^{-1/\beta} - 1)] \exp[-\alpha(x^{-1/\beta} - 1)] - \Phi_e x^{\gamma/\beta} \quad (20)$$

where $x = \rho/\rho_e$. The pair potential and the electron density in Johnson's model are not defined in the region where the distance R is unrealistically smaller than the ionic radius. Therefore, the embedding function is not defined when ρ is unrealistically large. The parameters in the above equation can be decided from the equilibrium atomic volume Ω_e , the sublimation energy E_s , the unrelaxed vacancy-formation energy E_v , the bulk modulus B and the Voigt average shear modulus G as follows [6]:

$$\alpha = \sqrt{\frac{9\Omega B}{E_s}} \quad (21)$$

$$\beta = \sqrt{\frac{15E_s\Omega G}{E_v(E_v + E_s)}} \quad (22)$$

$$\gamma = \sqrt{\frac{15\Omega G(E_s + E_v)}{E_s E_v}} \quad (23)$$

The unrelaxed vacancy-formation energies and the Voigt shear moduli for Cu, Au and Pd are taken from [4]. In order to test the effectiveness of Johnson's model for the monatomic system, we calculate the phonon dispersion relations for Cu, Au and Pd, respectively. We find Johnson's model predicts fairly good results for Cu but bad results for Au. The results for Pd are of moderate accuracy.

Table 1. The equilibrium lattice constants a_c (Å), the unit cell sublimation energies E_s (eV) and the bulk moduli B (Mbar) for Cu, Au, Pd, Cu₃Au and Cu₃Pd. The choices of the data for Cu₃Pd are stated in the text.

System	a_c	E_s	B
Cu	3.61 [22]	3.49 [22]	1.37 [22]
Au	4.08 [22]	3.81 [22]	1.73 [22]
Pd	3.89 [22]	3.89 [22]	1.81 [22]
Cu ₃ Au	3.74 [23]	14.57 [24]	1.51 [25]
Cu ₃ Pd	3.68	14.67	1.48

3. Lattice inversion method

Consider the FCC structure. The basic equations of LIM can be written as

$$F(R_1) = \sum_{n=1}^{\infty} w(n) f(\sqrt{n}R_1) \quad (24)$$

and

$$f(R_1) = \sum_{n=1}^{\infty} m(n) F(\sqrt{n}R_1) \quad (25)$$

where $m(n)$ is the three-dimensional Chen-Möbius function on the FCC lattice, which can be calculated according to the following relations [14]

$$m(n) = \mu(2n) \quad (26)$$

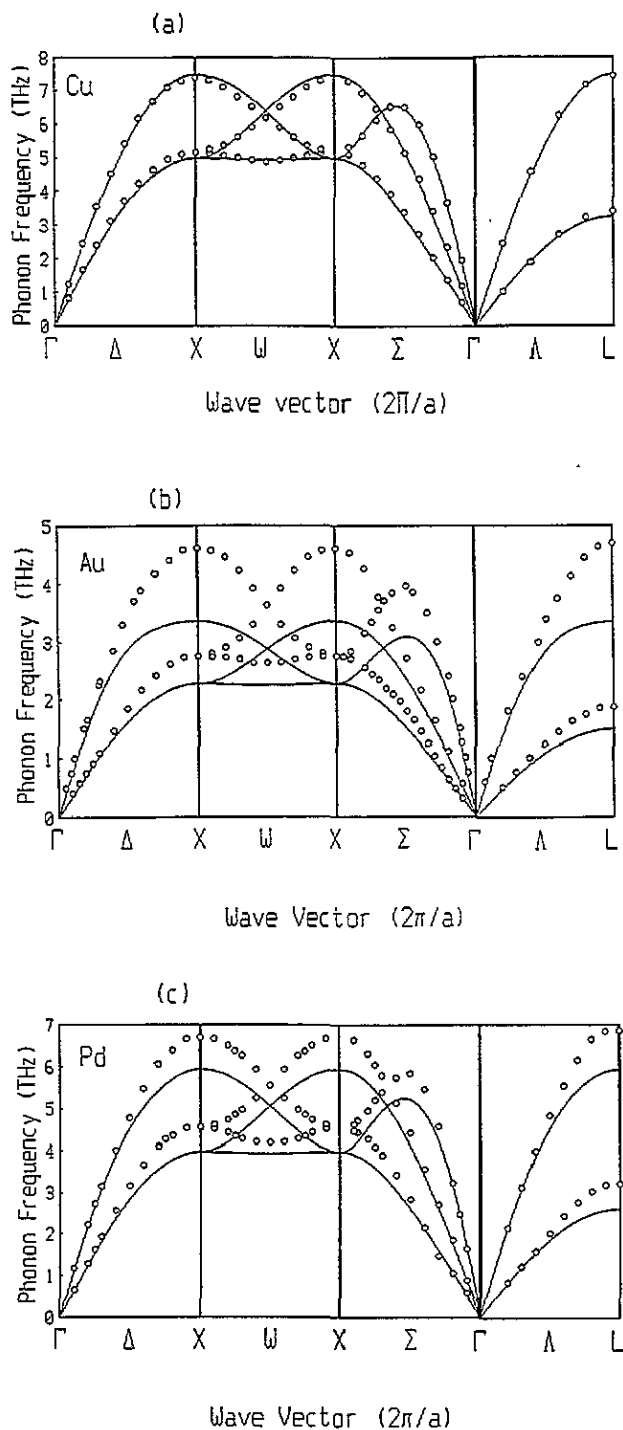


Figure 1. The phonon dispersion curves for Cu, Au and Pd. The open circles are experimental eigenfrequencies, taken from [19] (Cu measured at 80 K), [20] (Au measured at 296 K) and [21] (Pd measured at 296 K). (a) Cu; (b) Au; (c) Pd.

$$\sum_{n|\beta k} r(n)\mu(\beta k/n) = \delta_{\beta k} \quad (27)$$

with

$$r(2n-1) = 0 \quad r(2n) = w(n)$$

where $\beta = 2$ for the FCC lattice, k is a natural number. The sum runs over all the factors of βk including unity and βk . From the above equations, the inversion coefficients can be decided. However, the above formulae are not really plain enough to be understood. Here, we give an alternative but equivalent formula for calculating $m(n)$. For an arbitrary natural number n within the following interval

$$2^{q_m} \leq n < 2^{q_m+1} \quad \left(q_m = \left[\frac{\ln(n)}{\ln(2)} \right] \right)$$

$$m(n) = \frac{1}{w(1)}\delta(n, 1) - \sum_{p_1=2}^{\lfloor n/2^0 \rfloor} \frac{w(p_1)}{w(1)^2}\delta(n, p_1) + \sum_{p_1, p_2=2}^{\lfloor n/2^1 \rfloor} \frac{w(p_1)w(p_2)}{w(1)^3}\delta(n, p_1 p_2) - \dots$$

$$+ (-1)^{q_m} \sum_{p_1, p_2, \dots, p_{q_m}=2}^{\lfloor n/2^{q_m-1} \rfloor} \frac{w(p_1)w(p_2) \dots w(p_{q_m})}{w(1)^{q_m+1}} \delta(n, p_1 p_2 \dots p_{q_m}) \quad (28)$$

where $[x]$ is the maximum integer less than x , $\delta(x, y)$ is the Kronecker function. The above formula is a generalization of the Kronecker expansion of the Möbius function on a unitary semigroup to the FCC lattice [15]. The calculation of $m(n)$ based on equation (28) can be easily performed by a simple computer program.

The inversion of equation (17) then becomes

$$V_{ab}(r) = \sum_{n=1}^{\infty} m'(2n-1) \Phi_{ab}(\sqrt{2n-1}r) \quad (29)$$

where

$$m'(2n-1) = \frac{1}{w(1)}\delta(2n-1, 1)$$

$$+ \sum_{q=1}^{\infty} (-1)^q \sum_{p_1, p_2, \dots, p_q=2}^{\infty} \frac{w(2p_1-1)w(2p_2-1) \dots w(2p_q-1)}{w(1)^{q+1}}$$

$$\times \delta(2n-1, (2p_1-1)(2p_2-1) \dots (2p_q-1))$$

$$= \frac{1}{w(1)}\delta(2n-1, 1)$$

$$+ \sum_{q=1}^{\infty} (-1)^q \sum_{p_1, p_2, \dots, p_q=2}^{\infty} \frac{w(p_1)w(p_2) \dots w(p_q)}{w(1)^{q+1}} \delta(2n-1, p_1 p_2 \dots p_q)$$

$$= m(2n-1). \quad (30)$$

On deriving equation (30) we have for convenience changed the upper limits of each summation in equation (28) to infinity.

4. Results and discussion

The results of Au-Cu and Cu-Pd pair potentials are plotted in figure 2, by comparison with the alloy pair potentials of Johnson's average scheme and the FBD geometric average scheme. It is illustrated that the three curves coincide with each other in the region of small

interatomic distance. With increasing interatomic separation, the disagreements become greater and greater. The force range of $V_{\text{Cu-Au}}(r)$ is longer than those of Johnson and FBD, while the force range of $V_{\text{Cu-Pd}}(r)$ is shorter than those of Johnson and FBD.

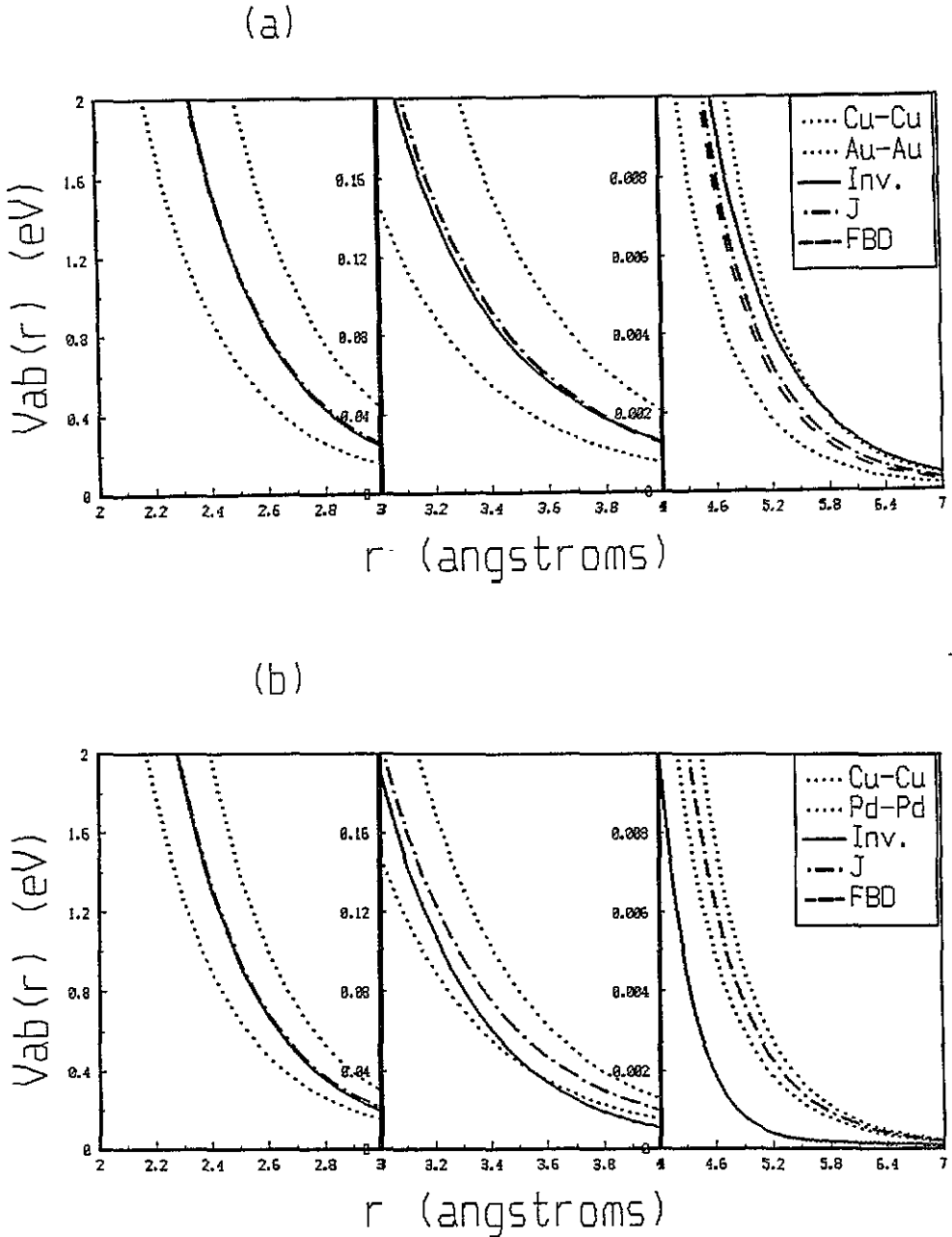


Figure 2. The pair potentials between a pair of different atoms in Cu-Au and Cu-Pd intermetallic alloys. Outer dotted— $V_{\text{A-A}}(r)$, inner dotted— $V_{\text{B-B}}(r)$, solid— $V_{\text{A-B}}(r)$ (inverted), dashed— $V_{\text{A-B}}(r)$ (FBD), dashed-dotted— $V_{\text{A-B}}(r)$ (Johnson) (A=Au, Pd; B=Cu). (a) Cu-Au; (b) Cu-Pd.

We calculate the excess heats of formation versus the NN distance for ordered Cu–Au and Cu–Pd superstructures. In the present calculations and the quoted first-principles calculations, the tetragonal distortion of the $L1_0$ superstructure is not considered. By comparison with *ab initio* results and Johnson's results, table 2 lists the corresponding numerical results at equilibrium. For the Cu–Pd system, the lattice constants of CuPd and CuPd₃ structures satisfy Vegard's law.

Table 2. Equilibrium lattice constants and excess heats of formation for three ordered stoichiometric superstructures Cu₃X(L1₂), CuX(L1₀) and CuX₃(L1₂)(X = Au, Pd). The first row is the results predicted by the present LIM. The second row is those from the first-principles calculation of Takizawa *et al* [8] and Terakura *et al* [9]. The lattice constants with asterisks are the predictions of Vegard's law. The third row is the results of Johnson [6].

System	a_e	ΔE	System	a_e	ΔE
Cu ₃ Au	3.74	-0.28	Cu ₃ Pd	3.68*	-0.31
	3.70	-0.26		3.68*	-0.31
	NA	-0.22		NA	0.06
(CuAu) ₂	3.86	-0.36	(CuPd) ₂	3.75	-0.39
	3.84	-0.28		3.75*	-0.28
	NA	-0.25		NA	0.08
CuAu ₃	3.98	-0.22	CuPd ₃	3.82	-0.28
	3.96	-0.14		3.82*	-0.21
	NA	-0.06		NA	0.06

The dilute-limit heat of solution of a guest atom of type b in a host lattice with type-a atoms can be calculated as the summation of the following five terms:

- (1) the energy needed for removing a host atom

$$E_1 = -F^a(\rho_e^a) - \sum_{n=1}^{\infty} w(n) V_{aa}(\sqrt{n} R_{1c}^a)$$

- (2) the energy needed for adding a guest atom

$$E_2 = F^b(\rho_e^a) + \sum_{n=1}^{\infty} w(n) V_{ab}(\sqrt{n} R_{1c}^a)$$

- (3) the energy results from the effects on the neighbouring atoms caused by adding a guest atom

$$E_3 = \sum_{n=1}^{\infty} w(n) [-F^a[\rho_e^a] + F^a[\rho_e^a + \Delta\rho(n)]]$$

with

$$\Delta\rho(n) = -f^a(\sqrt{n} R_{1c}^a) + f^b(\sqrt{n} R_{1c}^a)$$

- (4) the energy results from the change of cohesive energy after the host atom is replaced by the guest atom

$$E_4 = -E_s^a + E_s^b$$

- and (5) relaxation energy [4, 5]

$$E_5 = - \left[1.167 \left(\frac{\Omega_b}{\Omega_a} - 1 \right) \right]^2$$

Hence

$$E = E_1 + E_2 + E_3 + E_4 + E_5$$

The dilute-limit heats of solution of binary systems containing Pd predicted by Johnson [5] have remarkable disagreements with experimental data [24]. With the inverted alloy potential $V_{ab}(r)$, the errors are considerably reduced (see table 3).

Table 3. Dilute-limit heats of solution for binary alloys of Cu, Au, Pd. The data in parentheses are the results of Johnson. The experimental values are taken from [24]. G and H denote guest and host, respectively. All energies are in eV.

System	Unrelaxed	Relaxed	Experimental
Cu(G)Au(H)	-0.08(0.03)	-0.21(-0.10)	-0.13
Au(G)Cu(H)	-0.07(-0.03)	-0.34(-0.29)	-0.19
Cu(G)Pd(H)	-0.30(0.11)	-0.35(0.06)	-0.39
Pd(G)Cu(H)	-0.36(0.16)	-0.44(0.08)	-0.44

In conclusion, we have presented a useful method to construct the alloy pair potential in the EAM. The method needs no presupposition about the pair potential between unlike atoms. The difference between alloy pair potentials constructed by average schemes from pure metals and the inverted alloy pair potential lies in the fact that the inverted potential can reproduce the alloy cohesion equation of RSGF accurately whereas the average potentials cannot. As we have shown, the present method may provide a feasible solution for reducing the noticeable errors occurring in Johnson's calculations concerning palladium.

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