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Simple Relationships for Some Three-Parameter Interatomic-Potential Models for the Interactions between the Chemically-Different Types' Atoms

O. A. Likhachev, Yu. M. Koval, T. G. Sych, and V. A. Tatarenko

*G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,
36 Academician Vernadsky Blvd.,
UA-03142 Kyiv, Ukraine*

Three-parameter Lennard-Jones and Morse interatomic potentials are the simplest ones, which can be used to describe thermophysical properties of the liquid and solid substances. Upon adjusting the model parameters to real substance properties, the interatomic potentials can be used to describe simple single-component substance with good accuracy. Usually, these three parameters can be found from the cohesion energy, bulk moduli, and the molar volume data or the lattice parameters obtained experimentally for chemically-pure crystalline solids. In our paper, in case of chemically-different atoms, for both the Lennard-Jones potential and the Morse one, or any other three-parameter potential, we propose some convenient model relationships expressing the corresponding three parameters through the previously found ones for pure chemical elements.

Key words: solid substance, interatomic interactions, Lennard-Jones potential, Morse potential, lattice parameter, bonding energy, cohesive energy, bulk modulus, elastic stiffness, nearest-neighbour approximation.

Трипараметричні міжатомові потенціали Леннард-Джонса та Морзе є одними з найпростіших, що можуть використовуватися для одержання термодинамічних властивостей рідких і твердих речовин. За узгодження модельних параметрів з властивостями реальних речовин, міжатомові потенціали можуть використовуватися для опису простих однокомпонентних речовин з достатньою точністю. Зазвичай, ці параметри можуть бути

Corresponding author: Oleksandr Anatoliyovych Likhachev
E-mail: alexl@imp.kiev.ua

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знайдені з даних щодо енергії зв'язку, модуля стиску, мольного об'єму або параметрів кристалічної ґратниці, визначених експериментально для хемічно чистих кристалічних тіл. В нашій роботі для випадку хемічно різних атомів і потенціалів Леннард-Джонса, Морзе або будь-яких інших трипараметричних потенціалів пропонуються деякі зручні модельні співвідношення, що виражають відповідні три параметри через попередньо знайдені для хемічно однокомпонентних матеріалів.

Ключові слова: тверда речовина, міжатомові взаємодії, потенціал Леннард-Джонса, потенціал Морзе, параметер ґратниці, енергія зв'язку, енергія когезії, об'ємний модуль, пружня цупкість, наближення найближчих сусідів.

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1. INTRODUCTION

Finding the semi-empirical interatomic-interaction potentials is an important task for many aims. First, it may be initial starting point for the modelling of different thermodynamic properties of liquids and solids consisting of pure chemical element and of multiple chemical components.

The Lennard-Jones [1–3] and Morse [6] potentials are the simplest ones, which can be used to obtain thermophysical properties of the liquid and solid substances. These potentials are mathematically simple and, therefore, are often used in different computer simulation studies. Due to their mathematical simplicity and generic modelling capabilities, the mentioned potentials are probably still the most frequently studied model potentials. The Lennard-Jones potential is usually the standard choice for the development of theories for matter (especially soft-matter) as well as for the development and testing of computational methods and algorithms. Upon adjusting the model parameters to real substance properties, the interatomic potentials can be used to describe simple substance with good accuracy. Usually, these parameters can be found from the cohesive energy, bulk moduli and the molar volume data or the lattice parameters obtained experimentally for chemically pure single-component crystalline solids [4, 5, 7]. These ideas have been also applied to study some other properties of crystalline solids [8, 9, 11]. Nevertheless, finding similar parameters for interatomic potentials in case of chemically-different interacting atoms is not so easy, and the problem is still actual.

In our paper, in case of chemically-different atoms, for both the Lennard-Jones potential and the Morse one, or any other three-parameter potential, we propose some convenient model relationships expressing the corresponding three parameters through the previously found ones for pure chemical elements.

2. PARAMETERIZATIONS OF THE LENNARD-JONES AND MORSE POTENTIALS

Here, we introduce two three-parameter potentials, namely, the Lennard-Jones type (LJ-type) and the Morse type (M-type) potential, for the interaction energy between two neighbouring same atoms in the following form:

$$u_{\text{LJ}}(r) = \varepsilon((r/a)^{-2n} - 2(r/a)^{-n}) \text{ and } u_{\text{M}}(r) = \varepsilon(e^{-2\beta(r/a-1)} - 2e^{-\beta(r/a-1)}). \quad (1)$$

They have three parameters, LJ-type $\{\varepsilon, a, n\}$ and M-type $\{\varepsilon, a, \beta\}$, respectively. Here, r means the interatomic distance. Both interaction energy models $u_P(r)$ (with $\{\varepsilon, a, n\}$ for $P = \text{LJ}$ or $\{\varepsilon, a, \beta\}$ for $P = \text{M}$) have minima at $r = a$, where $u_P(a) = -\varepsilon$ characterizes the bonding energy of two same atoms at the equilibrium distance between them. The exponent parameters, n, β and $2n, 2\beta$, characterize the decrease or increase rate of the attractive energy parts and the repulsive ones, as the interatomic-separation distance r changes.

Instead of these three parameters, we can introduce a new set of universal parameters like the equilibrium interatomic bond length a , elastic stiffness of interatomic bonds k , and the elastic cut-off distance c , where

$$k = u''_P(a), \quad c = \sqrt{2\varepsilon/k}. \quad (2)$$

In particular, for the Lennard-Jones potential,

$$k_{\text{LJ}} = 2\varepsilon n^2 / a^2, \quad c = a / n, \quad (3)$$

and, for the Morse potential,

$$k_{\text{M}} = 2\varepsilon\beta^2 / a^2, \quad c = a / \beta. \quad (4)$$

Both interatomic potentials of LJ- and M-types, as well as so-called elastic-bond potential model, calculated at the $\beta = n = 5$ values are shown in Fig. 1. In these both cases and in any other three-parameter interatomic-potential models, we will use the following ‘model-independent’ (universal) relationships:

$$k = 2\varepsilon / c^2, \quad \varepsilon = 0.5kc^2. \quad (5)$$

Here, we have introduced so-called elastic-bond potential,

$$u_{\text{EB}}(r) = \varepsilon(-1 + (\gamma(r/a - 1))^2), \quad (6)$$

and, in addition, the equations similar to Eqs. (3), (4) obtained for the

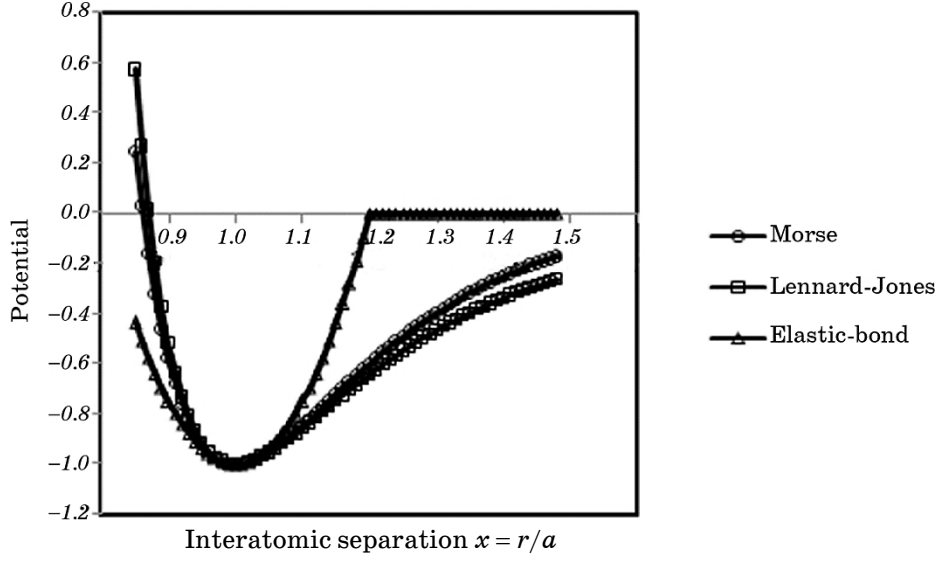


Fig. 1. Three-parameter Lennard-Jones, Morse and parabolic elastic-bond interatomic potentials calculated at equal bonding energy $\varepsilon = 1$ and $\beta = n = 5$.

Lennard-Jones and Morse potentials,

$$k_{\text{EB}} = 2\varepsilon\gamma^2 / a^2, \quad c = a / \gamma. \quad (7)$$

It also shown in Fig. 1 and calculated at $\gamma = \beta = n = 5$.

As it follows from Fig. 1, the elastic cut-off parameter c introduced in Eq. (2) characterizes interatomic distance, where elastic-bond potential takes a zero value, $u_{\text{EB}}(a + c) = 0$, that means that the elastic bond is broken at this distance. So, this parameter can be used for any interatomic-potential model as well.

In present subsection, for any three-parameter potential $u_p(r)$, instead of corresponding three parameters, we can introduce a new set of universal parameters like the equilibrium interatomic-bond length a , where $u_p'(a) = 0$, the interatomic-coupling energy $u_p(a) = -\varepsilon$, the elastic stiffness of interatomic bond $k = u_p''(a)$, and the elastic cut-off distance $c = \sqrt{2\varepsilon / k}$. Finally, we have introduced convenient dimensionless potential parameter $\eta = a/c$. Using these ones, the interatomic potential itself can be represented as follows:

$$u_p(r) = \varepsilon\varphi_\eta\left(\frac{r}{a}\right). \quad (8)$$

Here, the dimensionless potential function $\varphi_\eta(x)$ depends only on the dimensionless interatomic-separation distance x and a single potential

parameter η . In case of the Lennard-Jones and Morse potentials, $\eta = \beta = n$.

3. FINDING PARAMETERS FROM THE EXPERIMENTAL DATA

To find these parameters, most of researchers use the cohesive energy, bulk moduli and the molar volume (or lattice parameter) data such as represented in Table 1 for some f.c.c. and b.c.c. transition metals taken from [10, 12–14].

Using Eq. (1), one can write the molar internal energy at zero temperature for the crystalline solid as function of the nearest-neighbour distance r as follows:

$$U(r) = \frac{1}{2} N_A \sum_{i=1}^{K_c} z_i u_p(rp_i) = \frac{1}{2} N_A \varepsilon \sum_{i=1}^{K_c} z_i \phi_\eta \left(\frac{r}{a} p_i \right) = \frac{1}{2} N_A \varepsilon \Phi_\eta \left(\frac{r}{a} \right). \quad (9)$$

Here, summation is performed over a set of K_c nearest co-ordination spheres ($i = 1, 2, \dots, K_c$), where z_i denotes the number of atoms on the i -th co-ordination sphere. $N_A = 6.02214076 \cdot 10^{23}$ mole⁻¹ is the well-known Avogadro number, and p_i is a set of dimensionless distances to the i -th co-ordination sphere. We also introduce the dimensionless Lennard-Jones or Morse potential functions $\phi_\eta(x)$ having a minimum at $x = 1$, where $\phi_\eta(1) = -1$, and the second derivative value $\phi_\eta''(1) = 2\eta^2$ at $\eta = \beta = n$ for M- and LD-type potentials, respectively. Further, we will denote $\Psi_\eta(x) = 0.5\Phi_\eta(r/a) = 0.5\Phi_\eta(x)$ as the dimensionless crystal energy per atom. Normally, the internal energy of a crystal must be represented as a function of the molar volume $V_m = N_A v(r)$, where $v(r)$ is the volume per single atom in a given crystalline solid. For many ideal crystal structures like f.c.c., h.c.p. and b.c.c., there is a simple rela-

TABLE 1. Cohesive energy, bulk modulus and molar volume interpolated to 0 K for some f.c.c. and b.c.c. metals (experimental data).

	V	Nb	Ta	Cr	Mo	W	Fe	
Units	b.c.c.	b.c.c.	b.c.c.	b.c.c.	b.c.c.	b.c.c.	b.c.c.	
E_m , kJ/mol	512	730	782	395	658	859	413	
K , GPa	160	170	200	160	230	310	170	
V_m , $10^{-6} \cdot \text{m}^3$	8.337	10.84	10.87	7.232	9.334	9.550	7.092	
KV_m/E_m	2.59	2.52	2.78	2.93	3.26	3.45	2.92	
	Ni	Pd	Pt	Cu	Ag	Au	Rh	Ir
Units	f.c.c.	f.c.c.	f.c.c.	f.c.c.	f.c.c.	f.c.c.	f.c.c.	f.c.c.
E_m , kJ/mol	428	376	564	336	284	368	554	670
K , GPa	180	180	230	140	100	220	380	320
V_m , $10^{-6} \cdot \text{m}^3$	6.589	8.851	9.095	7.092	10.28	10.21	8.266	8.520
KV_m/E_m	2.77	4.23	3.71	2.95	3.61	6.32	5.47	3.42

tionship between the atomic volume and the nearest-neighbour distance: $v(r) = qr^3$, where q is a constant dependent on particular crystal geometry. At the equilibrium distance $r = r_e$, where

$$\left(\frac{d}{dr} U(V(r)) \right)_{r=r_e} = N_A \varepsilon \Psi'_\eta(x_e) = 0, \quad (10)$$

we can obtain a dimensionless ratio $x_e = r_e/a$ and the equilibrium molar volume

$$V_m(r_e) = N_A q r_e^3. \quad (11)$$

Therefore, using Eqs. (8), (9), one can obtain the bulk modulus K at zero temperature as follows:

$$K = V_m \left(\frac{d^2 U(V)}{dV^2} \right)_{V=V_m} = \varepsilon \frac{1}{9 q r_e a^2} \Psi''_\eta(x_e). \quad (12)$$

On the other hand, at zero temperature, the molar cohesive energy is

$$E_m = -U(V_m) = -N_A \varepsilon \Psi_\eta(x_e). \quad (13)$$

From Eqs. (12), (13), it follows an important dimensionless relationship between the cohesive energy, bulk modulus and the molar volume:

$$\frac{V_m K}{E_m} = -\frac{1}{9} x_e^2 \Psi''_\eta(x_e) / \Psi_\eta(x_e). \quad (14)$$

Here, $x_e = x_e(\eta)$ is a value minimizing the dimensionless cohesive-energy function that can be obtained solving Eq. (10). Obviously, it depends on the dimensionless parameter $\eta = \{n, \beta, \gamma\}$ of any interatomic potential discussed in the present paper or some other ones too. Therefore, Eq. (14) gives a possibility finding this one parameter as function of the experimental dimensionless quantity ($V_m K / E_m$):

$$\eta = \eta(V_m K / E_m). \quad (15)$$

The second parameter, namely, the bonding energy, one can find from Eq. (13):

$$\varepsilon = -\frac{E_m / N_A}{\Psi_\eta(x_e(\eta))}. \quad (16)$$

Lastly, the third parameter, *i.e.*, the bonding length a , is as follows:

$$a = d / x_e(\eta). \quad (17)$$

Here, d is the experimentally measured nearest-neighbour distance in b.c.c., f.c.c. or h.c.p. structure, or calculated from the known atomic volume:

$$v(d) = qd^3 = V_m / N_A, \quad (18)$$

where

$$q_{\text{b.c.c.}} = 4 / 3\sqrt{3} = 0.7698, \quad q_{\text{f.c.c.}} = 1 / \sqrt{2} = 0.7071$$

and, obviously,

$$d_{\text{b.c.c.}} = \sqrt{3}(2v_{\text{b.c.c.}})^{1/3} / 2, \quad d_{\text{f.c.c.}} = (4v_{\text{f.c.c.}})^{1/3} / \sqrt{2}. \quad (19)$$

The data given in Table 1 can be used to calculate all the interatomic-potential parameters. Normally, it can be done applying appropriate numerical methods. But here, we restrict ourselves by the simplest nearest-neighbour approximation by means of setting in Eq. (9) $K_c = 1$, $\Psi_\eta(x) = (z_1 / 2)\phi_\eta(x)$ and finding from Eq. (10) $\phi'(x_e) = 0 \Rightarrow x_e = 1$. After that, one can see: $\Psi_\eta(1) = -z_1 / 2$, $\Psi_\eta''(1) = (z_1 / 2)2\eta^2$ ($\eta = \{n, \beta, \gamma\}$). Finally, using Eq. (14), we obtain:

$$\frac{V_m K}{E_m} = \frac{2}{9}\eta^2 \quad \text{or} \quad \eta = 3\sqrt{V_m K / (2E_m)}. \quad (20)$$

At the same time, from Eqs. (16), (17), we find the two remained potential parameters:

$$\varepsilon = \frac{2}{z_1}(E_m / N_A) \quad \text{and} \quad a = d. \quad (21)$$

All the parameters characterizing the model Lennard-Jones and Morse potentials consistent with experimental data are collected in Tables 2, 3. It should be mentioned that the potential parameters for the b.c.c. lattice were calculated using both the first and second coordination spheres setting in Eq. (9) $K_c = 2$. The reason of that is the known elastic instability of b.c.c. lattices in the nearest-neighbour approximation in respect to its shear distortion.

Therefore, in present subsection, we have discussed a procedure of finding the potential parameters using the cohesive energy, bulk modulus and the molar volume (or lattice parameter) data represented in Table 1 for some f.c.c. and b.c.c. transition metals. The idea using these experimental data has been proposed quite long ago and, then, was applied by many other researchers mainly limiting themselves by the LJ- and M-cases [4, 5, 7]. The main reason for us is to formulate the finding procedure to be maximally independent on a particular poten-

TABLE 2. Cohesive energy per atom (eV), volume per atom (\AA^3) and the nearest-neighbour distance (\AA) together with the potential parameters calculated from the experimental data in the nearest-neighbour approximation for some b.c.c. metals.

Metal	ε_a , eV	v_a , \AA^3	d , \AA	β	ε , eV	k , eV/ \AA^3	c , \AA
V	5.31	13.84401	2.619959	3.413942	0.884493	3.003638	0.767429
Nb	7.57	18.00037	2.859572	3.367492	1.261094	3.497746	0.84917
Ta	8.11	18.05018	2.862208	3.536948	1.350925	4.125877	0.809231
Cr	4.09	12.00578	2.49845	3.631116	0.682373	2.882639	0.688067
Mo	6.82	15.49293	2.720102	3.830144	1.136712	4.507546	0.710183
W	8.90	15.85826	2.741316	3.940178	1.483945	6.131421	0.695734
Fe	4.28	11.7733	2.482219	3.624914	0.713468	3.043125	0.684766

tial type. Therefore, we did everything in dimensionless form. We have defined the basic crystal energy function as a sum of the individual dimensionless interatomic potentials taken over some appropriate number K_c of co-ordination spheres according to Eq.(9):

$$\Psi_\eta(x) = \frac{1}{2} \sum_{i=1}^{K_c} z_i \phi_\eta(x p_i). \quad (22)$$

Then, making minimizing procedure, one can find the equilibrium dimensionless nearest-neighbour distance $x = x_e(\eta)$ dependent on the potential parameter η in a given crystal lattice with a given set of co-ordination numbers $\{z_i\}$ and a set of dimensionless distances $\{p_i\}$ to the

TABLE 3. Cohesive energy per atom (eV), volume per atom (\AA^3), and the nearest-neighbour distance (\AA) together with the potential parameters calculated from the experimental data in the nearest-neighbour approximation for some f.c.c. metals.

Metal	ε_a , eV	v_a , \AA^3	d , \AA	β	ε , eV	k , eV/ \AA^3	c , \AA
Ni	4.44	10.94303	2.492016	3.530581	0.739381	2.968171	0.705837
Pd	3.90	14.69587	2.749393	4.362912	0.64955	3.27131	0.630174
Pt	5.85	15.11101	2.775041	4.085952	0.974325	4.224556	0.679167
Cu	3.48	11.7733	2.553511	3.643487	0.580449	2.363485	0.700843
Ag	2.94	17.07046	2.890148	4.030509	0.490617	1.908326	0.717068
Au	3.81	16.95422	2.883573	5.332917	0.63573	4.348807	0.540712
Rh	5.74	13.73275	2.687969	4.961351	0.957049	6.521024	0.541782
Ir	6.94	14.14789	2.714786	3.923009	1.157442	4.833891	0.692016

i -th co-ordination sphere. Finally, using Eq. (14), we obtain parameter η as a function of the only dimensionless experimental parameter $\chi = V_m K / E_m$, $\eta = \eta(\chi)$, as well as two remaining potential parameters:

$$\varepsilon(\chi) = -e_m / \Psi(x_e(\eta(\chi))) \text{ and } a(\chi) = d / x_e(\eta(\chi)). \quad (23)$$

Here, $e_m = E_m / N_A$ is the cohesive energy per atom, and d is the experimentally measured distance between the nearest atoms in b.c.c., f.c.c. or h.c.p. crystals.

4. MODELLING INTERATOMIC POTENTIALS FOR CHEMICALLY-DIFFERENT TYPES' ATOMS

In present section, we will propose some simple ideas, which allow constructing the interatomic potential for two chemically-different atoms A and B, shown schematically in Fig. 2. These atoms are placed at some interatomic distance $r_{AB} = (r_A + r_B)/2$, where r_A and r_B denote the bond length for A-A- or B-B-type interacting atoms, respectively. Here, f is a force taking zero value, if atoms A and B are at their equilibrium distances: $r_A = a_A$ and $r_B = a_B$. However, the interaction forces acting between the atoms (all equal due to Newton's third law) will change supposedly linearly, if r_A and r_B will experience some small changes: $r_A = a_A + \delta a_A$ and $r_B = a_B + \delta a_B$, as follows from equations below:

$$f = k_A \delta a_A \text{ and } f = k_B \delta a_B. \quad (24)$$

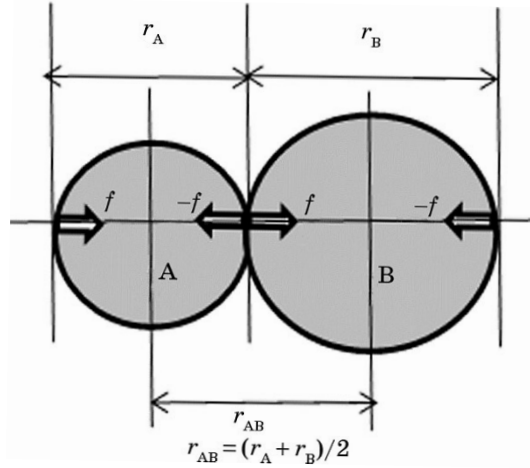


Fig. 2. The scheme represents two ball-shaped chemically-different atoms A and B producing weak forces, when the distance between them slightly changes.

Here, k_A , k_B are the elastic-bond stiffness parameters introduced in previous section. A similar relationship can be supposedly written for the A–B bonds:

$$f = k_{AB} \delta a_{AB}, \text{ where } \delta a_{AB} = (\delta a_A + \delta a_B) / 2. \quad (25)$$

Combining these equations, one can obtain relationships for the elastic-bond stiffness parameters for the A–B-type interatomic bonds as function of the stiffness parameters for the A–A and B–B ones, respectively:

$$1 / k_{AB} = (1 / k_A + 1 / k_B) / 2. \quad (26)$$

Along with this important equation, one can use a similar additive rule for the equilibrium bond length a . Besides, the elastic cut-off distance c_{AB} introduced in the previous section will be represented generally consisting of the half-additive contribution $(c_A + c_B) / 2$ and a difference $c_{AB}^{\text{exc}} = c_{AB} - (c_A + c_B) / 2$ as indicated in Eq. (27):

$$a_{AB} = (a_A + a_B) / 2, \quad c_{AB} = (c_A + c_B) / 2 + c_{AB}^{\text{exc}}. \quad (27)$$

Later, we will show that this so-called c -excess parameter c_{AB}^{exc} is small, but nevertheless, plays a very important role. These three relationships give us full description of all three parameters for the Lennard-Jones and Morse potentials, or any other three-parameter potentials as well. In particular, the bonding energy between the A–B atoms can be easily found from the following equation:

$$c_{AB}^2 / \varepsilon_{AB} = (c_A^2 / \varepsilon_A + c_B^2 / \varepsilon_B) / 2. \quad (28)$$

One can also obtain the following relationships for the exponent parameters n , β of the Lennard-Jones and Morse potentials: $n_{AB} = \beta_{AB} = a_{AB} / c_{AB}$.

Equation (28) is important for many applications for ordered or disordered binary alloys to predict their thermodynamic properties at different atomic concentrations.

In order to analyse and discuss this equation, it is more convenient to express it in a dimensionless form:

$$\frac{1}{(\varepsilon_{AB} / \varepsilon)} = \left(\frac{c_A^2 / c_{AB}^2}{(\varepsilon_A / \varepsilon)} + \frac{c_B^2 / c_{AB}^2}{(\varepsilon_B / \varepsilon)} \right) / 2, \text{ where } \varepsilon = \frac{\varepsilon_A + \varepsilon_B}{2}. \quad (29)$$

One can also express parameters ε_A , ε_B as follow:

$$\varepsilon_A = (\varepsilon_A + \varepsilon_B) / 2 + (\varepsilon_A - \varepsilon_B) / 2, \quad \varepsilon_B = (\varepsilon_A + \varepsilon_B) / 2 - (\varepsilon_A - \varepsilon_B) / 2. \quad (30)$$

The same can be done for parameters c_A, c_B as well:

$$c_A = (c_A + c_B) / 2 + (c_A - c_B) / 2, c_B = (c_A + c_B) / 2 - (c_A - c_B) / 2 \quad (31)$$

or the corresponding dimensionless relationships:

$$\varepsilon_A / \varepsilon = 1 + (\varepsilon_A - \varepsilon_B) / 2\varepsilon, \varepsilon_B / \varepsilon = 1 - (\varepsilon_A - \varepsilon_B) / 2\varepsilon \quad (32)$$

and

$$c_A / c_{AB} = 1 + (c_A - c_B) / 2c, c_B / c_{AB} = 1 - (c_A - c_B) / 2c. \quad (33)$$

Therefore, Eq. (28) is expressed through the following two dimensionless parameters with $c = (c_A + c_B) / 2$ and $\varepsilon = (\varepsilon_A + \varepsilon_B) / 2$:

$$w_{AB} = (c_A - c_B) / 2c (|w_{AB}| \leq 1), \omega_{AB} = (\varepsilon_A - \varepsilon_B) / 2\varepsilon (|\omega_{AB}| \leq 1). \quad (34)$$

So, finally, from Eq. (28)–(33), we obtain:

$$\frac{1}{(\varepsilon_{AB} / \varepsilon)} = \frac{1}{2} \left(\frac{c}{c_{AB}} \right)^2 \left(\frac{(1 + w_{AB})^2}{1 + \omega_{AB}} + \frac{(1 - w_{AB})^2}{1 - \omega_{AB}} \right), \quad (35)$$

and then find:

$$\frac{\varepsilon_{AB}}{\varepsilon} = 2 \left(\frac{c_{AB}}{c} \right)^2 \left(\frac{(1 + w_{AB})^2}{1 + \omega_{AB}} + \frac{(1 - w_{AB})^2}{1 - \omega_{AB}} \right)^{-1} = \left(\frac{c_{AB}}{c} \right)^2 F_{AB}(\omega_{AB}, w_{AB}). \quad (36)$$

One can observe (see Fig. 3) that $F_{AB}(\omega_{AB}, w_{AB})$ takes exactly unit value, $F_{AB}(\omega_{AB}, w_{AB}) = 1$, everywhere at the straight line $\omega_{AB} = w_{AB}$ within the square box region $-1 \leq \omega_{AB} \leq 1$ and $-1 \leq w_{AB} \leq 1$; however, $F_{AB}(\omega_{AB}, w_{AB}) < 1$ in other cases.

Therefore, in this section, we have proposed some simple ideas, which allowed constructing the interatomic-potential parameters for two chemically-different atoms A and B.

For this aim, we have considered the interatomic-distance changes $\delta_{AA}(f)$, $\delta_{BB}(f)$, $\delta_{AB}(f)$ produced by the same weak force f applied to A–A, B–B and A–B atomic pairs. We also assumed that, similarly to the equilibrium interatomic-bond length rule: $a_{AB} = (a_{AB} + a_{AB}) / 2$, the additional distance changes will follow the same rule: $\delta_{AB} = (\delta_{AB} + \delta_{AB}) / 2$. So, the important relationship between the interatomic-stiffness parameters, $1/k_{AB} = (1/k_A + 1/k_B)$, has been obtained in Eq. (25). It also gives a corresponding relationship for the energy coupling parameters: $c_{AB}^2 / \varepsilon_{AB} = (c_A^2 / \varepsilon_A + c_B^2 / \varepsilon_B) / 2$.

Finally, introducing two new parameters $w_{AB} = (c_A - c_B)(c_A + c_B)$ and $\omega_{AB} = (\varepsilon_A - \varepsilon_B)(\varepsilon_A + \varepsilon_B)$, one can obtain a fully dimensionless relationship:

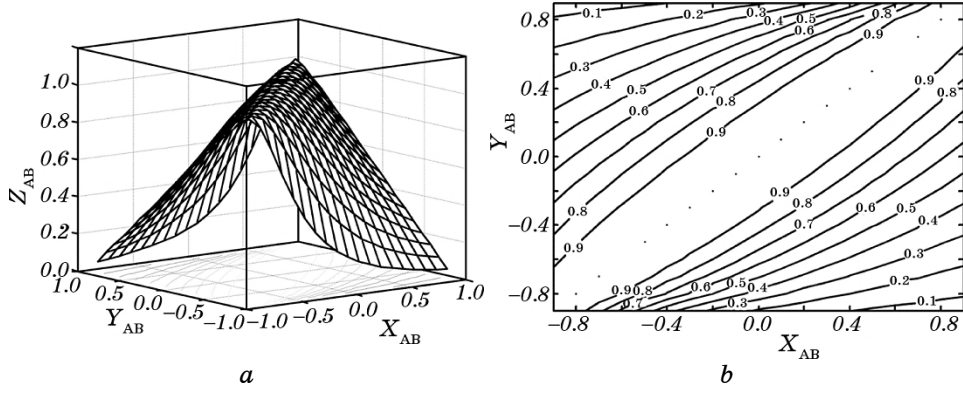


Fig. 3. Representing 3D image of the $F_{AB}(\omega_{AB}, w_{AB})$ -surface calculated from Eq. (36) (a); representing 2D image of the $F_{AB}(\omega_{AB}, w_{AB})$ -surface calculated from Eq. (36) (b). Here, $X_{AB} = w_{AB} = (c_A - c_B)(c_A + c_B)$, $Y_{AB} = \omega_{AB} = (\varepsilon_A - \varepsilon_B)(\varepsilon_A + \varepsilon_B)$ and $Z_{AB} = F_{AB}(\omega_{AB}, w_{AB})$.

$$\varepsilon_{AB} / \varepsilon = (c_{AB} / c)^2 F_{AB}(\omega_{AB}, w_{AB}), \quad (37)$$

where $c = (c_A + c_B)/2$, $\varepsilon = (\varepsilon_A + \varepsilon_B)/2$, and $F_{AB}(\omega_{AB}, w_{AB})$ is the function defined in Eq. (36). In present subsection in Eq. (27), we have also assumed that $c_{AB} = c + c_{AB}^{\text{exc}}$ and obtained Eq. (36). Therefore, there is a serious reason to introduce a new positively definite function $g_{AB}(\omega_{AB}, w_{AB}) = (c_{AB} / c)^2 = (1 + c_{AB}^{\text{exc}} / c)^2 \approx 1 + 2c_{AB}^{\text{exc}} / c$, which depends on the same parameters, like $F_{AB}(\omega_{AB}, w_{AB})$ does. As $F_{AB}(\omega_{AB}, w_{AB})$ and $g_{AB}(\omega_{AB}, w_{AB})$ must approach to the unit value as $\omega_{AB} \rightarrow 0$ and $w_{AB} \rightarrow 0$, both these functions can be expanded as $F_{AB}(\omega_{AB}, w_{AB}) \approx 1 - (\omega_{AB} - w_{AB})^2$ and $g_{AB}(\omega_{AB}, w_{AB}) \approx 1 + (P_1(\omega_{AB})^2 + P_2\omega_{AB}w_{AB} + P_3(w_{AB})^2)$ in this limit, accordingly. The fact that these expansions do not contain the linear terms with respect to parameters ω_{AB} , w_{AB} is due to the inversion-symmetry requirement: $g_{AB}(\omega_{AB}, w_{AB}) = g_{AB}(-\omega_{AB}, -w_{AB})$. Therefore, in this case we will have:

$$\varepsilon_{AB} / \varepsilon \approx 1 + ((P_1 - 1)\omega_{AB}^2 + P_2\omega_{AB}w_{AB} + P_3w_{AB}^2). \quad (38)$$

Here, P_1 , P_2 and P_3 are some fitting constants, which should be found from the analysis of some (minimum three) binary phase diagrams.

We are not going to discuss the appropriate procedure for that in details in the present paper and will do that somewhere else. We should only to mention that, for instance, it is convenient to consider the disordered binary alloys like f.c.c. lattice-based Cu–Ni, Ni–Au and Cu–Rh. All of them have a good solubility at high temperatures, but undergo decomposition reactions below some corresponding characteristic temperatures T_{max} and concentrations x_{max} . In case of Cu–Ni alloy, these

points are $T_{\max} = 355^{\circ}\text{C}$, $x_{\max} = 0.673$; for Ni–Au alloy, they are $T_{\max} = 812^{\circ}\text{C}$, $x_{\max} = 0.29$; and for Cu–Rh alloy, they are $T_{\max} = 812^{\circ}\text{C}$, $x_{\max} = 0.29$ [15]. Within the mean self-consistent field approximation, there is a simple relationship between these points and the interchange energy $\varepsilon^{\text{interch}}$ [16]: $kT_{\max}/(2z_1|\varepsilon^{\text{interch}}|) = x_{\max}(1 - x_{\max})$ describing the spinodal curve, if the nearest-neighbour interaction approximation is adopted, where T_{\max} is the absolute temperature in [K], and $z_1 = 12$ is the first co-ordination number in this case of f.c.c. lattice.

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