

## Empirical many-body interatomic potential for bcc transition metals

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A simple many-body interatomic potential is proposed. This is an empirical extension of the embedded-atom method (EAM). The EAM models the lattice energy and elastic compressibility using a pair interaction plus a many-body term. It does not include any contribution of many-body terms to the crystal elastic shear. This contribution is included in the model developed here. It implies a simplified treatment of the angularity inherent to covalent bonding in transition metals. A set of interatomic potentials is deduced for bcc Nb, Fe, and Cr. While in previous works in the literature the EAM has already been successfully applied to the fitting of interatomic potentials for Nb and Fe, this was not the case for Cr, for which the elastic-constant values implied a negative Cauchy pressure.

### I. INTRODUCTION

Computer simulation of defects in lattices has gone through different periods. In the early 1960s, the method was already applied to relatively complex defects like dislocations.<sup>1</sup> Computer speed and storage were the two major limitations of the technique until the mid-1970s. Recent advances in computing facilities as well as the development of efficient numerical algorithms have largely overcome these two drawbacks. However, even nowadays, the efforts to increase the complexity of problems studied using computer simulation are hindered because of the unavailability of simple, easy to compute, interatomic potentials, which, in addition, treat forces in a physically realistic way. To our knowledge, the pair interaction approximation has been used almost exclusively in the 1960s and 1970s. More realistic approaches to the interatomic forces in metals and semiconductors, which can also be used for the computer simulation of defects structure, have been only recently reported in the literature; see Refs. 2, 3, 4, 5, and 6 for a review. One must remember that, by using pair interaction potentials, the physical validity of the calculation is somewhat limited, the major drawbacks being that (i) if the experimental elastic constants are correctly reproduced, a fictitious pressure has to be imposed for holding the lattice at equilibrium; (ii) nearly equal cohesive and vacancy formation energies are predicted, at variance with the experimental observations; and (iii) those potentials generally predict unrealistic relaxation of the free-surface atoms.<sup>7</sup>

Finnis and Sinclair (FS),<sup>3</sup> Daw and Baskes (DB),<sup>4</sup> who named the method the embedded-atom method (EAM), and Ercolessi *et al.*<sup>5</sup> calculated the energy of an assembly of metal atoms defined through their atomic coordinates by including in the interatomic potential pair interaction terms plus the essential band character of the metallic cohesion. This latter was assumed as an explicit local volume dependence of the total energy. Their approach allows for the modeling of defect properties not accessible to the simple pair interaction potentials; in addition, the simplicity and speed in calculation are retained. Howev-

er, even nowadays if we want to simulate defects in covalent materials like Si or Ge or in transition metals, it is difficult to find appropriate interatomic potentials. For the case of Si bonding, the covalent interaction has been included in a potential function by Stillinger and Weber.<sup>2</sup> Those authors proposed a model of three-body interaction forces. Also for Si and Ge, Baskes<sup>8</sup> and Baskes *et al.*<sup>9</sup> developed a semiempirical potential based on a modified embedded-atom method (MEAM). This includes some dependence of the local electron density on the angle between the vectors joining two neighbor atoms to a central one.

In a previous paper,<sup>10</sup> we also proposed to extend the EAM, adopting an empirical approach based on considering each lattice atom as a defect embedded in an effective continuum host. That approach allows the contribution of a many-body term to the energy involved in shearing a crystal to be included. In Ref. 10 only many-body terms were considered in the fitting of the materials properties. The conclusions of that work are fully exploited below to develop interatomic potentials for bcc transition metals.

It is worthy to remember here that, as early as in 1981, Matthai *et al.*<sup>11</sup> discussed that experimental perfect lattice properties in bcc transition metals reflect departures from central force fields. They invoked, among others, (i) the deviation of the x-ray-scattering form factor from free-atom calculations, (ii) the wide range of elastic constants, and (iii) the negative Cauchy discrepancy observed in Cr. As a result of those experimental facts, Matthai *et al.* had to include bonding charges in their model of bcc transition metals. On the other hand, Johnson and Oh,<sup>12</sup> concerned about the large dispersion found in the elastic constant values in bcc metals, performed a careful study of the EAM parametric fitting procedure. Those authors found that their method for developing interatomic potentials failed in the case of Cr, for which the Cauchy pressure is negative. We show here how to overcome this situation, and shall conclude that, unless the contribution of the many-body terms to the shear elastic constants is included, the elastic constants of a crystal

with a negative Cauchy pressure cannot be fitted by physically valid expressions for a potential based solely on the EAM. Incidentally, that pressure is also strongly negative for the case of Si and Ge, this being a further justification for the need of developing for those crystals a MEAM, as already done by Baskes *et al.*<sup>8,9</sup> As promised in Ref. 10, we develop in this paper an empirical many-body potential that can be used easily in computer simulation studies. The metallic character of the interaction forces is similar to the one of EAM, whereas the covalent aspect of bonding is averaged within a pair interaction plus a many-body approach. The expressions deduced below allow for a clear separation between the pair and many-body contributions to the calculated elastic constants. We also deduce an expansion for the potential-energy parametric with the crystal cohesion and the vacancy formation energy. Although our procedure is somewhat similar to the MEAM,<sup>8,9</sup> we obtain simpler expressions for the potential function; this is achieved by taking full advantage of the crystal symmetry. Also the basic idea of considering each atom as an impurity embedded in the host field of the lattice appears very clearly as the basis of our approach, however empirical.

Consistently with that idea, we shall call our empirical-potential the embedded-defect (ED) potential. We expect ED to be particularly useful for the computer simulation of defects in transition metals with partially covalent bond character. As an application we deduce the interatomic potentials for Nb, Fe, and Cr.

## II. INTERATOMIC POTENTIAL

### A. Many-body terms

The EAM of FS (Ref. 3) and DB (Ref. 4) is based on considering every atom in the crystal as an impurity, a "quasiatom,"<sup>13</sup> embedded in the effective field<sup>14</sup> of the other crystal atoms. Around each atom  $i$ , a local electron density function  $\rho_i$  is defined. This function is taken as

$$\rho_i = \sum_{j (\neq i)} \phi(R_{ij}), \quad (1)$$

where  $R_{ij}$  is the distance between atom  $i$  and  $j$ , and  $\phi$  is a function which depends solely on  $R_{ij}$ . The total energy of an assembly of atoms is the addition of an  $N$ -body term,

$$U_N = -A \sum_i f_i(\rho_i), \quad (2)$$

and a standard pair interaction term,  $U_p$ , i.e.,

$$U = U_N + U_p. \quad (3)$$

In close analogy with the EAM, we shall also consider every atom in the crystal as an impurity embedded in the crystal effective field.

The theory of defects in a continuous media as developed, for example, by Kanzaki,<sup>15</sup> Flinn and Maradudin,<sup>16</sup> Tewary,<sup>17</sup> Nowick and Berry,<sup>18</sup> and Schober,<sup>19</sup> shows that the distortion field of an impurity within the harmonic approximation for the energy is determined by

the dipole tensor associated to the defect forces and the perfect lattice response.

The dipole tensor is defined as

$$P_i^{\alpha\beta} = \sum_{j (\neq i)} K_{ij}^{\alpha} R_{ij}^{\beta}, \quad (4)$$

where  $\bar{K}_{ij}$  is the Kanzaki force<sup>15</sup> acting on a displaced atom  $j$  due to an impurity located at site  $i$ .  $K_{ij}^{\alpha}$  and  $R_{ij}^{\beta}$  denote, respectively, the  $\alpha$  component of  $\bar{K}_{ij}$  and the  $\beta$  component of  $\bar{R}_{ij}$ .  $\bar{K}$  can be calculated consistently by deriving the crystal energy with respect to atomic displacements at the relaxed atom configuration, allowing therefore for the inharmonicity of the lattice straining.<sup>17</sup> One must realize that the dipole tensor represents the defect, source of the lattice distortion, as a set of forces and near-neighbor coordinates.

The approach of the preceding paragraph provides a hint of how to expand the local electronic density in a way consistent with the lattice symmetry and within the EAM spirit. A tensor function  $\lambda$  can be defined at each atomic site  $i$  in the lattice:

$$\bar{\lambda}_i = \sum_{j (\neq i)} \phi(R_{ij})(\bar{r}_{ij} \otimes \bar{r}_{ij}), \quad (5)$$

where  $\otimes$  is the tensor product, i.e.,  $(\bar{a} \otimes \bar{b})^{\alpha\beta} = a^{\alpha} b^{\beta}$ ,  $\phi$  is a function that depends only on the distance  $R_{ij}$  between atoms  $i$  and  $j$ ;  $\bar{r}_{ij}$  is the unit vector joining the  $i$  and  $j$  atom. The vector  $\bar{K}(R_{ij}) = [\phi(R_{ij})/R_{ij}] \bar{r}_{ij}$  mimics, therefore, the Kanzaki force of the impurity, Eq. (4), while, as discussed below, the function  $\phi$  will be related to the one in Eq. (1). At the perfect lattice configuration, the tensor  $\lambda$  of Eq. (5) can be written as a function of the atomic shells around atom  $i$  and within the range of  $\phi$ :

$$\bar{\lambda}_i = \sum_{\nu} \phi_{\nu} \sum_{j \in \nu} (\bar{r}_{ij} \otimes \bar{r}_{ij}), \quad (6)$$

where  $j \in \nu$  denotes all the atoms at the atomic shell  $\nu$  around the atom  $i$ .

It is convenient to decompose the tensor  $\lambda$  as a sum of two terms:

$$\begin{aligned} \bar{\lambda} &= \bar{S} + \bar{D}, \\ S^{\alpha\beta} &= \frac{1}{3} \text{tr}(\bar{\lambda}) \delta^{\alpha\beta}, \\ D^{\alpha\beta} &= \begin{cases} \lambda^{\alpha\beta}, & \alpha \neq \beta, \\ \lambda^{\alpha\beta} - \frac{1}{3} \text{tr}(\bar{\lambda}), & \alpha = \beta. \end{cases} \end{aligned} \quad (7)$$

The first term in Eq. (7) is isotropic and the second, so-called deviatoric tensor, has null trace. These two tensorial quantities belong to orthogonal subspaces. The  $N$ -body energy contribution being a scalar magnitude, its dependence on the tensor field  $\lambda$  must be through invariants of the latter. If we only consider up to the second-order ones, these are the trace of  $\bar{S}$  (normalized), and the norm of  $\bar{D}$ , namely,

$$I_1^i = \frac{1}{\sqrt{3}} \text{tr}(\bar{\lambda}_i) = \frac{1}{\sqrt{3}} \sum_{j (\neq i)} \phi_{ij}, \quad (8)$$

$$Y_2^i = \sum_{\alpha, \beta} D_i^{\alpha\beta} D_i^{\alpha\beta} \equiv \langle \bar{D}_i | \bar{D}_i \rangle = \langle \bar{\lambda}_i | \bar{\lambda}_i \rangle - (I_1^i)^2. \quad (9)$$

Equation (9) also defines the product  $\langle \bar{D} | \bar{D} \rangle$ , further used below.

Note that the above decomposition of the tensor  $\lambda$  is independent of the lattice symmetry. However, for any particular symmetry, a set of tensors can always be found that constitutes a natural basis for expanding the physical magnitudes.

We now propose to associate the local tensor  $\lambda$  with the electronic density and we shall call this tensor the dipole electron-density tensor. If  $\phi$  in Eq. (5) is taken as the same function  $\phi$  in the electron density equation (1), we have  $I_1^i \equiv \rho_i / \sqrt{3}$ . Therefore, the above separation of  $\lambda$  in two contributions qualitatively agrees with the separation of the electron density into an  $s$ -electron-density part, modeled by the  $I_1^i$  term, and a  $d$ -electron-density part, modeled by  $Y_2^i$  plus a pair interaction contribution.

Following Harrison's remark, according to Keating,<sup>20</sup> that "an arbitrary potential energy which is suitably invariant is decomposable into parts which are separately invariant," the energy associated to a site  $i$  can be written as

$$E_i = \frac{1}{2} \sum_{j (\neq i)} V_{ij} + F(I_1^i) + G(Y_2^i), \quad (10)$$

where  $V_{ij}$  is a pair interaction term,  $F$  agrees with the many-body cohesive function of the EAM, and the new term  $G(Y_2^i)$  is a many-body shear term related to bond angles in a global (average) sense. We call this empirical expression for the energy of an ensemble of atoms the embedded-defect (ED) potential.

### B. Forces, force constants, and elastic constants

Hereafter, we assume, without loss of generality, that in Eq. (10)  $dF/dI_1^i = 0$  for the perfect lattice at equilibrium. This is a convenient choice that transforms the function  $V$  into an effective pair interaction potential.<sup>3,5</sup> In this scheme, algebraic expressions are simpler. We also take  $G(Y_2^i) = 0$  for the perfect lattice value of  $Y_2^i$  ( $= 0$  for cubic symmetry).

The crystal cohesive energy is

$$E_{\text{coh}} = U_p^i + U_N^i = \frac{1}{2} \sum_{j \neq i} V_{ij} + F_0, \quad (11)$$

where  $F_0 = F(I_1^i)$  for  $I_1^i$  calculated at the perfect-lattice configuration.

The forces on an atom can be calculated through the principle of the virtual displacements. If a crystal atom  $i$  suffers an infinitesimal displacement  $\delta \bar{x}(i)$ , the variation of the  $N$ -body term contribution to the energy near the equilibrium state results:

$$\delta U_N^i = G'_0 \delta Y_2^i, \quad (12)$$

where  $G'_0$  is the first derivative of  $G$  with respect to its argument.

Replacing the variation of  $\lambda$  in Eq. (12) as deduced in the Appendix [Eq. (A1)], and applying Eqs. (8) and (9), the force equilibrium condition at the perfect lattice state is given by

$$\sum_{k (\neq i)} V'_{ik} \bar{r}_{ik} + 8G'_0 \bar{D} \left| \sum_{k (\neq i)} \frac{\phi_{ik}}{R_{ik}} \bar{r}_{ik} \right\rangle = 0, \quad (13)$$

which is identically null for a centrosymmetric lattice.

While Eq. (13) holds for the equilibrium configuration, for computer simulation the forces at any configuration are needed. The many-body-term contribution to the force on an atom  $i$  due to the neighboring ensemble of atoms is

$$\begin{aligned} \bar{f}_{Ni} = & -\frac{1}{\sqrt{3}} \sum_{k (\neq i)} \phi'_{ik} (F'_i + F'_k) \bar{r}_{ik} \\ & - 4 \sum_{k (\neq i)} \frac{\phi_{ik}}{R_{ik}} (G'_i \bar{D}_i | \bar{r}_{ik} \rangle + G'_k \bar{D}_k | \bar{r}_{ik} \rangle). \end{aligned} \quad (14)$$

In Eqs. (13) and (14) the compact vector notation has been used, namely

$$(\bar{D} | \bar{r} \rangle)_i \equiv \sum_k D_{ik} r_k.$$

In the Appendix the expression for the many-body-terms contribution to the force constants is deduced [Eq. (A2)]. There, it can be seen that if  $F'' > 0$  and  $G' > 0$ , the Einstein eigenvalues for the many-body part of the force-constant matrix are positively defined.

The elastic constants are either deduced from the force-constant matrix or calculated by applying a uniform infinitesimal strain to the perfect lattice configuration and evaluating the corresponding change of the energy. The algebra is relatively simple if the proper symmetry tensor basis is used. For a cubic element, one obtains

$$\Omega \frac{C_{11} + 2C_{12}}{2} = \frac{1}{12} \sum_{\nu} N_{\nu} R_{\nu}^2 V''_{\nu} + \frac{1}{2} F''_0 P_1^2, \quad (15a)$$

$$\Omega \frac{C_{11} - C_{12}}{2} = \frac{1}{4} \sum_{\nu} N_{\nu} \beta_{\nu}^2 (R_{\nu}^2 V''_{\nu} - R_{\nu} V'_{\nu}) + G'_0 P_2^2, \quad (15b)$$

$$\Omega C_{44} = \frac{1}{4} \sum_{\nu} N_{\nu} \gamma_{\nu}^2 (R_{\nu}^2 V''_{\nu} - R_{\nu} V'_{\nu}) + G'_0 P_3^2, \quad (15c)$$

being

$$P_1 = \sum_{\nu} N_{\nu} R_{\nu} \phi'_{\nu} / 3,$$

$$P_2 = \sum_{\nu} [(\frac{1}{3} - \beta_{\nu}^2) 2\phi_{\nu} + \beta_{\nu}^2 R_{\nu} \phi'_{\nu}] N_{\nu},$$

$$P_3 = \sum_{\nu} [(\frac{1}{3} - \gamma_{\nu}^2) 2\phi_{\nu} + \gamma_{\nu}^2 R_{\nu} \phi'_{\nu}] N_{\nu},$$

where  $\Omega$  is the atomic volume,  $\nu$  is a shell index,  $N_{\nu}$  is the number of atoms in shell  $\nu$ , and  $\beta_{\nu}^2$  and  $\gamma_{\nu}^2$  are cubic symmetry-shell-related fractions (see the Appendix). The first terms of the above expressions are the effective pair contributions, whereas the second terms are the many-body contributions. Further details on deriving Eq. (15) are given in the Appendix. Note that the term  $G$ , as expected, only contributes to shear modes. Also the many-body-terms contribution to the crystal shear and bulk elasticity appear clearly separated.

Within the above scheme to the Cauchy pressure<sup>3</sup> re-

sults

$$P_c = \frac{(C_{12} - C_{44})}{2} = \frac{1}{6\Omega} [F''_0 P_1^2 - G'_0 (2P_2^2 + 3P_3^2)] . \quad (16)$$

As on physical grounds  $F''$  is expected to be positive for the equilibrium lattice configuration (also  $F'' < 0$  for the equilibrium lattice would imply a maximum in the many-body contribution to the energy), it is clear from Eq. (16) why simple EAM schemes, where the term  $G$  is not included ( $G' = 0$  and  $F'' > 0$ ), are not suited in cases in which experimentally  $P_c < 0$ .

### III. VACANCY FORMATION ENERGY IN A bcc LATTICE

As the vacancy formation energy will be used in the next section for fitting the interatomic potentials, we deduce the expression here. From Eq. (10), the formation energy of a vacancy at site 0 in an unrelaxed lattice is given by

$$E_f^v = -\frac{1}{2} \sum_{i \neq 0} V_{0i} + \sum_{i \neq 0} [F(I_{1d}^i) - F(I_{1p}^i) + G(Y_{2d}^i) - G(Y_{2p}^i)] , \quad (17)$$

where  $I_{1d}^i, I_{1p}^i$  and  $Y_{2d}^i, Y_{2p}^i$  correspond to the values of  $I_1^i$  and  $Y_2^i$  at the defect and perfect lattice, respectively. A finite range is generally assumed for the function  $\phi$ ; for example, FS (Ref. 3) took a second-neighbor range. For that range the formation energy of the vacancy (17) in a bcc lattice results in the following expression:

$$E_f^v = -\frac{1}{2} \sum_{i \neq 0} V_{0i} + \left[ 8F \left[ \frac{7\phi_1 + 6\phi_2}{\sqrt{3}} \right] + 6F \left[ \frac{8\phi_1 + 5\phi_2}{\sqrt{3}} \right] - 14F \left[ \frac{8\phi_1 + 6\phi_2}{\sqrt{3}} \right] \right] + 8G \left( \frac{2}{3}\phi_1^2 \right) + 6G \left( \frac{2}{3}\phi_2^2 \right) , \quad (18)$$

where the pair (term  $V_{0i}$ ) and many-body contributions are explicitly shown.  $\phi_1$  and  $\phi_2$  stand, respectively, for the values of  $\phi$  at first- and second-neighbor distance. If we assume the differences between perfect and defect values for the arguments,  $I_1$  and  $Y_2$  of the many-body functions to be small, Eq. (12) can be consistently applied. This implies that the formation energy can be obtained by varying the perfect lattice energy as

$$E_f^v = -\frac{1}{2} \sum_v N_v V_v + \frac{1}{3} \left[ \frac{F''_0}{2} + 2G'_0 \right] \sum_v N_v \phi_v^2 . \quad (19)$$

Here the subscript 0 stands for the perfect lattice configuration. Equation (19) will be used in Sec. IV as a first-order approximation, i.e., previous to lattice relaxation, for the fitting of the potential to the vacancy formation energy.

The unrelaxed lattice Kanzaki forces,<sup>15</sup> i.e., the forces induced onto an atom of an otherwise perfect lattice by

creating a vacant site, can be deduced either from Eq. (17) or Eq. (19). It is interesting to realize that if, for example, a second-neighbor interaction range is assumed for the function  $\phi$  in a bcc lattice, the forces on atoms at the unrelaxed perfect lattice configuration reach the sixth-neighbor shell around the vacancy. Also the lattice symmetry imposes those forces to be generally radial (towards or away from the origin at the vacant site) except for the (311) shell. A further study of the vacancy relaxation will be included in a forthcoming paper.

### IV. INTERATOMIC POTENTIAL FOR TRANSITION METALS

#### A. Fitting procedure

In this section we develop a scheme to construct the potential outlined in the preceding sections, and treat below the cases of Nb, Fe, and Cr. The parameters to be fitted are cohesive energy  $E_{\text{coh}}$ , lattice constant  $a$ , elastic constants  $C_{11}, C_{12}, C_{44}$ , and the vacancy formation energy  $E_f^v$ .

The cohesive energy is fitted to the Rose *et al.*<sup>21</sup> universal expression as a function of the first-neighbor distance  $R_1$ ,

$$\frac{E(\bar{a})}{E_{\text{coh}}} = -(1 + \bar{a}) \exp(-\bar{a}) , \quad (20)$$

where  $\bar{a} = \alpha(R_1/R_{1e} - 1)$ ,  $R_{1e}$  being the equilibrium value of  $R_1$  and  $\alpha^2 = 9\Omega B/E_{\text{coh}}$ , where  $\Omega$  is atomic volume and  $B$  the bulk modulus. Once the pair function has been fixed, this equation is used to extend the range of the embedding function beyond the vicinity of the equilibrium state.

The condition of zero pressure at the equilibrium lattice constant results in the simple equation

$$\sum_v N_v R_v V'_v = 0 , \quad (21)$$

where  $F'_0 = 0$ ; only the effective pair interaction term is involved.

For the vacancy formation energy we use Eq. (19) as a zeroth-order approximation but the calculated value is fitted to the experimental one by allowing for the relaxation of the lattice configuration.

The problem of finding an appropriate interatomic potential is reduced to satisfy the system of equations formed by (i) Eqs. (15) (three equations for the eigenvalues of the matrix of elastic constants), (ii) Eq. (20) for the lattice cohesive energy, (iii) Eq. (21) for null pressure at the equilibrium lattice configuration, and (iv) Eq. (19) for the vacancy-formation energy. This constitutes a system of six equations. For fitting an interatomic potential to the above equations we have to find somewhat arbitrary functions for the different-term contributions. To obtain the dipole electron-density tensor  $\lambda$ , we must choose an expression for the function  $\phi$ . For this purpose, we select a simple Thomas-Fermi screening function,

$$\phi = \left[ \exp \left[ -\beta \frac{r}{r_{1e}} \right] \right] / \left[ \frac{r}{r_{1e}} \right]. \quad (22)$$

With electronic calculations that consistently predict a range of  $\beta$  between 4 and 5, we have fixed the value at 5. We find minor variations between predicted values of  $\beta$  are not critical to the fitting scheme.

For the pair part of the interaction we propose a polynomial form,

$$V(x) = \begin{cases} (x-d)^2(a_3x^3 + a_2x^2 + a_1x + a_0), & x \leq d, \\ 0, & x > d, \end{cases} \quad (23)$$

where  $x = R/R_{1e}$ ,  $R$  being the distance between atom positions and  $d$  a cutoff parameter. For a fixed value of  $d$  Eq. (23) leaves four unknowns free for fitting material properties. The remaining unknowns to be fitted come from the many-body part of the ED potential, Eq. (10). Those are  $F_0$ ,  $F_0'$ , and  $G_0'$ . It can be seen that  $F_0$  is solely determined by the cohesive energy. On physical grounds we must impose  $F'' > 0$  at the equilibrium configuration. Also, in order to avoid possible instabilities, we shall require that  $G_0' > 0$ . Even within those restrictions the above seven quantities are only required to fit six equations. Therefore one parameter remains to be determined. One of the main advantages of the EAM type of potentials is that they can be accommodated to model the local electronic charge distribution in the neighborhood of a lattice defect; we choose this parameter to be the many-body contribution to the unrelaxed vacancy-formation energy. We define this as a positive fraction,

$$\xi = \frac{\frac{1}{3}(F_0''/2 + 2G_0') \sum_v N_v \phi_v^2}{E_f^y}. \quad (24)$$

The variable  $\xi$  can also be taken as a measure of the relative contributions of the many-body terms to the bulk modulus  $(c_{11} + 2c_{12})/3$ , to the shear mode  $(c_{11} - c_{12})/2$ , and to the shear mode  $c_{44}$ . Those contributions will be called  $\theta_1$ ,  $\theta_2$ , and  $\theta_3$  respectively.

### B. Interatomic potentials for Nb, Fe, and Cr

As an application of the theory and procedure developed above, the interatomic potentials for Nb, Fe, and Cr are computed. First, the matrix  $\lambda$  is fixed by  $\phi$ , the Thomas-Fermi function,<sup>22</sup> and the lattice symmetry (the electron density  $\rho$  is normalized to the equilibrium value). Then a given value of  $\xi$  is selected; for the time being this value is arbitrarily chosen by an educated guess. The feasible values are restricted by constraining the relative contribution of the many-body terms to the elastic constants to be a positive fraction.

Once  $\xi$  has been selected, an appropriate effective potential pair potential can be determined. This should satisfy the system of equations discussed in the preceding section. Also, the pair part of the interaction plus the many-body function  $F$  must satisfy the Rose *et al.* expression [Eq. (20)], while the second derivative of  $F$  at equilibrium is constrained to give the correct bulk modulus.

For  $G$  we shall choose here a straight line through the origin with  $G' > 0$ . In turn, this implies that the potentials fitted below can be considered as a first-order expansion of the EAM with respect to a many-body angular term  $Y_2^i$ .

For Fe and Nb we fit a simple EAM potential and our ED potential, which includes the linear term  $G$ . As discussed above, for Cr, a metal with a negative Cauchy pressure, only ED is able to provide a fitting to the measured elastic constants. Therefore, only an ED potential is reported for Cr. The ED effective pair functions are shown in Fig. 1, whereas the experimental values used for the fitting are reported in Table I, and the parameters defining the above functions are given in Table II for the three metals. Those experimental values are exactly reproduced by the different potentials reported in Table II (with small deviations in the relaxed vacancy-formation energy). The calculated difference in cohesive energy with respect to the fcc phase is reported also. The fcc phase is metastable under the corresponding potential; its first-neighbor distance, relative to the one of the bcc phase, is also given. As already pointed out by Johnson and Oh,<sup>12</sup> the stability of the bcc lattice with respect to the fcc one is mainly determined by the pair part of the potential. bcc stability is favored, for instance, if the pair function remains relatively flat between first and second neighbors.

All potentials are fitted to provide the largest possible difference in energy between the bcc and fcc lattice. This procedure implies that other material properties could also have been fitted (within certain limits) while keeping the relative stability of the bcc lattice. In that respect the potential parameters reported in Table II should be taken as preliminary and further development is forthcoming.

For the case of Cr we find that imposing the function and its first derivative to be null at the end of the range, forces a small positive value of  $V$  between the second and third neighbors. This feature helps the stability of the bcc lattice against the fcc one. However a shorter-range potential, obtained by suppressing any pair interaction beyond the second-neighbor distance, can also be fitted to determine a stable bcc lattice. Therefore the results for this second, shorter-range potential for Cr are also re-

TABLE I. Fitted experimental values.

	Cr	Fe	Nb
$\Omega$ (Å <sup>3</sup> )	12.00	11.78	17.98
$E_{\text{coh}}$ (eV)	4.10 <sup>a</sup>	4.28 <sup>a</sup>	7.57 <sup>a</sup>
$E_f^y$ (eV)	1.2 <sup>b</sup>	1.79 <sup>c</sup>	2.04 <sup>b</sup>
$C_{11}$ (eV/Å <sup>3</sup> )	2.215 <sup>d</sup>	1.510 <sup>e</sup>	1.536 <sup>e</sup>
$C_{12}$ (eV/Å <sup>3</sup> )	0.443 <sup>d</sup>	0.914 <sup>e</sup>	0.836 <sup>e</sup>
$C_{44}$ (eV/Å <sup>3</sup> )	0.630 <sup>d</sup>	0.699 <sup>e</sup>	0.179 <sup>e</sup>

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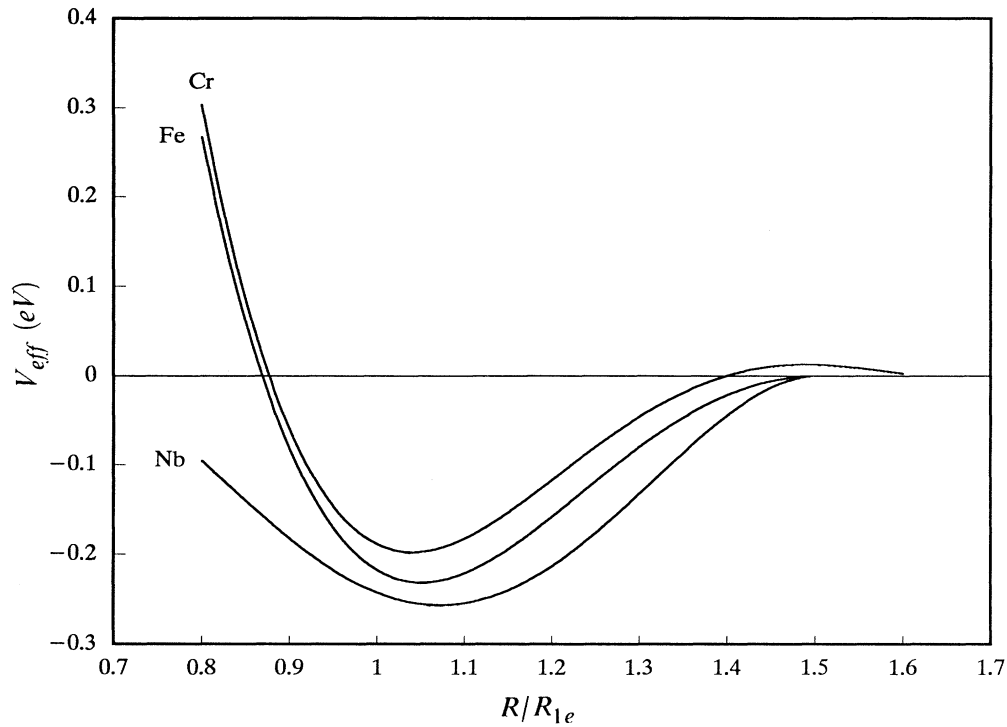


FIG. 1. ED effective pair potentials for Cr, Fe, and Nb.

ported in Table II.

If for a feasible value of  $\xi$  it turns out to be  $G'_0=0$ , then our potentials should be equivalent to a simple EAM. This is the case indeed for Fe and Nb. The effective pair functions so obtained are drawn in Figs. 2 and 3, respectively, together with the corresponding functions of FS.<sup>3</sup> It is seen that the agreement is good, particularly for Fe. The differences may be attributed to higher

values of the unrelaxed vacancy-formation energy used in Ref. 3, namely 2.05 and 2.64 eV for Fe and Nb, respectively.

## V. CONCLUSIONS

In this paper, we have extended the EAM interatomic potential<sup>3-5</sup> by expressing the energy of an ensemble of

TABLE II. Potential parameters for Cr, Fe, and Nb.

	Cr	ED	Nb	Fe	EAM
		Fe			Nb
$a_3$	-0.2795 90	0.481 147	-0.686 114 0	0.308 839 2	28.981 68
$a_2$	10.012 28	5.116 408	-5.709 385	12.583 42	-92.165 65
$a_1$	-21.668 08	-17.445 40	8.803 652	-33.674 37	90.006 36
$a_0$	11.498 81	10.980 53	-2.656 076	19.694 71	-27.989 78
$d$	165; 1.4	1.5	1.5	1.5	1.5
$\xi$	0.2	0.2	0.2	0.012	0.048
$\theta_1$	0.061 5	0.436 7	0.771 3	0.193 4	0.614 6
$\theta_2$	$6.34 \times 10^{-4}$	$2.04 \times 10^{-3}$	$3.19 \times 10^{-4}$	0.0	0.0
$\theta_3$	0.397	0.387	0.934	0.0	0.0
$F''_0$	47.73	716.6	1856	317.4	1479
$G'_0$	1081	1147	1083	0.0	0.0
$E_f^{ya}$ (eV)	1.5	1.8	2.1	1.8	2.1
$E_f^{yb}$ (eV)	1.5; 1.3	1.7	2.1	1.6	2.0
$E_{fcc}$ (eV)	4.05; 4.08	4.22	7.43	4.24	7.44
$r_{fcc}/r_{bcc}$	103; 1.04	1.035	1.025	1.04	1.04

<sup>a</sup>Unrelaxed.

<sup>b</sup>After relaxation.

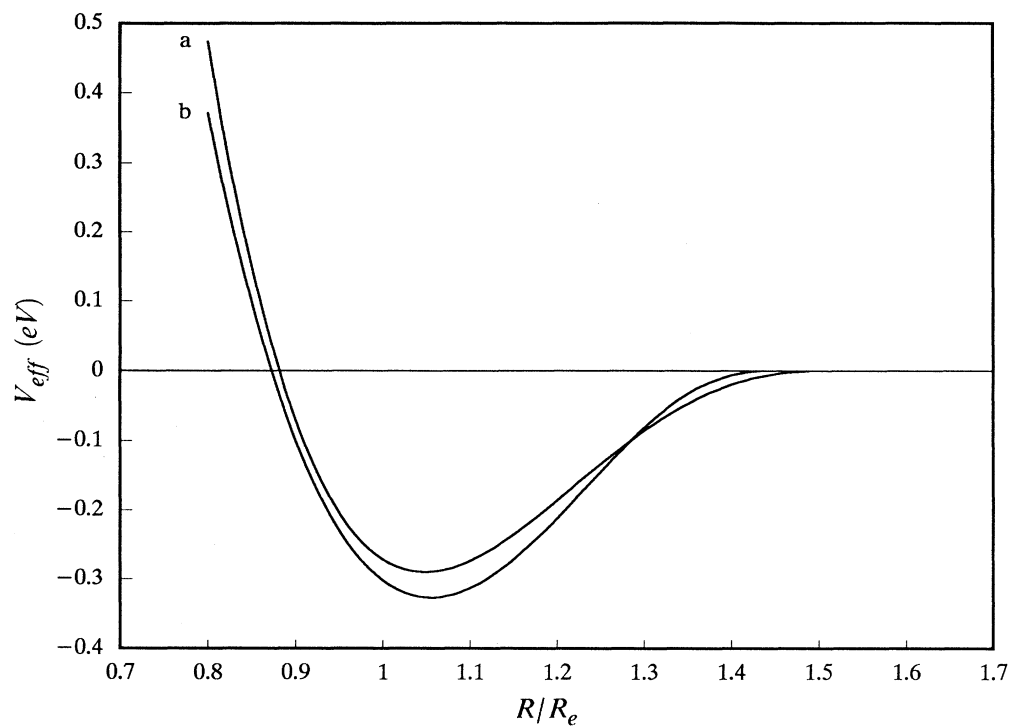


FIG. 2. EAM effective pair potential for Fe: (a) this work (b) from Ref. 3.

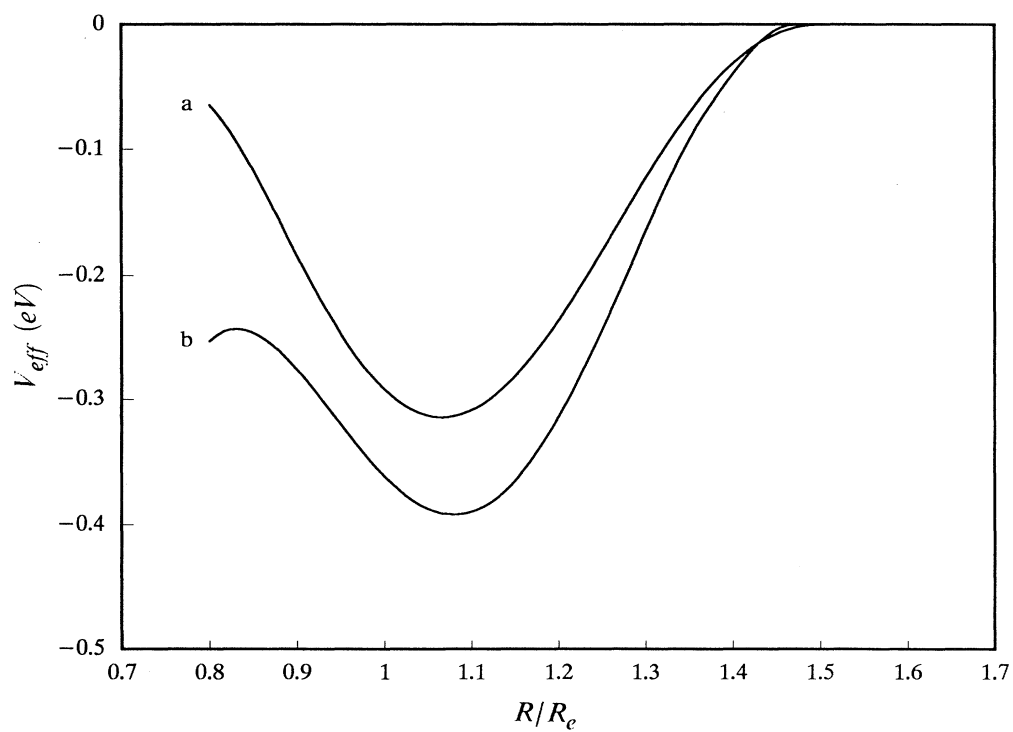


FIG. 3. EAM effective pair potential for Nb: (a) this work (b) from Ref. 3.

atoms as the addition of a pair and a many-body function, already included in the EAM plus a new term, a function  $G$  in Eq. (10). This term introduces many-body contributions to the shear elastic moduli, which in the EAM are fitted only by the effective pair interaction contribution. We consider each lattice atom to be embedded in an effective continuum host. The embedding is obtained as perturbation of the perfect lattice electron density. By arguments based on the theory of point defects, the source of distortion is simulated by a set of forces on neighbor atomic locations. This allows the electron density and distribution to be related to a tensor parameter, called above the dipole electron-density tensor. The approach provides, therefore, a simple way of introducing many-body angle-dependent forces within the EAM spirit. Recognizing the basis of the model, we have called the empirical potential obtained above the embedded defect (ED) potential.

The idea of including angular force many-body terms into an empirical extension of the EAM was previously developed by us in Ref. 10. There, we found that the elastic constants of cubic lattices could be used to fit a many-body empirical potential with no pair-term contribution. In the case of cubic symmetry defects  $\langle \bar{\lambda} | \bar{\lambda} \rangle$  can be expanded in its cubic symmetry invariants and a separate function can be assigned to each. Consistent with that idea, in Ref. 10, we proposed three different many-body terms in the energy: the term  $F$  already used in the EAM, and two new ones,  $H$  and  $G$ . Both of them are connected with shear modes of the lattice but each one depends on different cubic symmetry components of the density tensor  $\lambda$ . These shear contributions proved to be relevant to the simulation of the static configuration of an octahedral interstitial. However the arguments of those functions are not invariants for a distorted lattice whenever a lattice atom or a defect separates from the cubic symmetry. As said above, in the ED potential we include the pair and many-body term  $F$  of the EAM plus a function  $G$  in Eq. (10), which accounts for the many-body contribution to the energy of "shearing" the lattice. The arguments of  $F$  and  $G$  are, respectively, the trace and an invariant related to the deviatoric part of  $\lambda$ . These two functions are fully rotational invariant and not related therefore to any lattice symmetry. We expect the many-body function  $G$  to be mainly determined by the  $d$ -electron contribution to lattice cohesion. To reinforce that expectation, we want to stress that the tensor  $\bar{D}$  of Eq. (7) can be decomposed into a five tensor basis, where each tensor keeps the symmetry of a  $d$  orbital. We have obtained very simple relations between physical measured quantities and the functions used both in the EAM and in ED. In the scheme presented above for generating the ED potential, all elastic constants can be fitted without some of the drawbacks that appear in the classical EAM. Particularly, the physical condition of positive curvature of the embedding function  $F$  is preserved, which would not be the case within the EAM for lattices with negative Cauchy pressure (this being the case of Cr and the reason why Johnson and Oh<sup>12</sup> failed to fit an appropriate EAM potential to this metal). As reported in the literature<sup>11</sup> and summarized in Sec. I, several properties of transition

metals show departures from a central force field, among those the negative value of the Cauchy discrepancy in Cr. In that  $d$ -band metal, Finnis *et al.*<sup>22</sup> claim that the many-body part of the EAM should stand mainly for the difference between the sum of one-electron energies resulting from embedding the atom into the jellium with respect to creating a vacancy plus a free atom, while in an  $s$ -band solid the main contribution should come from the embedding energy of the atom in a jellium. This implies in turn that the expression for the many-body term should not necessarily agree in both metals. Therefore the ED potential is expected to be particularly useful for calculating perfect lattice properties and computer simulating defects in transition metals.

We shall now comment on the fitting of the interatomic potentials to Nb, Fe, and Cr. It can be seen in Table II that, for ED, the many-body-term contribution to the shear elastic constants ( $\theta_2$  and  $\theta_3$  fractions) is nearly null for  $(c_{11} - c_{12})/2$ , while it is relatively important for  $c_{44}$ . This latter,  $\theta_3$  seems to be the largest for Nb, the metal with the largest value for the Cauchy pressure. However, for Fe or Nb we cannot claim that ED should in principle provide any better potential than the EAM. Finally, we want to stress that if  $G'$  is taken as null for the ED interatomic potentials reported here, then they have the characteristics of an EAM potential for which the experimental elastic constants are those reported in Table I, except for the shear constants  $(c_{11} - c_{44})/2$  and  $c_{44}$ ; fractions  $\theta_2$  and  $\theta_3$  have to be subtracted, respectively, to get the proper values.

Our scheme for fitting the potential energy provides a nice way not only of expanding the elastic and force constants but also of differentiating between the many-body-terms contribution to the cohesive energy and vacancy formation energy. Our definition of the parameter  $\xi$ , Eq. (24), implies that the cohesive energy and the formation energy for the vacancy are approximately related by

$$E_{\text{coh}} \simeq E_f^v(1 - \xi) + F_0. \quad (25)$$

Equation (25) shows that the difference between cohesive energy and vacancy formation energy is given by the many-body contribution to cohesion  $F_0$ , and to the vacancy formation energy  $\xi E_f^v$ . Also, within the procedure previously discussed, the many-body terms contribution to the elastic constants depends solely on the parameter  $\xi$ .

For fitting pure covalent bonds, like those of Si and Ge, materials that also show a negative value for the Cauchy pressure, Baskes *et al.*<sup>8,9</sup> developed a modified embedded-atom method (MEAM). Those authors assumed an electron density that includes angular term contributions as an argument of the many-body function  $F$  of the EAM. Baskes<sup>8</sup> adopted in his paper an angular expansion of the electron density that is further extended by Baskes *et al.*<sup>9</sup> in Eq. (14) in their paper. It is interesting to realize that Baskes's<sup>8</sup> expression for the electron density reduces to

$$\rho_i = aI_1^i + bY_2^i, \quad (26)$$

where  $I_1$  and  $Y_2$  are the invariants of the dipole density



tensor  $\lambda$  in Eq. (6). Baskes<sup>8</sup> fit the electron density to theoretical calculations, which is equivalent to finding a value for the ratio  $a/b$  in Eq. (26). Therefore, his model is quite equivalent to ours. Essentially, both models fix independent many-body contributions to the force on a lattice atom. We model separately the many-body contribution to an angular dependent energy from the one due to local-density changes, which allows for a clear relationship between potential parameters and experimental quantities. On the other hand, Baskes *et al.*<sup>9</sup> included new terms in their density function with respect to the one of Baskes;<sup>8</sup> this might, in turn, allow properties of the lattice not accessible to our potential to fit.

#### ACKNOWLEDGMENTS

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#### APPENDIX: FORCE, FORCE CONSTANTS, AND ELASTIC CONSTANTS CALCULATIONS

Forces on a lattice atom and force constants are obtained by expanding the cohesive energy with respect to the virtual displacements of the atomic coordinates. Under such virtual displacement, the corresponding variation of the tensor  $\lambda$  at a lattice point  $k$ , Eq. (6), is

$$\begin{aligned} \delta\bar{\lambda}_k &= \sum_m \delta\psi_{km} (\bar{R}_{km} \otimes \bar{R}_{km}) \\ &+ \sum_m \psi_{km} (\delta\bar{R}_{km} \otimes \bar{R}_{km} + \bar{R}_{km} \otimes \delta\bar{R}_{km}) \\ &+ \sum_m \psi_{km} (\delta\bar{R}_{km} \otimes \delta\bar{R}_{km}), \end{aligned} \quad (\text{A1})$$

where

$$\psi(R_{ij}) = \frac{K(R_{ij})}{R_{ij}} = \frac{\phi(R_{ij})}{R_{ij}^2}.$$

$K(R_{ij})$  is the module of the pseudo-Kanzaki force in Eq. (5), and

$$\begin{aligned} \delta\psi_{km} &= \psi'_{km} \langle \bar{r}_{km} | \delta\bar{R}_{km} \rangle + \frac{1}{2} \left[ \psi''_{km} - \frac{\psi'_{km}}{R_{km}} \right] \langle \bar{r}_{km} | \delta\bar{R}_{km} \rangle^2 \\ &+ \frac{1}{2} \frac{\psi'_{km}}{R_{km}} \langle \delta\bar{R}_{km} | \delta\bar{R}_{km} \rangle. \end{aligned}$$

In Eq. (A1) either a  $k$  or  $m$  atom coordinate must have imposed a virtual variation  $\delta\bar{x}$  for a given term  $km$  to be non-null. The force on an atom, Eq. (13), is obtained by replacing the above variation of  $\lambda$  in the corresponding terms of Eq. (12).

The derivation of the force constants for the ED potential energy (10) is straightforward. For a given component  $\alpha\beta$  that relates an atom  $i$  with an atom  $j$ , the corresponding variations in the atomic coordinates must be imposed and the energy change calculated. The general result is, however, cumbersome. For a cubic symmetry lattice at equilibrium, the many-body contributions are given by

$$\begin{aligned} \frac{1}{2}\chi_{ii}^{\alpha\beta} &= \delta^{\alpha\beta} \left[ \frac{1}{9} \left( \frac{F''_0}{2} + 2G'_0 \right) \sum_v N_v (\phi'_v)^2 + \frac{4}{3} G'_0 \sum_v N_v R_v^2 \psi_v^2 \right], \\ \chi_{ij}^{\alpha\beta} &= \delta^{\alpha\beta} 4G'_0 \sum_{k(\neq ij)} \psi_{ik} \psi_{jk} \langle \bar{R}_{ik} | \bar{R}_{jk} \rangle + \sum_{k(\neq ij)} r_{ij}^{\alpha} r_{jk}^{\beta} \left[ \frac{2}{3} \phi'_{ik} \phi'_{jk} \left( \frac{F''_0}{2} - 2G'_0 \right) + 2G'_0 \psi'_{ik} \psi'_{jk} \langle \bar{R}_{ik} | \bar{R}_{jk} \rangle^2 \right] \\ &+ 4G'_0 \sum_{k(\neq ij)} \langle \bar{R}_{ik} | \bar{R}_{jk} \rangle (r_{ik}^{\alpha} r_{jk}^{\beta} \psi'_{ik} \psi_{jk} R_{ik} + r_{jk}^{\alpha} r_{ik}^{\beta} \psi'_{jk} \psi_{ik} R_{jk}), \end{aligned} \quad (\text{A2})$$

where the  $i, j, k$  indexes stand for atomic positions and the Greek indexes for Cartesian components.

We said in the main text that the fitting of interatomic potentials to experimental elastic constants can be simplified by using an appropriate tensor base (see, for instance, Ref. 23). For cubic symmetry such a base (normalized) can be written as

$$\begin{aligned} A_g: \quad \bar{A} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \frac{1}{\sqrt{3}}; \\ E_g: \quad \bar{B}_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \frac{1}{\sqrt{6}}, \quad \bar{B}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}}; \\ T_{2g}: \quad \bar{C}_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}}, \quad \bar{C}_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}}, \quad \bar{C}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}}. \end{aligned} \quad (\text{A3})$$

The above tensors span nonequivalent irreducible representations of the cubic group  $O_h$ , indicated by the appropriate symbols at the left in (A3).<sup>24</sup> Therefore, the tensors (A1) are eigenvectors of the elastic constants matrix  $C_{ijkl}$ , with eigenvalues (in Voigt's notation):  $(c_{11} + 2c_{12}), (c_{11} - c_{12}), 2c_{44}$ .

The strain tensor may be expanded as

$$\bar{\epsilon} = a\bar{A} + \sum_{i=1}^2 b_i\bar{B}_i + \sum_{i=1}^3 c_i\bar{C}_i, \quad (\text{A4})$$

resulting in the elastic energy density,

$$U_{el} = \frac{C_{11} + 2C_{12}}{2} a^2 + \frac{C_{11} - C_{12}}{2} \sum_i b_i^2 + C_{44} \sum_i c_i^2, \quad (\text{A5})$$

where

$$I_1(\bar{\epsilon}) = a, \\ Y_2(\bar{\epsilon}) = \sum_{i=1}^2 b_i^2 + \sum_{i=1}^3 c_i^2.$$

In order to find the expression for the elastic constants, we must now expand the ED energy, Eq. (10), for a uniform lattice deformation (A4), i.e., the atomic positions change by

$$\delta\bar{R} = \bar{\epsilon} \cdot \bar{R}, \quad (\text{A6})$$

while the tensor  $\lambda$  varies by

$$\delta\bar{\lambda} = \left[ \sum_{\nu} \frac{2}{3} N_{\nu} \phi_{\nu} \right] \bar{\epsilon} + \sum_{\nu} R_{\nu}^3 \psi'_{\nu} \bar{\epsilon} \cdot \sum_{j \in \nu} (\bar{r}_j \otimes \bar{r}_j) \otimes (\bar{r}_j \otimes \bar{r}_j). \quad (\text{A7})$$

In the base (A3), Eq. (A7) is expanded as

$$\delta\bar{\lambda} = \frac{1}{3} \left[ \sum_{\nu} N_{\nu} R_{\nu} \phi'_{\nu} \right] a\bar{A} \\ + \left[ \sum_{\nu} \frac{2}{3} N_{\nu} \phi_{\nu} + \sum_{\nu} N_{\nu} R_{\nu}^3 \psi'_{\nu} \beta_{\nu}^2 \right] \sum_{i=1}^2 b_i \bar{B}_i \\ + \left[ \sum_{\nu} \frac{2}{3} N_{\nu} \phi_{\nu} + \sum_{\nu} N_{\nu} R_{\nu}^3 \psi'_{\nu} \gamma_{\nu}^2 \right] \sum_{i=1}^3 c_i \bar{C}_i, \quad (\text{A8})$$

where

$$\beta_{\nu}^2 = \frac{1}{6} [(r_x^2 - r_y^2)^2 + (r_x^2 - r_z^2)^2 + (r_y^2 - r_z^2)^2]_{\nu}, \\ \gamma_{\nu}^2 = \frac{2}{3} [(r_x r_y)^2 + (r_x r_z)^2 + (r_y r_z)^2]_{\nu}.$$

$r_x, r_y, r_z$  in (A8) are the Cartesian components of a unit vector pointing to an atom at the  $\nu$ th shell of neighbors. Note that the following relation holds:

$$\beta_{\nu}^2 + \frac{3}{2} \gamma_{\nu}^2 = \frac{1}{3}.$$

(A8) can be replaced in Eq. (12) and the many-body contribution to the elastic constants (15) may be obtained by comparison with (A5). On the other hand, the pair interaction contribution agrees with the standard one reported in the literature.<sup>23</sup>

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