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A simple empirical N-body potential for transition metals

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ABSTRACT

A simple form of multi-ion interaction has been constructed for the purpose of atomistic simulation of transition metals. The model energy consists of a bonding term, which is the square-root of a site density ρ_i , summed over atoms i , and a repulsive pairwise term of the form $\sum_{ij} \frac{1}{2} V(R_{ij})$. The site density ρ_i is defined as a sum over neighbouring sites j of a cohesive potential $\phi(R_{ij})$. Both V and ϕ are assumed to be short-ranged and are parameterized to fit the lattice constant, cohesive energy and elastic moduli of the seven body-centred-cubic (b.c.c.) transition metals. The result is a simple model which, unlike a pair-potential model, can account for experimental vacancy-formation energies and does not require an externally applied pressure to balance the 'Cauchy pressure'.

§ 1. INTRODUCTION

The use of pair-potentials for describing the energetics of transition metals has, until recently, been the only way to attempt to simulate defects such as dislocations, grain boundaries and cracks. Although the pair-potential description has no theoretical foundation, it can still be useful for generating qualitative information, such as the possible local configurations of atoms (Maeda, Vitek and Sutton 1982). However, even at a practical level the pair-potential model has drawbacks. For example, unless the elastic constants in a cubic crystal satisfy the Cauchy relation $C_{12} = C_{44}$, which is seldom the case in real metals, an equilibrium pair-potential model cannot reproduce them. It is customary to deal with this problem by adding to the pair-potential in the total energy a term which depends on the macroscopic volume of the crystal (Maeda *et al.* 1982), by analogy with simple-metal perturbation theory. The elastic constants can then be adjusted arbitrarily at equilibrium because the volume-dependent term supplies a fictitious external pressure to balance the so-called Cauchy pressure, $\frac{1}{2}(C_{12} - C_{44})$. However, the introduction of the macroscopic volume as a variable in the total energy leads to the familiar paradox that the bulk modulus calculated by the method of long waves (constant volume) differs from its value calculated by homogeneous deformation, unless the volume-dependent term is linear in volume. In general, internal distortions of the crystal which leave its surface fixed do not involve this volume-dependent term, which enters only when the surface of the crystal is displaced. The difficulty becomes acute when we contemplate the simulation of internal cavities or cracks within a metal, and one may consider the application of special surface forces as unsatisfactory in principle.

A second shortcoming of the pair-potential description is related to the first. If we resign ourselves to a model without surface forces, and accept $C_{12} = C_{44}$, the vacancy formation energy is always found to be about equal to the cohesive energy. Experimentally (see table 2) it is about one-third of the cohesive energy (table 1). Even at a qualitative level we may suspect that such a gross misrepresentation of the cohesive properties might not allow us to simulate even some qualitative aspects of crack-tip opening or vacancy clustering, which we would like to explore with a wide range of possible potentials.

Table 1. Experimental quantities to be fitted.

	a Å	u_{tot}^\dagger (eV)	C_{11}^\ddagger	C_{12}	C_{44} (10^{11} Pa)	C'	B	P_c
Vanadium	3.0399	5.31	2.279	1.187	0.426	0.546	1.551	0.3805
Niobium	3.3008	7.57	2.466	1.332	0.281	0.567	1.710	0.5255
Tantalum	3.3058	8.10	2.660	1.612	0.824	0.524	1.961	0.394
Chromium	2.8845	4.10	3.871	1.035	1.008	1.418	1.980	0.0135
Molybdenum	3.1472	6.82	4.647	1.615	1.089	1.516	2.626	0.263
Tungsten	3.1652	8.90	5.224	2.044	1.606	1.590	3.104	0.219
Iron	2.8665	4.28	1.519	0.862	0.762	0.3285	1.081	0.050

† Cohesive energies, u_{tot} , are taken from table 3 of Kittel (1976).

‡ Elastic constants are from the compilation in Bujard (1982) except for iron, which are taken from Rayne and Chandrasekhar (1961).

The solution we propose here is to incorporate in a simple model the essential band character of metallic cohesion. The simplest expression of band character is in the second-moment approximation to the tight-binding model, in which the cohesive energy per atom varies as \sqrt{z} , where z is the atomic coordination which can range from one (diatomic molecule) to about 12 (f.c.c. crystal). This difference to the pair-potential model explains the low value of vacancy formation energies, and we build it into the present model. (Carlsson and Ashcroft (1983) discuss these points in more detail.)

§ 2. THE MODEL

We write the total energy of an assembly of atoms at positions $\{\mathbf{R}_i\}$ as

$$U_{\text{tot}} = U_N + U_P. \quad (1)$$

U_N is the N -body term and U_P is a conventional central pair-potential summation. We proceed in a purely empirical way to write U_N as a sum over all atoms of a 'cohesive function', as follows:

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

where

$$\rho_i = \sum_j \phi(R_{ij}), \quad (3)$$

$$R_{ij} = |\mathbf{R}_{ij}| = |\mathbf{R}_j - \mathbf{R}_i|,$$

	Fitting parameters			Calculated		Experimental		Semi-empirical
	d (Å) A (eV) β	c (Å) c_0 c_1 c_2	E_v^t (eV)	γ_{100} (mJ m ⁻²) [†]	E_v^t	$\gamma_t^†$		
Vanadium	3.692767 2.010637 0	3.80 -0.8816318 1.4907756 -0.3976370	1.97	1761			2600	
Niobium	3.915354 3.013789 0	4.20 -1.5640104 2.0055779 -0.4663764	2.64	2046 (2380)	2.04	2300	2700	
Tantalum	4.076980 2.591061 0	4.20 1.2157373 0.0271471 -0.1217350	3.13	2345 (2540)	2.90	2780	3050	
Chromium	3.915720 1.453418 1.8	2.90 29.1429813 -23.3975027 4.7578297	1.97	1780	1.20	2200	2400	
Molybdenum	4.114825 1.887117 0	3.25 43.4475218 -31.9332978 6.0804249	2.58	2112 (2220)	2.24	2200	2950	
Tungsten	4.400224 1.896373 0	3.25 47.1346499 -33.7665655 6.2541999	3.71	2926 (2800)	3.15	2800	3300	
Iron	3.699579 1.889846 1.8	3.4 1.2110601 -0.7510840 0.1380773	1.77	1693	1.79	2200	2500	

† The experimental E_v^t are from the compilation of Górecki (1974) except for iron, which is from De Schepper *et al.* (1983).
 ‡ The experimental γ and semi-empirical γ_{100} are from Miedema (1978). The calculated γ_{100} in parentheses are due to Desjonquères and Cyrot-Lackmann (1975).

and A is a constant which we anticipate to be positive. The function ϕ will be interpreted later. Equations (2) and (3) have also been used by Daw and Baskes (1983).

We choose $f(\rho)$ to be $\sqrt{\rho}$, so as to mimic the result of tight-binding theory in which $\phi(R)$ would be interpreted as a sum of squares of overlap integrals (Masuda and Sato 1981). The remaining input to the model will be based on computational convenience and empirical fitting. The term U_P can be written as

$$U_P = \frac{1}{2} \sum_{ij} V(R_{ij}).$$

Our tight-binding interpretation is that U_N represents the band energy, which is bonding in character, while U_P is a repulsive core-core interaction. However, two further physical interpretations of this form of model are possible :

- (a) ρ_i is the local electronic charge density at site i which is constructed by a rigid superposition of atomic charge densities ϕ . This was the viewpoint of Daw and Baskes (1983). The energy of the atom at site i is then assumed to be, to a first approximation, the same as if it were in a uniform electron gas of that density, for which $f(\rho)$ can be calculated and tabulated.
- (b) ρ_i is a measure of the local density of atomic sites. Equation (1) is then interpreted as the sum of a volume-dependent energy U_N and the pairwise summation U_P . In this sense the model is a prescription for defining a 'local' volume, which may be appropriate in the usual simple-metal theory (Maeda *et al.* 1983, Finnis and Sachdev 1976).

Since the present approach is empirical any or all of these interpretations could be made ; the consequences of the form of the model which we now derive, and the fitting to experimental data which follows, do not depend on the physical interpretation.

2.1. The pressure and elastic moduli

In this section we derive from the model expressions for the pressure and elastic moduli of a perfect crystal. For simplicity we shall restrict the discussion to the b.c.c. structure and for subsequent computational convenience we shall assume that the interactions ϕ and V do not extend further than the second shell of neighbours. Since we are now dealing with a crystal in which all the atoms are equivalent we can work with the energy per atom (the cohesive energy, with reversed sign) which, following eqn. (1), is

$$u_{\text{tot}} = u_N + u_P, \quad (4)$$

where

$$u_N = -Af(\rho), \quad (5)$$

$$\rho = \sum_{i \neq 0} \phi(R_i), \quad (6)$$

and

$$u_P = \frac{1}{2} \sum_{i \neq 0} V(R_i), \quad (7)$$

where the positions $\{\mathbf{R}_i\}$ are referred to an atom at the origin.

The first neighbours in the b.c.c. structure are at a distance $\sqrt{3}a/2$ and the second are at a . Restricting the ranges of ϕ and V to first and second neighbours, we introduce the notation $\phi_1 = \phi(\sqrt{3}a/2)$; $\phi_2 = \phi(a)$; $V_1 = V(\sqrt{3}a/2)$ and $V_2 = V(a)$, in order to write

$$\rho = 8\phi_1 + 6\phi_2 \quad (8)$$

and

$$u_P = 4V_1 + 3V_2. \quad (9)$$

The pressure is given by $P = -du_{\text{tot}}/d\Omega$, where Ω , the atomic volume, is given by

$$\Omega = a^3/2.$$

From eqn. (4),

$$P = P_N + P_P,$$

where $P_N = -du_N/d\Omega$ and $P_P = -du_P/d\Omega$.

By substituting eqns. (8) and (9) we find that

$$P_N = \frac{4A}{3a^2} (2\sqrt{3}\phi'_1 + 3\phi'_2)f' \quad (10)$$

and

$$P_P = \frac{-2}{3a^2} (2\sqrt{3}V'_1 + 3V'_2), \quad (11)$$

where

$$f' = \frac{1}{2}\rho^{-1/2},$$

and primes denote differentiation with respect to R .

We note that the derivatives of u_P can be obtained systematically from those of u_N by setting $f = -\frac{1}{2}\rho/A$ in place of $f = \rho^{1/2}$, and by replacing ϕ by V . We can now take the appropriate second derivatives of u_{tot} with respect to strain in order to obtain expressions for the elastic moduli. Omitting details of the derivations, the results are as follows.

For the bulk modulus,

$$B = B_N + B_P,$$

where

$$B_N = -\frac{4A}{9a^2} (3a\phi''_1 + 3a\phi''_2 - 4\sqrt{3}\phi'_1 - 6\phi'_2)f' - \frac{8A}{9a} (2\sqrt{3}\phi'_1 + 3\phi'_2)^2 f'' \quad (12)$$

and

$$B_P = \frac{2}{9a^2} (3aV''_1 + 3aV''_2 - 4\sqrt{3}V'_1 - 6V'_2). \quad (13)$$

For the rhombohedral shear modulus,

$$C_{44} = C_{44N} + C_{44P},$$

where

$$C_{44N} = -\frac{4A}{9a^2} (3a\phi''_1 + 4\sqrt{3}\phi'_1 + 9\phi'_2)f' \quad (14)$$

and

$$C_{44P} = \frac{2}{9a^2} (3aV''_1 + 4\sqrt{3}V'_1 + 9V'_2). \quad (15)$$

For the tetragonal shear modulus,

$$C' = \frac{1}{2}(C_{11} - C_{12}) = C'_N + C'_P,$$

where

$$C'_N = -\frac{2A}{3a^2} (3a\phi''_2 + 4\sqrt{3}\phi'_1 + 3\phi'_2)f' \quad (16)$$

and

$$C'_P = \frac{1}{3a^2} (3aV''_2 + 4\sqrt{3}V'_1 + 3V'_2). \quad (17)$$

In deriving these expressions we have not made use of the equilibrium condition $P = 0$.

It is interesting that the results do not differ formally from the results one would obtain from an effective central pairwise potential,

$$V_{\text{eff}}(R) = V(R) - 2A f' \phi(R), \quad (18)$$

except for the presence in B of a term in f'' . In fact we can generalize this observation: if the second and higher derivatives of f are ignored, the energy change associated with any change in configuration $\{\mathbf{R}_i\}$ can be calculated on the assumption that the atoms interact with the effective pairwise interaction V_{eff} .

For the case of vacancy formation we can easily demonstrate that it is not serious to neglect f'' because the coordination change is relatively small. To see this, suppose that the coordination of atoms neighbouring a vacancy has changed from 12 to 11 during its creation. Within our model the exact change in the total bonding energy is (in units of the cohesive energy $-A\rho^{1/2}$) $\Delta V_{\text{exact}} = 12 - 12(11/12)^{1/2}$ which in the effective pair-potential approximation becomes, by linearizing the square root $\Delta V_{\text{pairwise}} = 1/2$. The difference is only 2.2%. Nevertheless, the second derivative of f does have a significant contribution to make in the bulk modulus, eqn. (12), and it accounts for the Cauchy discrepancy which we now discuss.

2.2. The Cauchy relation

We define the Cauchy pressure as

$$P_c = \frac{1}{2}(C_{12} - C_{44}) = \frac{1}{2}(B - C_{44} - \frac{2}{3}C'). \quad (19)$$

It is well known that for a cubic crystal in equilibrium under pairwise central potentials $P_c = 0$. This is the Cauchy relation.

For the present model we obtain from the expressions of § 2.1

$$P_c = P - \frac{4A}{9a} (2\sqrt{3}\phi'_1 + 3\phi'_2)^2 f'',$$

which on applying the equilibrium condition $P = 0$ becomes

$$P_c = -\frac{4A}{9a} (2\sqrt{3}\phi'_1 + 3\phi'_2)^2 f''. \quad (20)$$

Thus it is just the term in f'' , shown in the previous section to differentiate our model from an effective pair-potential description, which provides a non-vanishing Cauchy pressure. Furthermore, assuming that A is a positive bonding energy, the square-root form of f ensures that P_c is positive, which is observed experimentally for all the b.c.c. transition metals (see table 1).

2.3. Forces and force constants

In order to perform atomistic simulations of crystals containing defects it is essential to have a rapid algorithm for calculating the force on each atom. Within the present model, the pairwise term U_p is of the conventional form and forces are calculated conventionally by summing terms of the form $V'(R)\mathbf{R}/R$. The x_α component of force on the i th atom arising from U_N is given by

$$-\frac{1}{A} \frac{\partial U_N}{\partial R_{i\alpha}} = f'_i \sum_{k \neq i} \phi'(R_{ik}) R_{ik\alpha} / R_{ik} - \sum_{k \neq i} f'_k \phi'(R_{ki}) R_{ki\alpha} / R_{ki} \\ = - \sum_{k \neq i} (f'_i + f'_k) \phi'(R_{ik}) R_{ik\alpha} / R_{ik}, \quad (21)$$

where

$$f'_i = \left. \frac{df}{d\rho} \right|_{\rho=\rho_i}$$

and

$$\mathbf{R}_{ik} = \mathbf{R}_k - \mathbf{R}_i.$$

The first term expresses the change in energy due to change in density at the site i itself as atom i moves. The second term expresses the change in energy due to the change in density at all the other sites as atom i moves. Compared to a simple pairwise expression, an extra lattice summation of ϕ is required to obtain the densities ρ_k before the forces can be calculated; however, we restrict ϕ in practice to first and second neighbours, so the additional computation is small.

For future calculation of dynamical matrices and phonon dispersion it will be useful to evaluate the force constants. The derivation is straightforward, and we obtain for the N -body part

$$-\frac{1}{A} \frac{\partial^2 U_N}{\partial R_{i\alpha} \partial R_{j\beta}} = -(f'_i + f'_j) \frac{\partial^2 \phi(R_{ij})}{\partial R_{ij\alpha} \partial R_{ij\beta}} + \sum_{k \neq i, j} f''_k \phi'(R_{ki}) \frac{R_{ki\alpha}}{R_{ki}} \\ \times \phi'(R_{kj}) \frac{R_{kj\beta}}{R_{kj}} - f''_i \phi'(R_{ij}) \frac{R_{ij\beta}}{R_{ij}} \sum_k \phi'(R_{ik}) \frac{R_{ik\alpha}}{R_{ik}} \\ - f''_j \phi'(R_{ji}) \frac{R_{ji\alpha}}{R_{ji}} \sum_k \phi'(R_{jk}) \frac{R_{jk\beta}}{R_{jk}}. \quad (22)$$

It is noteworthy that the force constants are of longer range than ϕ itself, since pairs of atoms are coupled by the density changes induced on intermediary atoms. In fact, for b.c.c. crystals, if the range of ϕ is to second neighbours $a\langle 100 \rangle$, the range of the force constants is to sixth neighbours $a\langle 200 \rangle$.

2.4. Surface and vacancy formation energies

We only consider here the unrelaxed formation energies of a surface and a vacancy, in order to illustrate the formalism. Fully relaxed formation energies would be straightforward to calculate by a computer minimization of the energy. The way we approach both the vacancy and surface energies is to sum ϕ and V over the neighbours of those atoms within range of the defect, i.e. those whose first- or second-neighbour coordination is changed by the presence of the defect, and to subtract the corresponding perfect lattice terms.

Consider the (100) surface. Only atoms in the first and second layers need be counted and there is one of each in an area a^2 .

The bonding contribution to γ_{100} is therefore

$$-\frac{A}{a^2} [(4\phi_1 + 5\phi_2)^{1/2} + (8\phi_1 + 5\phi_2)^{1/2} - 2f]$$

where

$$f = (8\phi_1 + 6\phi_2)^{1/2}. \quad (23)$$

The pairwise contribution is

$$-\frac{1}{a^2} (2V_1 + V_2). \quad (24)$$

In a similar way we find that for the vacancy, the bonding contribution to E_v^f is :

$$-A[8(7\phi_1 + 6\phi_2)^{1/2} + 6(8\phi_1 + 5\phi_2)^{1/2} - 14f] \quad (25)$$

and the pairwise contribution is

$$-(4V_1 + 3V_2). \quad (26)$$

2.5. Parameterization and fitting to experimental data

In this section we describe a simple parameterized version of the model with which we have fitted the cohesive energy, equilibrium volume and all three elastic moduli for the b.c.c. transition metals.

For the cohesive potential ϕ we adopted the parabolic form

$$\left. \begin{aligned} \phi(r) &= (r-d)^2, & r \leq d \\ &= 0, & r > d. \end{aligned} \right\} \quad (27)$$

The range d is a disposable parameter which we assume to lie between the second and third neighbours, thus

$$a < d < \sqrt{2}a.$$

For the pair-potential V we adopted the quartic polynomial

$$\left. \begin{aligned} V(r) &= (r-c)^2(c_0 + c_1r + c_2r^2), & r \leq c \\ &= 0, & r > c. \end{aligned} \right\} \quad (28)$$

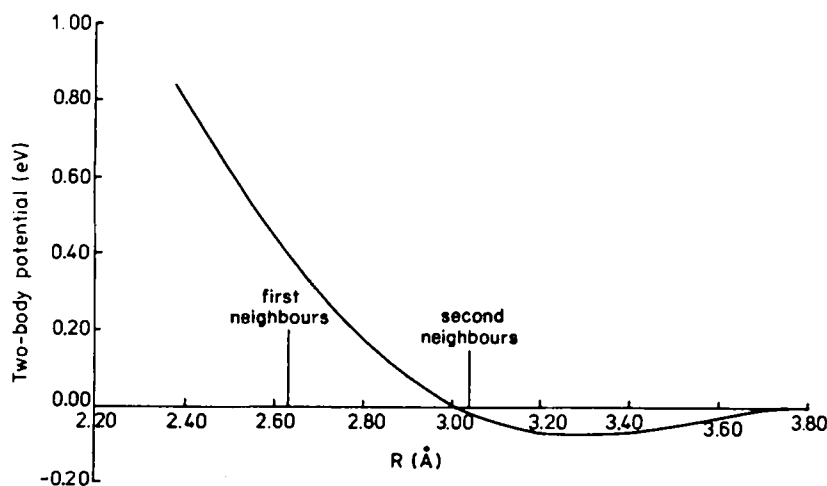
We assume that c , like d , lies between the second and third neighbours. The three parameters c_0 , c_1 and c_2 are free for fitting experimental data. The fitting is helped by the fact that all the physical quantities referred to are linear in c_0 , c_1 and c_2 , in addition to A . We adopted the following procedure, for which a simple computer program was written. Firstly, values of the cut-offs c and d were selected from an array of feasible pairs. Next, the experimental values of u_{tot} , P ($=0$), B and P_c were fitted by solving a set of linear equations in c_0 , c_1 , c_2 and A . C_{44} was then fitted by an iteration on d . This is not sufficient to specify c uniquely. However, a further condition was found to limit the range of possible c , namely that the unrelaxed vacancy formation energy E_v^f should lie in the range $0.3u_{\text{tot}} \leq E_v^f \leq 0.5u_{\text{tot}}$, to ensure a physically reasonable value. The restriction was imposed while scanning c and d before the iteration to fit C_{44} . The results are still not unique, except for A ; they could be made so by a precise fit to the experimental E_v^f including relaxation, but we did not feel that this refinement was warranted, considering the crudity of the model. The experimental and calculated quantities are shown in tables 1 and 2. Examples of $V(R)$ for vanadium and molybdenum are shown in figs. 1 and 2.

The cases of chromium and iron were treated slightly differently. Because of their anomalously low value of P_c it proved impossible to fit all the elastic constants within the above parameterization scheme. From eqn. (20) it was clear that smaller values of ϕ' would be required, so we tried modifying eqn. (27) to reduce ϕ' , thus :

$$\phi(r) = (r-d)^2 + \beta(r-d)^3/d, \quad (29)$$

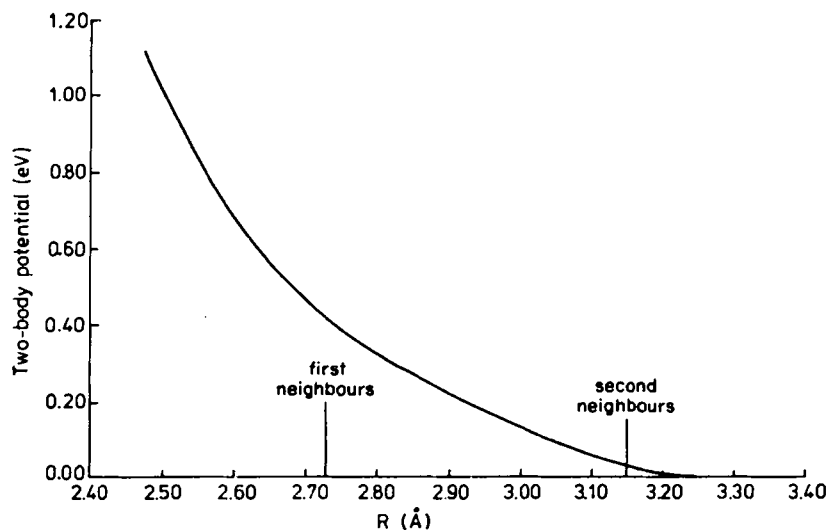
where β was chosen to introduce a maximum in ϕ within the first-neighbour distance which, for the extreme values of d , requires $\beta < 4.975$ if $d=a$ and $\beta < 1.7199$ if $d=\sqrt{2}a$.

Fig. 1



The repulsive two-body potential for vanadium which contributes to the total energy.

Fig. 2



The repulsive two-body potential for molybdenum which contributes to the total energy.

Fits were then obtained with $\beta=1.8$ for Cr and Fe; this is an arbitrary value which gave plausible results for both elements.

Applying the results of § 2.4, we calculated E_v^f (unrelaxed), the values of which, compared with experiment in table 2, are very reasonable. The tendency to exceed the experimental values would be counteracted by relaxation, which from previous experience with simple pairwise potentials can reduce E_v^f by about 20%.

It is more difficult to assess the quality of the calculated values of γ_{100} because experimental data for solid surface energies are subject to large uncertainty. Some experimental estimates of the mean surface energy at high temperature are included in table 2, and are in fair agreement with the present calculations. According to Miedema's (1978) semi-empirical model, γ at zero temperature (see table 2) should be somewhat higher, which suggests that our values are systematically too low. However, the Miedema model assumes that both γ and u_{tot} are proportional to the electron density at the boundary of a Wigner-Seitz sphere in the bulk metal, and it is therefore subject to some of the same criticism as other pairwise additive bond models. Our values also agree fairly well with the tight-binding calculations of Desjonquères and Cyrot-Lackmann (1975), also shown in table 2.

§ 3. DISCUSSION

We have derived an empirical parameterized model to represent the multi-centre interactions in b.c.c. transition metals. It involves two short-ranged interatomic 'potentials'; a cohesive one, $\phi(r)$, and a repulsive one, $V(r)$. The cohesive potential is summed over neighbours and the square-root of the

result describes the bonding energy. $V(r)$ is simply summed in the usual way to describe the repulsive core-core interaction. The potentials were fitted to the experimental quantities given in table 1, with the results shown in table 2. The cohesive and repulsive character of these potentials was expected on physical grounds and indeed it came naturally out of the fitting procedure, although it was not constrained to be so. However, we do not read any quantitative physical significance in the values of the fitting parameters. Examples of the repulsive potentials found for V and Mo are given in figs. 1 and 2. The latter is seen to have a weakly attractive tail but this is probably dependent on the form of the function assumed to fit V , because information about V is only obtained at the neighbour positions.

We conclude that the multi-centre potential derived here extends the range of situations which could be readily studied by atomistic simulation to include the possibilities of internal cavities and surfaces, without the problems of simple pair-potentials which arise because of the Cauchy discrepancy. The potential has been defined by fitting to experimental data for a perfect crystal. The fit would therefore not be changed if the potential were modified elsewhere than at the first- and second-neighbour positions. In particular, modification at short range may be necessary for use in damage or shock studies. It remains to be seen if the model gives qualitatively correct energy differences between different crystal structures, so as to predict a stable b.c.c. structure. The potentials are certainly too short-ranged to distinguish f.c.c. and h.c.p. structures, for which purpose they would have to be extended to the third-neighbour distance in those structures.

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