

## The elastic moduli, the volume contribution and the Cauchy ratio for $d$ and $f$ shell metals

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**Abstract.** The elastic constants of nine transition metals and four rare-earths and actinides are calculated using the ion–ion interaction defined by us recently. The volume contribution to elastic moduli is calculated by exploiting the density dependence of the screening function. The calculated volume contribution to bulk modulus is found to vary between 17.1% and 62.4% for a number of metals, which is quite significant and play an important role for describing quantitatively the violation of the Cauchy ratio for these metals.

**Keywords.** Elastic constants; Cauchy ratio; bulk modulus.

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### 1. Introduction

In the past there have been many attempts to obtain different analytical forms of the pair interaction  $V(r)$  between ions in solids based on pseudopotentials, linear screening theory and second-order perturbation in the energy. Previous attempts to obtain such analytical forms have met with partial success [1–3]. Pettifor and Ward [4, 5] have shown that fitting a rational function to the Lindhard [6] susceptibility  $\chi(\mathbf{q})$  leads to an analytical form for  $V(r)$ . The ion–ion interaction obtained by them is fast converging and can be used to get quick calculations. Inspired by Pettifor and Ward's work, Hafner and Heine [7] obtained a simple form of the pair potential by solving the integral appearing in band-structure part of it. Their form of  $V(r)$  exhibits the Friedel [8] oscillations through the oscillatory terms. The Friedel oscillations are found to be necessary for the physical stability of the solids.

The pair potentials have been popular in describing metallic bonding because of their computational simplicity. But they do not describe properly the violation of the Cauchy ratio. This problem can be overcome by including a volume dependent energy term [9], introducing many-body interactions. Finnis [10] has shown that for simple metals violation of the Cauchy ratio can be obtained by calculating the derivatives of the density dependent total energy. Walker and Taylor [11] have obtained density dependent pair potential following the approach of Pettifor and Ward [4]. They have used the non-local pseudopotential instead of the local pseudopotential and have made energy-wave-number characteristic function rational rather than the logarithmic term of the Lindhard [6] dielectric function.

The problem of the Cauchy ratio violation can also be overcome by introducing many-body interaction in the pair potential. Daw and Baskes [12] and Foiles *et al* [13] have developed the model pair potential known as the embedded-atom model

(EAM), which is based on the density functional and the effective-medium theory [14–16]. Finnis and Sinclair [17] developed independently a model which is mathematically equivalent to the EAM, using the second-moment approximation to the density of states in the tight-binding method [18]. Ercolessi *et al* [19] have used the same approach forgetting N-body potential. In non-centrosymmetric lattices the elastic constants are composed of a homogeneous and an inhomogeneous contribution [20]. The elastic constants of hcp solids have been calculated by van Midden and Sasse [21] using embedded-atom potential. Wallace [22] and Martin [23] showed that influence of sublattice relations for hcp and diamond crystals does not cancel out when we use many-body potentials.

The rare earths and actinides have comparatively complex electronic structure. In these solids some of the *d* and *f* electrons are itinerant and some of them are tightly bound. Therefore, not many attempts have been made to obtain the simple analytical form of the ion–ion interaction for these metals. Wills and Harrison [24] and Harrison [25] in their classic work, have obtained the attractive and overlap contributions due to *d* and *f* electrons considering the following approximations: (i) the non-interacting band model scheme for *s*, *d* and *f* electrons, (ii) Friedel model of density of states and (iii) Andersen model of muffin-tin orbital theory for *d* and *f* orbitals. Following the approach of Wills and Harrison [24], Walzer [26] has written the total energy for transition metals as a function of volume and calculated the elastic and bulk properties of a number of transition and rare earth metals. The first principle method based on density functional idea has been used by Per Soderlind *et al* [27, 28] to calculate the elastic constants of transition metals and rare earths. The work of Hafner and Heine [7] has inspired us [29] to obtain the pair potential for simple metals, using two-parameter Heine–Abarenkov [30] model potential instead of Ashcroft [31] model potential. Combining this interaction with ion–ion interaction obtained by Wills and Harrison [24] and Harrison [25], we define the pair potential for rare earth metals. This ion–ion interaction is then used to calculate the elastic constants and binding energy of transition metals, rare-earths and actinides in fcc and bcc phase. The volume dependent contribution to elastic moduli is calculated by taking the derivatives of the density dependent part of the total energy. As has been suggested by Hafner and Heine [7], the local-field corrections due to Ichimaru and Utsumi [32] are considered to normalize the screening function.

## 2. Theory

The total energy of a solid in second-order perturbation theory combined with local pseudopotential can be written as [22, 33] and [34]:

$$E = E_{\text{eg}}(n_0) + \frac{1}{2} V_{\text{bs}}(r=0) + \frac{1}{2} \sum_{i \neq 0} V(\mathbf{r}_i). \quad (1)$$

$E_{\text{eg}}(n_0)$  is the energy of all electrons in a homogeneous electron gas of density  $n_0 = Z_s/V_0$ , where  $V_0$  is the atomic volume and  $Z_s$  is the valence of the ion. The exchange-correlation corrections appropriate to the metallic densities [35] have been included in  $E_{\text{eg}}(n_0)$ . All the structure dependence has been included in the sum over pairwise interaction between atoms,  $V(\mathbf{r}_i)$ ,  $\mathbf{r}_i$  being the position of the *i*th ion. The volume dependence in this term is included through the dielectric screening function  $\epsilon(\mathbf{q})$ , where  $\mathbf{q}$  is the phonon wave vector. The volume dependent energy  $V_{\text{bs}}(r=0)$  is

really a multi-ion interaction of sufficiently long range and sufficiently weak structure; so that it does not contribute to the volume dependent part of bulk modulus.

Considering the non-interacting band model for  $s$ ,  $d$  and  $f$  electrons, the ion-ion interaction for rare earths is written as the sum of  $s-s$  contribution,  $d-d$  and  $f-f$  attractive and repulsive contributions as follows:

$$V(r) = [V_{FE}(r) + V_d(r) + V_{dd}(r) + V_f(r) + V_{ff}(r)] \exp(-\pi K_B T r / \hbar v_F). \quad (2)$$

The free electron part of pair interaction  $V_{FE}(r)$  is obtained in second-order perturbation theory using two-parameter Heine-Abarenhov [30] model potential. The integral appearing in the band structure term can be solved following the procedure devised by Hafner and Heine [7]. After a lengthy but straightforward algebra, we arrive at the following results [29]:

$$V_{FE}(r) = \frac{Z^2}{r} [H_1(r - 2r_c) + \frac{1}{4}H_3(r - 2r_c) + \frac{1}{2}H_2(r) + \frac{1}{4}H_1(r + 2r_c) - \frac{1}{4}H_3(r + 2r_c)]. \quad (3)$$

$H_1$ ,  $H_2$  and  $H_3$  are represented as the sum of the repulsive and the oscillatory contributions. The analytical expressions for these functions are given in [29]. The coupling between the local nonoverlapping  $d$  states and orthogonalized plane waves is obtained by Wills and Harrison [24] in second-moment approximation and using Friedel model of density of states. The  $s-d$  hybridization in  $V_d(r)$  is included through the factor  $Z_d \left(1 - \frac{Z_d}{10}\right)$  which represents the continuous filling of bonding levels,

where  $Z_d$  is the occupation number of  $d$  states. The overlapping contribution due to different  $d$  orbitals  $V_{dd}(r)$  is obtained using Andersen's model of muffin-tin orbital theory. In rare earth metals the  $f$  bands play the same role as the  $d$  bands play in transition metals. Therefore, Harrison [25], in his subsequent paper, has obtained the attractive  $V_f(r)$  and overlapping  $V_{ff}(r)$  contributions by treating  $f$  electrons just like  $d$  electrons. The analytical expressions for  $V_d(r)$ ,  $V_{dd}(r)$ ,  $V_f(r)$  and  $V_{ff}(r)$  are given in [36]. The temperature dependence in the pair potential is included through the damping factor [37],  $\exp(-\pi K_B T r / \hbar v_F)$ . Here  $v_F = \hbar K_F / m$  is the Fermi velocity and  $K_B$  is the Boltzmann constant. The band structure energy  $V_{bs}(r = 0)$  can be obtained from the band structure part of  $V_{FE}(r)$  by putting  $r = 0$  and then solving the integrals following the procedure of Hafner and Heine [7].

The pressure required to hold a solid can be evaluated by differentiating (1) with respect to its volume  $V$ . Differentiating (1) once more, we get the bulk modulus [22, 33]:

$$B = V \frac{\partial^2}{\partial V^2} \left( \frac{1}{2} \sum_{i \neq 0} V(\mathbf{r}_i) \right) + \Delta_{bs}. \quad (4)$$

The first term in (4) is identical to the contribution obtained using dynamical longwave method.  $\Delta_{bs}$  is the additional contribution to  $B$  arising from the volume dependence of the band structure part of the energy  $\sum_q V_{bs}(\mathbf{q})$ , i.e.,

$$\Delta_{bs} = V \left( 2 \frac{\partial^2}{\partial V_0 \partial V_{osc}} + \frac{\partial^2}{\partial V_{osc}^2} \right) \sum_q V_{bs}(\mathbf{q}). \quad (5)$$

$\partial/\partial V_0$  operates on explicit volume term while  $\partial/\partial V_{osc}$  operates on volume dependence of the dielectric function  $\epsilon(\mathbf{q})$  only.

If we now choose to differentiate  $V_{bs}(\mathbf{q})$  with respect to  $\mathbf{q}$  rather than  $V$  and  $K_F$  rather than  $V_{osc}$ , eq. (5) may be written as [22]:

$$\Delta_{bs} = \frac{1}{9V_0} \sum_{\mathbf{q}} \left( 10K_F \frac{\partial}{\partial K_F} + K_F^2 \frac{\partial^2}{\partial K_F^2} + 2qK_F \frac{\partial^2}{\partial q \partial K_F} \right) V_{bs}(\mathbf{q}). \quad (6)$$

The elastic constants for cubic crystals in longwave length limit [20]  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  can be calculated easily once the force constants are known. Including the volume-dependent contribution obtained using (6), we can get the elastic moduli using the following relations:

$$C_{11} = C_{11} + \Delta_{bs}, \quad (7a)$$

$$C_{12} = C_{12} + \Delta_{bs}, \quad (7b)$$

$$C_{44} = C_{44}, \quad (7c)$$

It is to be noted that  $C_{44}$  remains unaffected by volume forces because it only involves homogeneous strain at constant volume [22, 34]. The bulk modulus defined by eq. (4) can now be written as:

$$B = \tilde{B} + \Delta_{bs}. \quad (8)$$

### 3. Calculation and results

The atomic radius  $r_0$  is taken corresponding to the observed [38] volume for all metals. The number of  $s$  electrons per atom [24]  $Z_s$  for each Cu, Ag, Ni, Pd and Pt is taken as 1.5.  $Z_s$  is taken equal to 2 for Au. The number of electrons in  $s$  and  $d$  shells are taken to be 2 and 4, respectively, for all the three metals Cr, Mo and W. The number of electrons in  $d$  and  $f$  shells are taken from [24] and [25]. The  $d$  and  $f$  shell radii  $r_d$  and  $r_f$  are calculated from the respective  $d$  and  $f$  band widths, as has been suggested in [24] and [25]. The calculations for La, Ce, Yb and Th are done for the configuration  $5d^1 6s^2$ ,  $5d^{0.5} 4f^1 6s^{2.5}$ ,  $5d^{0.5} 4f^{1.4} 6s^{1.5}$  and  $6d^{0.5} 5f^{1.7} s^3$ , respectively, because these configurations have been found to yield overall better results of phonon frequencies in [36]. The potential parameters  $D$  and  $r_c$  for a metal are determined by matching the calculated values of the binding energy  $E_{BI}$  and the elastic constant  $C_{44}$ . The damping parameter  $\delta = 2$  is found to yield overall better results. It is to be noted that the value of  $C_{44}$  remains unaffected by the volume forces. The values of  $D$  and  $r_c$  so obtained are given in table 1. The contributions up to 7th shell have been found sufficient to achieve convergence. The theoretical values of the binding energy are presented in table 1 alongwith its estimated [39], [40] results from the cohesive energy and the ionization energies. The calculated and estimated values of the binding energy for fcc transition metals, bcc transition metals and rare earths and actinides to within 10–20% except for Pb, Pt and W. The maximum discrepancy between calculated and experimental values of binding energy is found to be 36.2% for Pt. The calculated results of elastic constants are presented in table 2 alongwith the observed [41–46] values. It is found that the radial force constants play a dominant role in yielding the elastic constants.

The volume contribution to bulk modulus is found to vary between 17.1% and

**Table 1.**  $r_0$  is the observed [38] atomic radius.  $D$  and  $r_c$  are the fitted values of the potential parameters.  $E_{BI}$  represents the binding energy. The estimated values of the binding energy  $E_{BI} = E_{coh} + E_I + E_Z$  are obtained from the experimental values of the cohesive energy,  $E_{coh}$  [39] and using the first, second and third ionization energies [39–40],  $E_I$ ,  $E_{II}$  and  $E_{III}$ , respectively.  $E_Z$  represents  $\frac{1}{4}(E_I + E_{II})$ ,  $E_{II}$ ,  $E_{II} + \frac{1}{4}(E_{II} + E_{III})$  and  $E_{II} + E_{III}$  for  $Z_s = 1.5, 2.0, 2.5$  and  $3.0$ , respectively. The values in the parantheses represent the difference (in per cent) between the theoretical and estimated values.

Element	$r_0$ (a.u.)	$D$ (a.u.)	$r_c$ (a.u.)	$-E_{BI}$ (eV/atom)	
				Theor.	Expt.
Cu	2.664	0.98	2.0	14.99 (-17.6)	18.19
Ag	3.005	1.14	2.4	14.95 (-15.7)	17.73
Au	3.005	1.20	2.4	27.00 (-19.4)	33.51
Ni	2.608	0.275	1.447	14.61 (-21.1)	18.51
Pd	2.872	0.99	2.749	13.94 (-27.2)	19.15
Pt	2.891	1.0	2.80	13.84 (-36.2)	21.68
Cr	2.684	0.60	2.132	24.66 (-9.9)	27.36
Mo	2.930	0.40	2.30	24.90 (-17.2)	30.07
W	2.949	0.37	2.345	24.89 (-28.0)	34.58
La	3.961	0.70	2.44	19.17 (-9.2)	21.11
Ce	3.819	0.95	2.76	32.18 (+13.3)	28.40
Yb	3.762	0.80	2.72	12.50 (+0)	12.45
Th	3.762	0.80	2.635	41.48 (+7.0)	44.60

**Table 2.** Values of the elastic moduli ( $C_{ij}$ ), Bulk modulus ( $B$ ), volume contribution ( $\Delta_{bs}$ ) (in  $10^{12}$  dyn/cm<sup>2</sup>) at 300 K and the volume contribution to  $B$  in per cent ( $\% \Delta_{bs}$ ). (a) and (b) represent the theoretical results obtained without including  $\Delta_{bs}$  and by including  $\Delta_{bs}$ , respectively. (c) represents the observed values of the elastic constants and are taken from [41–46], \*represents that the value of  $C_{12}$  is estimated from the experimental values of  $C_{11}$  and bulk modulus  $B$  of Cr.\*\*

Element	$C_{11}$	$C_{12}$	$C_{44}$	$B$	$\Delta_{bs}$	$\% \Delta_{bs}$	$C_{12}/C_{44}$
Cu (a)	1.579	1.412	0.628	1.468	—	—	2.25
(b)	1.537	1.370	0.628	1.426	-0.042	-2.9	2.18
[41] (c)	1.684	1.214	0.754	1.371	—	—	1.61
(d)	1.93	1.51	0.82	1.65	—	—	1.84
(e)	1.67	1.24	0.76	1.38	—	—	1.63
Ag (a)	1.107	0.929	0.442	0.989	—	—	2.10
(b)	1.128	0.950	0.442	1.010	+0.021	+2.1	2.15
[41] (c)	1.240	0.937	0.461	1.010	—	—	2.03
(d)	1.28	0.86	0.61	1.00	—	—	1.41
(e)	1.29	0.91	0.57	1.04	—	—	1.60
Au (a)	1.520	1.147	0.598	1.271	—	—	1.92
(b)	1.570	1.197	0.598	1.321	+0.050	+3.8	2.00
[41] (c)	1.94	1.61	0.47	1.72	—	—	3.40
(d)	2.09	1.75	0.31	1.86	—	—	5.64
(e)	1.83	1.59	0.45	1.67	—	—	3.53

(Continued)

**Table 2.** (Continued)

Element		$C_{11}$	$C_{12}$	$C_{44}$	$B$	$\Delta_{bs}$	$\% \Delta_{bs}$	$C_{12}/C_{44}$
Ni	(a)	2.393	2.081	1.442	2.185	—	—	1.44
	(b)	2.044	1.732	1.442	1.836	-0.349	-19.0	1.20
[41]	(c)	2.508	1.500	1.235	1.86	—	—	1.21
	(d)	3.33	1.54	1.28	1.80	—	—	1.20
Pd	(a)	1.823	1.747	0.719	1.772	—	—	2.43
	(b)	1.723	1.648	0.719	1.673	-0.100	-6.0	2.29
[41]	(c)	2.271	1.760	0.717	1.810	—	—	2.45
	(d)	1.95	1.76	0.73	1.82	—	—	2.41
	(e)	2.18	1.84	0.65	1.95	—	—	2.83
Pt	(a)	2.811	2.528	1.118	2.622	—	—	2.26
	(b)	2.714	2.431	1.118	2.525	-0.097	-3.8	2.17
[41]	(c)	3.467	2.507	0.765	2.78	—	—	3.28
	(d)	3.72	2.53	0.85	2.93	—	—	2.98
	(e)	3.03	2.73	0.68	2.83	—	—	4.01
Cr	(a)	3.205	1.599	1.094	2.134	—	—	1.46
	(b)	2.727	1.122	1.094	1.657	-0.477	-28.8	1.03
[41]	(c)	3.47	1.12*	1.00	1.90	—	—	1.12
Mo	(a)	4.289	2.227	1.570	2.914	—	—	1.42
	(b)	3.742	1.681	1.570	2.368	-0.546	-23.0	1.07
[42]	(c)	4.75	1.67	1.08	2.73	—	—	1.55
	(d)	4.06	1.50	1.07	2.35	—	—	1.40
W	(a)	4.720	2.543	1.657	3.269	—	—	1.53
	(b)	4.242	2.065	1.657	2.790	-0.478	-17.1	1.25
[42]	(c)	5.13	2.06	1.53	3.23	—	—	1.35
	(d)	5.53	2.07	1.78	3.22	—	—	1.16
La	(a)	0.320	0.230	0.184	0.260	—	—	1.25
	(b)	0.310	0.210	0.184	0.243	-0.019	-7.9	1.14
[43]	(c)	0.285	0.204	0.165	0.24	—	—	1.24
	(d)	0.29	0.17	0.16	0.21	—	—	1.06
Ce	(a)	0.294	0.102	0.168	0.166	—	—	0.61
	(b)	0.249	0.057	0.168	0.121	-0.045	-37.2	0.34
[44]	(c)	0.241	0.102	0.194	0.148	—	—	0.53
Yb	(a)	0.226	0.172	0.192	0.190	—	—	0.90
	(b)	0.152	0.099	0.192	0.117	-0.073	-62.4	0.52
[45]	(c)	0.186	0.104	0.177	0.131	—	—	0.59
Th	(a)	0.907	0.582	0.467	0.690	—	—	1.25
	(b)	0.766	0.442	0.467	0.550	-0.141	-25.6	0.95
[45]	(c)	0.753	0.489	0.478	0.577	—	—	1.02

\*\* (d) and (e) represent the theoretical results of elastic constants taken from [27] and [13] respectively.

62.4% for Ni, Cr, Mo, W, Ce, Yb and Th, which is quite significant and important for describing quantitatively the Cauchy ratio for these metals. The volume contribution for Au and Pt metals is found to be +3.8% to -3.8%, respectively, which is quite negligible. Even though the discrepancy between calculated and experimental values of the elastic constants and the Cauchy ratio for these two metals are found comparatively large. The large discrepancy found between the calculated and experimental results of binding energy for Pt and W is also reflected in our

calculated results of elastic constants for these metals. This is because of the limitation of the central pair potential. The angular forces [47] and many-body contributions [48] play a significant role in yielding good results of elastic constants. Recently, Per Soderlind *et al* [27] and Foiles *et al* [13] have calculated the elastic constants of transition metals including many-body contributions. In table 2, we have compared our calculated results of elastic constants with those obtained in [27] and [13]. It is found that many-body contributions improve the results of elastic constants in Au, Pt, Mo and W to a great extent. However, the central potential yield equally good results of elastic constants for rest of the metals considered so far.

#### 4. Conclusions

The interionic potential is determined by assuming simple forms for  $s$ ,  $d$  for  $f$  electron contributions. We have endeavoured here to use the simplest parametrized forms possible with the lowest number of parameters. The validity of the ionic interaction has been tested by calculating the bulk properties for as many as 13 cubic metals.  $\Delta_{bs}$  makes up typically 62.4% of the bulk modulus in Yb. It is therefore significant to include  $\Delta_{bs}$  to describe the Cauchy ratio and the elastic constants properly.  $\Delta_{bs}$  is found to be positive or negative and depends markedly on the pseudopotential and the screening considered. The present treatment can be extended easily to study the bulk properties of metallic alloys.

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