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Pressure derivatives of some FCC metals

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Abstract
A model is developed on the two-body Morse potential. This potential is controlled by a factor P. The elastic constants Second (SOEC), Third (TOEC) and Fourth (FOEC) are calculated earlier. Here Pressure derivatives of the Some FCC metals are explained on the basis of elastic constants. The other then elastic constants for parameters are also explained.

Keywords: Dynamical matrix, phonon frequencies, pair potential, pseudo potential, A- G Parameters and F- G Parameter

Introduction
Overview of H.264 Video Codec
The involvement of d-electron in transition metals like platinum, palladium and lead calls for the significant role of non-pair coupling forces in determining the static and dynamic properties of the metals. Second order perturbation theory considers only the linear response of the electrons towards weak electron–ion potential. Direct integration of the contribution from ring diagram has lead Brovman and Kagan [1] to deduce the third order term. To derive these terms Llyod and Sholl [2] have analysed the one electron Hamiltonian. Pasch *et al*. [3], Machlaren and Sholl [4] have carried out the further refinement of the higher order perturbation theory. Brovman *et al*. [5] have employed third order pseudo potential theory to compute the elastic moduli, binding energies, phonon spectra etc in Mg. Harrsion[6]
have resorted to similar course to investigate the structural properties of some metals. Bertoni *et al*. [7] Varius authors have analysed the role of the three-body forces in metals on phenomenological lines. The much used angular forces by Delaunay [8] and Clark *et al*. [9] bear identity with either Upadhyay [10], Rathore [11], Rathore and Verma [12] or with axially symmetric Rathore [13] or with general tenso forces by Moore and Upahyay [14].
In view of this situation, we have developed a three – body potential. Which account for the non-linear response of the electron in the metals. This potential bearing attractive as well as repulsive character is combined with the two-body Morse potential [15] to get a simple and realistic total potential, coupling by various constituents of the face contretred cubic metals Pd, Pt and Pb which show vide variation in their Cauchy's discrepancy [16].
The potential is used to derive Second order (SO), Third order (TO) and Fourth order (FO) elastic constants in these metals. Pressure derivatives of the SOEC, Anderson Gruneisen, frequency dependent Gruneisen parameters and expansion co-efficient are also computed. The phonon dispersion pridicted by the potential are finally compared with the neutron scattering data and other theoretical studies.

Theory: Here the three-body Morse potential on the lines of Mishra *et al*[17] in conjugation with the scheme of Animalu[18]. The three-body potential coupling the atom (l, k) with two common nearest neighbor's (l', k') and (l'', k'') is written as

$$\theta^{(3)}_{(r_1,r_2)} = \sum_{\substack{l',k'\\ l'',k''}}{}' \sum_{l,k} \frac{A(k)}{2}\left[\beta^2 \exp\left\{-2\alpha\left(r_1+r_2\right)\right\} - 2\beta\, \exp\left\{-\alpha\left(r_1+r_2\right)\right\}\right] \quad \ldots. (1)$$

Here A (k) is the three-body parameter, r_1 and r_2 are separation of the atoms (l',k') and (l'',k'') from the atom (l,k) respectively. α and β are the parameters of the potential. We can calculate the value of β for suitable value of α and a. The matching value of β with corresponding value of α to evaluate the equilibrium separation. The two-body potential mainly governs the lattice stability gives approximate value of β and it is used in three-body potential which implies the satisfaction of lattice equilibrium by the three-body forces.

Dynamical Matrix: Diagonal $\left[D_{\alpha'\alpha'}(q)\right]$ and off diagonal $\left[D_{\alpha'\beta'}(q)\right]$ elements of dynamical matrix for the fcc crystal may be written as in two body or pairwise part:
Two body part:

$$D^{(2)}_{\alpha'\alpha'}(q) = 4(\beta_1 + 2\alpha_1) - 2(\beta_1 + \alpha_1)C_{\alpha'}\left(C_{\beta'} + C_{\gamma'}\right)$$

$$4\alpha_1 C_{\beta'}C_{\gamma'} + 4\beta_2 S^2_{\alpha'} + 4\alpha_2\left(S^2_{\beta'} + S^2_{\gamma'}\right)$$

$$D^2_{\alpha'\beta'}(q) = 2(\beta_1 - \alpha_1)S_{\alpha'}S_{\beta'} \qquad \ldots\ldots. (2)$$

Where

$$\alpha_1, \beta_1 = 1,2,3;\ C_{\alpha'} = \mathrm{Cos}\left[\frac{aq\ \alpha'}{2}\right] \text{and } S_{\alpha'}$$

$$= \mathrm{Sin}\left(\frac{aq\alpha'}{2}\right), q_{\alpha'}$$

is the α'th component of the phonon wave vector q and

$$\alpha_1 = 1/r_1\left[\frac{\partial\theta}{\partial r}\right]r_1 \ ;\ \alpha_2 = 1/r_2\ \left[\frac{\partial\theta}{\partial r}\right]r_2$$

$$\beta_1 = \left[\frac{\partial^2\theta}{\partial r^2}\right]r_1 \ ;\ \beta_2 = \left[\frac{\partial^2\theta}{\partial r^2}\right]r_2 \qquad \ldots.. (3)$$

Where, r_1 and r_2 are the separations from the first and the second neighbours respectively.

The phonon dispersion:- The phonon frequencies (γ) are obtained by solving the usual secular equation i.e,

$$D_{\alpha'\beta'}(q) - 4\pi^2\gamma^2 \mathrm{mI} = 0 \qquad \ldots\ldots\ldots (4)$$

Where m is the mass of the atom and I is the unit matrix of 3×3 order.

Equation (4) yields following dispersion relation along the three major symmetry directions;

Along [100] $q_{\alpha'} = q \ ;\ q_{\beta'} = 0 \ ;\ q_{\gamma'} = 0$

$$4\pi^2 mv^2 L = \left[D_{\alpha'\alpha'}(q)\right]_{(100)}$$

$$4\pi^2 mv^2 T = \left[D_{\beta'\beta'}(q)\right]_{(100)}$$

Along $[110]$ $q_{\alpha'} = q_{\beta'} = \frac{q}{\sqrt{2}}\ q_{r'} = 0$

$$4\pi^2 mv^2 L = \left[D_{\alpha'\alpha'}(q) + D_{\alpha'\beta'}(q)\right]_{(110)}$$

$$4\pi^2 mv^2 T_1 = \left[D_{\gamma'\gamma'}(q)\right]_{(110)}$$

$$4\pi^2 mv^2 T_2 = \left[D_{\alpha'\alpha'}(q) - D_{\alpha'\beta'}(q)\right]_{(110)}$$

Along $[111]$ $q_{\alpha'} = q_{\beta'} = q_{v'} = \frac{q}{\sqrt{3}}$

$$4\pi^2 mv^2 L = \left[D_{\alpha'\alpha'}(q) + D_{\alpha'\beta'}(q)\right]_{(111)}$$

$$4\pi^2 mv^2 T = \left[D_{\alpha'\alpha'}(q) + D_{\alpha'\beta'}(q)\right]_{(111)}$$

The Three body part:- The non-pair potential $\theta^{(3)}_{(r_1, r_2)}$ is first used to be build up the dynamical matrix. The procedure leads to the following diagonal and off-diagonal elements of the matrix.

$$D^{(3)}_{\alpha'\alpha'}(q) + 4\beta_3\left[4 - 2C_{2\alpha'} - C_{2\alpha'}\left(C_{2\beta'} + C_{\gamma'}\right)\right]$$

$$D^{(3)}_{\alpha'\beta'}(q) + 4\beta_3\left[C_{\alpha'}\left(C_{\beta'} + C_{\gamma'}\right) - 2\right] \qquad \ldots\ldots (5)$$

Where β_3 is the second derivate of $\theta^{(3)}_{(r_1, r_2)}$

$$C_{\alpha'} = \mathrm{Cos}\left[\frac{aq\ \alpha'}{2}\right] \text{and } C_{2\alpha'} = \mathrm{Cos}(aq\alpha')$$

Elastic constants:- Three expression for the second, third and fourth order elastic constants are given by

$$C_{11} = \frac{a^4}{2\Omega}\sum_j l_1^4\ D_j^2\ \theta^{(2)}(\gamma_j) \qquad \ldots (6)$$

$$C_{111} = \frac{a^6}{2\Omega}\sum_j l_1^6 \; D_j^3 \; \theta^{(2)}\left(\gamma_j\right) \quad \text{.....} \quad (7)$$

$$C_{1111} = \frac{a^8}{2\Omega}\sum_j l_1^8 \; D_j^4 \; \theta^{(2)}\left(\gamma_j\right) \quad \text{..... (8)}$$

Where

Ω is the atomic volume and $D_j = \frac{1}{r_j}\frac{d}{dr_j}$; other symbols has their usual meanings. The remaining values of the second, third and fourth order elastic constants are obtained by replacing $l_1^2,\ l_2^2,\ l_3^2$ by the appropriate combinations of the l_1^2, l_2^2, l_3^2 in the above expression.

In the above equation, elastic constants are not related to the forces constants. Elastic constant has been derived from the theory of Sharma and Mathur [19].

Table 1: Computed Pressure Derivatives of SCEC, A-G parameter, F-G parameter and expansion Co-efficient of Pt, Pd and Pb

Metals	Pressure derivatives of SOEC			The A-G paramet		The F –G Parameter	The expansion Coefficient $(\times 10^{-6}/^0\,C)$
	$\partial C_e/\partial P$	$\partial K/\partial P$	$\partial C_i/\partial P$	By elastic constant	By Pressure derivatives		
Pt	0.560	6.089	1.831	4.310	4.066	3.742	0.153
Pd	0.673	6.660	2.017	4.487	4.485	4.990	0.090
Pb	0.384	5.468	0.900	4.244	4.468	3.885	0.106

Table 2: Percentage Contribution of composite two and three body interaction at various points of Brllouin Zone

Wave Vector	Pt		Pd		Pb	
	ν_L	ν_T	ν_L	ν_T	ν_L	ν_T
.1,0,0	-	138.0	118.7	101.2	110.6	111.3
.2,0,0	-	138.0	124.7	100.8	111.4	111.0
.3,0,0	117.2	136.6	128.8	99.6	111.0	112.7
.4,0,0	115.7	127.9	126.9	98.6	114.3	112.8
.5,0,0	113.3	124.8	116.7	93.4	115.1	114.9
.6,0,0	108.4	118.4	110.2	92.8	118.5	115.9
.7,0,0	104.6	116.5	104.4	90.4	117.4	118.8
.8,0,0	96.1	133.8	106.1	91.1	118.6	119.4
.9,0,0	94.4	112.7	95.2	89.0	121.3	119.5
1,0,0	89.7	111.4	94.1	90.8	122.8	120.6

Wave Vector	Pt			Pd			Pb		
	ν_L	ν_{T_1}	ν_{T_2}	ν_L	ν_{T_1}	ν_{T_2}	ν_L	ν_{T_1}	ν_{T_2}
.1,1,0	115.7	112.0	138.2	120.2	127.9	146.2	99.1	106.2	111.5
.2,2,0	117.1	122.6	137.3	118.4	135.5	135.6	102.2	106.3	111.5
.3,3,0	116.4	131.4	133.5	115.7	141.1	134.6	104.5	108.3	111.6
.4,4,0	114.7	134.8	128.9	114.9	125.1	127.1	106.5	111.7	113.6
.5,5,0	118.8	127.6	118.7	118.6	110.9	118.7	106.6	111.8	116.6
.6,6,0	118.9	121.2	107.3	113.8	103.2	112.1	101.2	113.8	111.8
.7,7,0	119.2	117.1	101.3	110.1	97.8	104.7	96.2	115.0	117.8
.8,8,0	117.2	116.2	95.8	99.3	93.7	98.1	91.3	117.8	119.9
.9,9,0	116.2	123.6	92.6	96.2	92.4	96.5	86.5	119.2	121.9
.1,1,0	112.6	112.8	-	92.0	92.2	95.3	84.7	121.8	123.9

Result and Discussion: The three body forces developed in a consistent manner from the Morse potential explain adequately the Cauchy's discrepancy contained in various orders of the constants. The predicted phonon dispersion show satisfactory agreement with the precise experimental findings by Dutton *et al.* [20], Table - 2 enlists the percentage contribution of composite two and three body intersections at various points of Brillouin Zone for the metals under consideration. Thus Table - 2 speaks about deviation of phonon frequencies at various lattice vectors along with the major symmetry directions. This model predicts excellently phonon dispersion curves in Pb given by Mishra *et al.* [21] and elastic constants by angle dependent Morse potential. The intersections considered in developing the model fairly explain the elastic, the thermo physical behaviours and the lattice dynamical behaviour of the FCC metals.

References

1. Brovman EC, Kagan YU. Sovt. Phys JEPT. 1967;25:365.
2. Llyod P, Sholl CA. J Phys.1968;C-1:1620.
3. Pasch G, Schiberdther Tripta. J Phys. 1973;C-5:2991,.
4. Maclaren RE, Sholl CA. J Phys. 1974;F-4:2172.
5. Brovman EG, Kagan YU, Kholas A. Govt. Phys. JEPT. 1972;35:738.
6. Harrison W. Phys. Rev. 1973;B-8:4487.
7. Bertoni CM, Bertoni V, Calandra C, March F. J Phys. 1974;F-3:L-244.
8. J Delaunay in Solid State Physics, edited by F. Seitz and D. Turabull, Academic press, New York. 1956;2:249.
9. Clark BC, Gazis DG, Wallis RF. Phys. Rev. 1964;134:A1484.
10. Upadhyay JC. J Chem, and Phys. of Solids. 1976;37:664.
11. Rathore RPS. Ind JP And Appld. Phys. 1997;15:730.
12. Rathore RPS, Verma MP. Ind. JP and Applied. Phys, 1977, 15.
13. Rathore RPS. Ind. JP and Applied. Phys. 1978;16:267.
14. Moore RA, Upadhyay JC. Can. J Phys. 1979;57:2053.
15. Morse PM. Phys. Rev. 1920;34:57.
16. Mishra MK, Pawan Srivastava, Mishra SK. Phys. Stat. 1992;Sol(b):171, K-5.
17. Mishra MK, Pawan Srivastava, Vikas Mishra, Acta Physica Hungerica. 1992;72(2-4):213-221.
18. Animalu AOE. Phys. Rev. 1973;B-8:3542-3555.
19. Sharma YP, Mathur SS. Cam. J Phys. 1995, 47.
20. Dutton DH, Brochouse BN, Miller AP, Can. J Phys. 50, 2915, 1972.
21. Mishra MK, Bajpai AK, Pawan Srivastava, Vikas Mishra. Journal of Pure & Applied Physics. 1993;5(1):61-74.