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Elastic behaviour of the FCC metals

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Abstract
A model is developed to explain elastic and lattice dynamical behaviour of FCC metals. The elastic constants Second, Third and Fourth order for FCC metals are computed with two-body Morse potential. The potential is controlled by a factor P. The phonon dispersion predicted by the model show satisfactory agreement with experimental findings.

Keywords: Elastic, lattice dynamical, FCC metals

Introduction
In the last decades a number of authors [1-9] have put much emphasis on lattice dynamical studies based on Morse potential [10]. Above studies explain lattice dynamical behaviour all types of cubic metals. Morse potential has a peculiar nature to explain the properties i.e. elastic, lattice dynamical and thermal. The three body forces derived by Rathore *et al*. [11] including ionic part of the compressibility and cohesive energy have been used as input parameters. The second, third & fourth order elastic constants are assigned value of the exponent P.

Theory
The necessity of ionic displacement of coupled electrons is inclusion of three body force in the system. This potential coupling the atom (l, k) with two common neighbours (l',k') and (l'',k'') of attractive as well as repulsive characters is written as

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

Where $A(k)$ three is body parameter, r_1 and r_2 are the separations of atom (l',k') and (l'',k'') from the atom (l,k) and α, β are the parameters of two body Morse potential. α measures the hardness of the potential [12].

The two body Morse potential may be written as

$$\theta^2_{(r_j)} = \frac{D}{2}\sum\left[\exp\left\{-2\alpha\left(r_j - r_0\right)\right\} - \exp\left\{-\alpha\left(r_j - r_0\right)\right\}\right] \quad \ldots\ldots (2)$$

The parameter β depending upon equilibrium separation r_0, then

$$\beta = \exp\left(\alpha,\, r_0\right) \quad \ldots\ldots (3)$$

Now the equation (2) is written as

$$\theta^{(2)}_{(r_j)} = \frac{D}{2}\sum\left[\beta^2 \exp\left(-2\alpha r_j\right) - 2\beta \exp\left(-\alpha r_j\right)\right] \ldots (4)$$

Here D is dissociation energy of the pair, r_j is distance of j^{th} atom from the origin.

$$\text{So, } r_j = \left(l_1^2 + l_2^2 + l_3^2\right)^{1/2} \text{ a} = L_j \text{ a} \quad \ldots\ldots (5)$$

In equation (5), a is the semi-lattice constant and (l_1, l_2, l_3) are integers representing the co-ordinates of j^{th} atom,
In the equation (1) prime at the first summation means.

$$l'k' \neq l''k'' \quad \ldots\ldots (6)$$

The non pair potential $\theta^{(3)}_{(r_1, r_2)}$ is first used to build up the dynamical matrix[13]. The procedure leads to the following diagonal and off-diagonal elements of the matrix.

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

$$\text{Or } D^{(3)}_{(\alpha',\beta')}(q) + 4\beta_3\left[C_{\alpha'}\left\{C_{\beta'} + C_{\gamma'}\right\} - 2\right] \quad \ldots\ldots (7)$$

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

$$C_{\alpha'} = \cos\left[\frac{aq_{\alpha'}}{2}\right] \text{ and } C_{2\alpha'} = \cos\left(aq_{\alpha'}\right)$$

Table 1: Second Order Elastic Constants ($\times 10^{12}$ dyne / cm^2)

Metals	C_{11}		C_{12}		C_{44}	
	Theoretical	**Experimental**	**Theoretical**	**Experimental**	**Theor**	**Experim**
Pt	3.465	3.510 Ref. No-14	2.350	2.575	0.417	0.718
Cu	2.439	2.327 Ref. No-15	1.758	1.942	0.612	0.731
Al	0.727	0.618 Ref. No-16	0.442	0.517	0.091	0.156

Table 2: Third Order Elastic Constants ($\times 10^{12}$ dyne / cm^2)

Metals	C_{111}	C_{112}	C_{123}	C_{166}	C_{456}	C_{144}
Pt	-18.817	-9.221	4.550	-6.167	0.137	-1.779 Ref. No-17
Cu	-14.158	-8.675	3.541	-5.427	0.250	-0.875 Ref. No-18
Al	-4.451	-3.127	0.671	-0.815	0.007	-0.541 Ref. No-19

Table 3: Fourth Order Elastic Constants ($\times 10^{12}$ dyne / cm^2)

FOEC	Pt	Cu	Al
C_{1111}	119.861	123.942	26.005
C_{1112}	43.115	54.531	9.953
C_{1166}	34.207	37.711	7.150
C_{1122}	37.917	50.754	9.755
C_{4444}	29.340	31.435	5.409
C_{1144}	8.005	13.307	2.840
C_{1244}	3.765	7.740	1.346
C_{4466}	4.508	6.527	1.448

Result and Discussion

Table 1, 2 and 3 show results of the present study on Second Order (SOEC), Third Order (TOEC) and Fourth Order (FOEC) elastic constants along with measured data and compaired with other studies.

Table 1 predicts the second order Elastic constants in Pt, Cu & Al. The results shows a good agreement with experimental data. The ratio $C_{11} / C_{12} > 1$. Table 2 shows the third order elastic constants. It is found C_{123} and $C_{456} > 0$. All the other TOEC - C_{111}, C_{112}, C_{166} and C_{114} are negative [20] for FCC metallic crystals which means C_{123} is not sensitive to the short range while other constants are sensitive to the value of α. The forth order elastic constants are negative in sign, which shows the interaction parameter with the value of hardness [21]. In Table -3 predicts the FOEC.

The interaction considered is developing the model fairly explains the elastic, thermo physical behaviour and the lattice dynamical behaviour of the FCC metals.

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