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***RESEARCH ARTICLE***

**ELASTIC BEHAVIOUR OF THE FCC METALS**

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## Abstract

A model comprising two and three body potential has been developed to explain the elastic behaviour of fcc metals i.e, Pt, Cu and Al. The force constants and parameters for fcc metals are computed here. The phonon dispersion pridected by the model shows satisfactory results with experimental findings.



## Introduction:-

In the present communication, I have dealt with paired part of potential having a specific nature of Morse potential. This two body part has been added to modified three body generalised part. The present scheme uses a minimal number of parameters for expressing two and three body forces. The many body forces formulated by Das et al[1] and Sarkar et al[2] show improvement in the phonon dispersion of complicated metals and explain the shear modulii but at the same time assumes only the repulsive character. The three-body forces put forward by Keating[3] show angular character. Prakash and Upadhyay[4 - 5] modified the model potential due to Animalu[6] by included the three body forces. These author's[4 - 5] have assigned the repulsive character to these forces and affect only I – modes in metals like Ni, Cu, Au and Pd. This Morse Potential[7] bearing attractive as well as repulsive characters. The ionic part of the compressibility and of the cohesive energy have been used as input for the evaluation of parameters of the two-body potential[8]. This potential is used to derive parameters for fccmetels and force constants.

**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 neighbour $(l', k')$ and $(l'', k'')$ of attractive as well as repulsive characters is written as

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

Where $A(k)$ is three body parameter, $r_1$ and $r_2$ are the separations of atom $(l', k')$ and $(l'', k'')$ from the atom $(l, k)$ and $\alpha$, $\beta$ are the parameters of two body Morse potential. $\alpha$ measures the hardness of the potential.

The two body Morse potential may be written as

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

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The parameter $\beta$ depending upon equilibrium separation $r_0$ , then

$$\beta = \exp\left(\alpha, r_0\right) \qquad \text{...... (3)}$$

Now the equation (2) is written as

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

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

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

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.

$$l'k' \neq l''k'' \qquad \text{...... (6)}$$

The non pair potential $\theta^{(3)}_{(r_1, r_2)}$ is first used to build up the dynamical matrix[9]. The procedure leads to the following diagonal and off-diagonal elements of the matrix.

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

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

Here $\beta_3$ 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 I**:- Input data for fcc Metals.

| Metals | Semi lattice constant (a) (nm) | Ionic part of cohesive energy $\theta\left(\times 10^{-12}\text{erg}\right)$ | Two body bulk modulus $K^{(2)}\left(\times 10^{12}\text{ dyne/ cm}^2\right)$ | P |
|---|---|---|---|---|
| Pt | 0.1960 | 9.287 | 1.085 | 2.25 |
| Cu | 0.1805 | 2.405 | 0.927 | 2.25 |
| Al | 0.2025 | 2.367 | 0.368 | 2.25 |

**Table II:-** Computed parameters for fcc Metals.

| Metals | $\alpha\left(\text{nm}\right)^{-1}$ | $\gamma_0\left(\text{nm}\right)$ | $D\left(\times 10^{-12}\text{ergs}\right)$ | $A\left(k\right)\left(\times 10^{+12}\text{ ergs}\right)$ |
|---|---|---|---|---|
| Pt | 0.0771 | 0.3640 | 0.468 | 1.665 Ref. (10) |
| Cu | 0.1220 | 0.2945 | 5.109 | 0.543 Ref. (11) |
| Al | 0.1001 | 0.3224 | 5.655 | 0.445 Ref. (12) |

**Table III:-** Computed force constants ($\times 10^4$ dyns / cm).

| Metals | $\alpha_1$ | $\alpha_2$ | $\beta_1$ | $\beta_2$ | $\beta_3$ |
|---|---|---|---|---|---|
| Pt | - 0.249 | 0.033 | 2.032 | 0.940 | 0.295 |
| Cu | - 0.175 | 0.0387 | 2.740 | -0.085 | 0.092 |
| Al | - 0.221 | 0.046 | 2.050 | -0.022 | 0.073 |

## Result and Discussion:-

The three parameters $D, \alpha$ and $\gamma_0$ are evaluated in terms of semi lattice constant, Ionic part of cohesive energy and two body bulk modulus $K^{(2)}$ as per procedure, which is earlier by Girifalco and Weizer[13]. While evaluating these parameters, the lattice stability is maintained by first derivative of the potential upto zero. The two body potential is assumed to couple the eight nearest neighbours and three body potential is short range and couple only common nearest neighbour. The force constants required to compute the phonon dispersion in metals are give in Table–III.

The findings of Pt has been compared with theoretical study of Rajput[14] and with the study of Vrati[15]also. Experimental points[16] are well satisfied. For metal Cu is very close to experimental points[17] by using TMMP model and another Study by Sharma and Joshi[18]. For metal Al we have better results than the other studies given byBehari and Tripathi[19] and Wang and Overhauser[20]. Experimental Points[21-23] are in good agreement with this approach for Al. This interaction is fairly explains the elastic and thermo physical behaviour of fcc metals.

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