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RESEARCH ARTICLE

A LATTICEDYNAMICALSTUDY OF COBALTBASEDONTHE MORSE POTENTIAL

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Abstract

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The present investigation used modified Morse potential to explain the lattice dynamical behaviour of cobalt. This study finds better agreement between experimental and theoretical results. These findings have been compared with other studies.

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Introduction:-

Recently Prakash and Upadhyaya [1, 2] and Upadhyaya and Prakash [3] investigatedthe lattice dynamicsof some f.c.c. metals using the transition metalmodel potential (TMMP) incorporating many body forces. It is to be remembered that the TMMP of Animalu [4] is local approximation and also the scheme of Eschrig and Wonn [5] use only central pairwise forces in the interaction system. As we known, compressibility and cohesive energy are the sum of ionic interaction and interaction due to electrons. Earlier studies based on separation of two and three body part of the compressibility. Then used Morse potential for the lattice dynamical study.

Here, I developed a three-body potential based on Morse potential to predict the lattice dynamical behaviour. The ionic part of the compressibility and of the cohesive energy have been used as input to evaluate the parameters.

Theory:-

The necessity of ionic displacement of loosely coupled electrons is inclusion of a three body force in the system. Here I considered a third common nearest (l',k') neighbour into the coupling of the atom (l',k') with the atom (l,k). These vertices are located on a equilateral triangle. The Morse potential[6]modified to represent the three-body intersection among the atoms $(l,k),(l',k')$ and (l'',k'') as is this form.

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

Where r_1 and r_2 are the respective separations of the atoms (l',k') and (l'',k'') from the atom (l,k). $A(k)$ is the three-body parameter, α measures the hardness of the potential, and β is a parameter depending upon the equilibrium separation r_0, then it should be written as

$$\beta = \exp(\alpha r_0) \quad \ldots\ldots (2)$$

In the equation (1) prime at the first summation means

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$$l'k' \neq l''k''$$

The two body Morse potential is expressed as

$$\phi_{(r_j)}^{(2)} = \frac{D}{2}\sum_j \left[\beta^2 \exp\left(-2\alpha r_j\right) - 2\beta \exp\left(-\alpha r_j\right)\right] \quad \ldots\ldots. (3)$$

Where D is dissociation energy of the pair, j goes over 140 atoms (including neighbouring atoms) in f.c.c. metals and r_j is the distance of j^{th} atom from the origin.

So $$r_j = \left(l_1^2 + l_2^2 + l_3^2\right)^{1/2} a = L_j a \quad \ldots\ldots. (4)$$

Here a is the semi-lattice constant and $\left(l_1, l_2, l_3\right)$ are integers representing the co-ordinates of j^{th} atom.

The elements of the diagonal and off-diagonal matrix may be given, after solving the usual secular determinant, as

$$D_{\alpha'\alpha'}\left(\vec{q}\right) = 4\left(\beta_1 + 2\alpha_1\right) - 2\left(\beta_1 + \alpha_1\right) C_{\alpha'}\left(C_{\beta'} + C_{r'}\right) - 4\alpha_1 C_{\beta'} C_{r'} + 4\beta_2 S_{r'} + 4\alpha_2\left(S_{\beta'}^2 + S_{r'}^2\right)$$

$$D_{\alpha'\beta'}\left(\vec{q}\right) = 2\left(\beta_1 - \alpha_1\right) S_{\alpha'} S_{\beta'} + 4\beta_3\left\{\left(C_{\alpha'} + C_{r'}\right) - 2\right\}$$

Here $C_{\alpha'} = \cos\left(aq_{\alpha'}/2\right)$ and $S_{\alpha'} = \sin x\left(aq\alpha'/2\right)$ ….. (5)

Where α_1, α_2 are the first and β_1, β_2 are the second derivatives of the potential $\phi_{(rj)}^{(2)}$

While β_3 is the second derivative of $\phi_{(r_1, r_2)}^{(3)}$.

Computation and Discussions:-

Mishra etal[7] have used the total cohesive energy for the evaluation of the two-body parameters means only two body interaction. Now it is required to elaborate paired and unpaired parts is terms of cohesive energy. To solve this paired and unpaired parts we adopt this purpose.

$$\phi = \phi_i + \phi_e \quad \ldots.. (6)$$

Here ϕ is total cohesive energy, ϕ_i is the energy due to ions & ϕ_e is energy due to electrons.

This energy due to electrons is combination of other energy, which is as

$$\phi_e = E_f + E_x + E_c \quad \ldots\ldots (7)$$

Where E_f is fermi energy $= 2.21/r^2$ Ryd

E_x is exchange energy $= -0.916/r$ Ryd.

And E_c is correlation energy $= \left(0.06221nr - 0.096\right)$ Ryd

As we know

$$1\text{Ryd} = 13.0 \times 1.6 \times 10^{-24} \text{ erg.}$$

Hence the energy due to electrons is equal to

$$\phi_e = \left[\frac{2.21}{r^2} - \frac{0.916}{r} + \left(0.0622 \,\text{In r} - 0.0961\right)\right] \text{Ryd} \quad \ldots. (8)$$

Here r is a dimensionless quantity and may be any value i.e 2,3,4, ….

The three parameters of the two-body potential $\phi_{(r_j)}^{(2)}$ are evaluated by equilibrium lattice constant laid down by Girifalco and Weizer[8]. The cohesive energy of the solid as well as compressibility of the ionic part is procedure laid down by Mishra et al[12]. Finally the three body parameter A(k) is evaluated by the cauchi discrepancy in the second-order elastic constants.

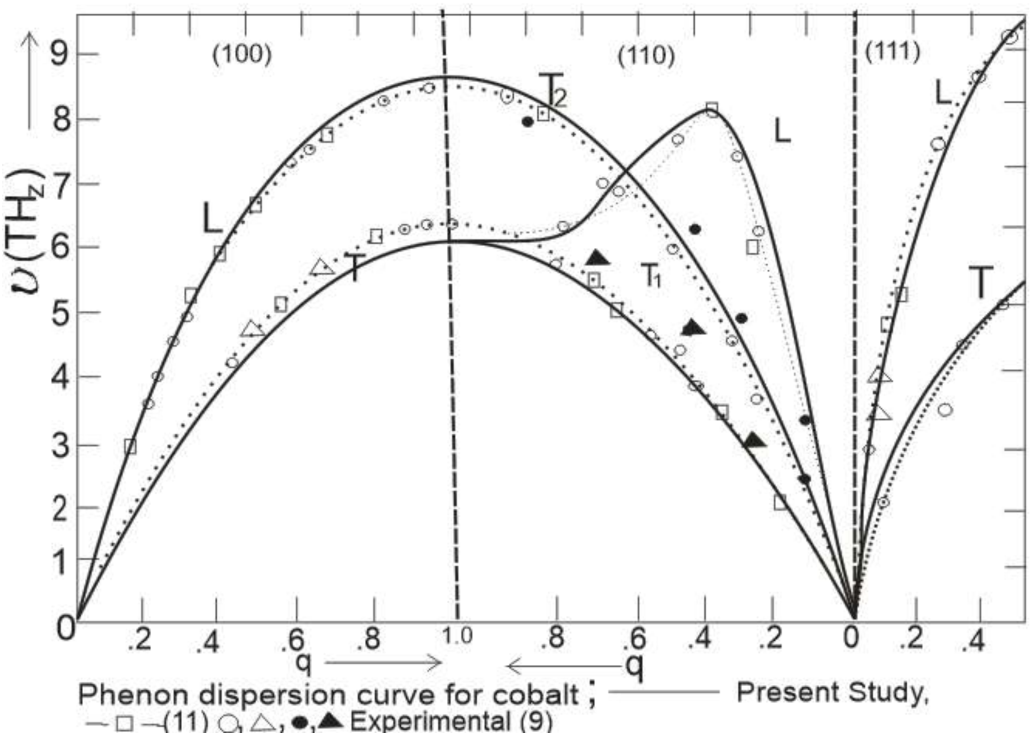

Figure shows the dispersion curve for cobalt. My prediction is cobalt follows closely to the experimental data[9]. The theoretical findings of verma[10], however, exhibit deviations from the experimental findings[11].

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