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Lattice Dynamical Study of Phonon Dispersion in Thorium: Cubic Metal

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Abstract:-Dispersion curve in Th(Thorium) has been Computed with Morse Potential for Lattice dynamical study of fcc Metal . Results obtained are very excellent and very close to experimental Values.

Key Words:-Morse, Lattice dynamical study, fcc, SOEC

Introduction:- On the basis of generalized Morse Potential[2] Singh and Ratore[1] have studied the lattice dynamics of some cubic metals input data for empirical Morse potential[2] are Cohesive energy, Lattice constants and Compressibility. But the compressibility and cohesive energy are the sum of Ionic interaction and interaction due to electrons.

In my study, I have separated the two and three body part of the compressibility on the lives of Mohdetal[4] and then I have used to Morse potential for a lattice dynamical study of fcc metal. The most important contribution to the binding energy which produces from the interaction between ions and electrons is not included in the potential even though the potential is fitted to the total cohesive energy. In this we used the input, the ionic part of compressibility and of the cohesive energy for evaluation of parameters of the two body potential.

Discussion and calculation:- We used the total cohesive energy which means the whole cohesive comes from the two body interaction. Now we discuss paired and unpaired parts in terms of cohesive energy following procedure has been adopted for this purpose.

$$\phi = \phi_i + \phi_e$$

where, ϕ is the total cohesive energy, ϕ_i is the energy due to ions and ϕ_e is the energy due to electrons.

Further,

$$\phi_e = E_f + E_x + Ec$$

where, E_f (Fermi energy) = $2.21/r^2$Ryd.

E_x (Exchange energy) = - 0.916/r Ryd.

E_c (Correlation energy) = (0.0622 Lnr – 0.096) Ryd.

While 1 Ryd = $13.0 \times 1.6 \times 10^{-24}$ ergs.

Hence the energy due to electrons is-

$$\phi_e = \left(\frac{2.21}{r^2} - \frac{0.916}{r} + (0.0622\ \mathrm{Lnr} - 0.0961)\right)\mathrm{Ryd.}$$

Here r is dimensionless quantity and may be valued 2, 3, 4 or 5.

The three parameters (D, α and r_0) defining the two body potential $\phi^{(2)}_{(r_j)}$ are evaluated by the knowledge of the equilibrium lattice constant, the ionic part of the compressibility as well as by the cohesive energy of the solids by the procedure laid down by Girifalco and Weizer[4].

The two and three body components of total potential are computed from such eq.

$$D\alpha'\beta'(\vec{q}) - (4\pi^2)^2 mI = 0$$

Where m is the man of atom, I is the unit matrix of 3×3 order and Dα'β' is the total dynamical matrix. The total dynamical matrix. The dispersion relations have been obtained in the tree major symmetry directions.

The total potential

$$\phi^{(3)}(r_1, r_2) = \sum_{\substack{l'k' \\ l''k''}}^{l} \sum_{l'k'} A/2\left[\beta^2 e\times p\{-2\lambda(r_1 r_2)\} - 2\beta e\times p\{-\lambda(r_1 + r_2)\}\right]$$

Where r_1 and r_2 are the separation of the atoms (l', k') and (l'', k'') from the atom (l,k). A is the tree body parameter. The prime on the first summation means l'k'≠l''k'' β can evaluated in such a way,

$$\beta = \mathrm{e} \times \mathrm{p}(\alpha ro)$$

This scheme centered on the separation of two and three body parts in terms of Bulk Modules as well as cohesive energy explain the SOEC as given in the table-1. The theoretical values are very close to experimental results (5-10) in SOEC. Our results on the TOEC are in good agreement with other workers (11-19) in table-2. This study predicts widely and compares results on FOEC as well as pressure derivatives with other studies [12 and 14-19] shown in table-3.

Conclusion:- Finally phonon dispersion curves have been drawn and compare with experimental findings. Dispersion curve of Thorium, very slight deviation is found in this can with experimental study of Re are et.al.

TABLE – 1

The Predicted SOEC ($\times 10^{-12}$ dyne-cm^{-2})

Sr. No.	Solid	C_{11}				C_{12}				C_{13}			
		Two Body	Three Body	Total	Expt	Two Body	Three Body	Total	Expt	Two Body	Three Body	Total	Expt
1	Th	0.693	0.009	0.702	0.753 (10)	0.481	0.009	0.490	0.489	0.481	-0.002	0.479	0.478

TABLE – 2

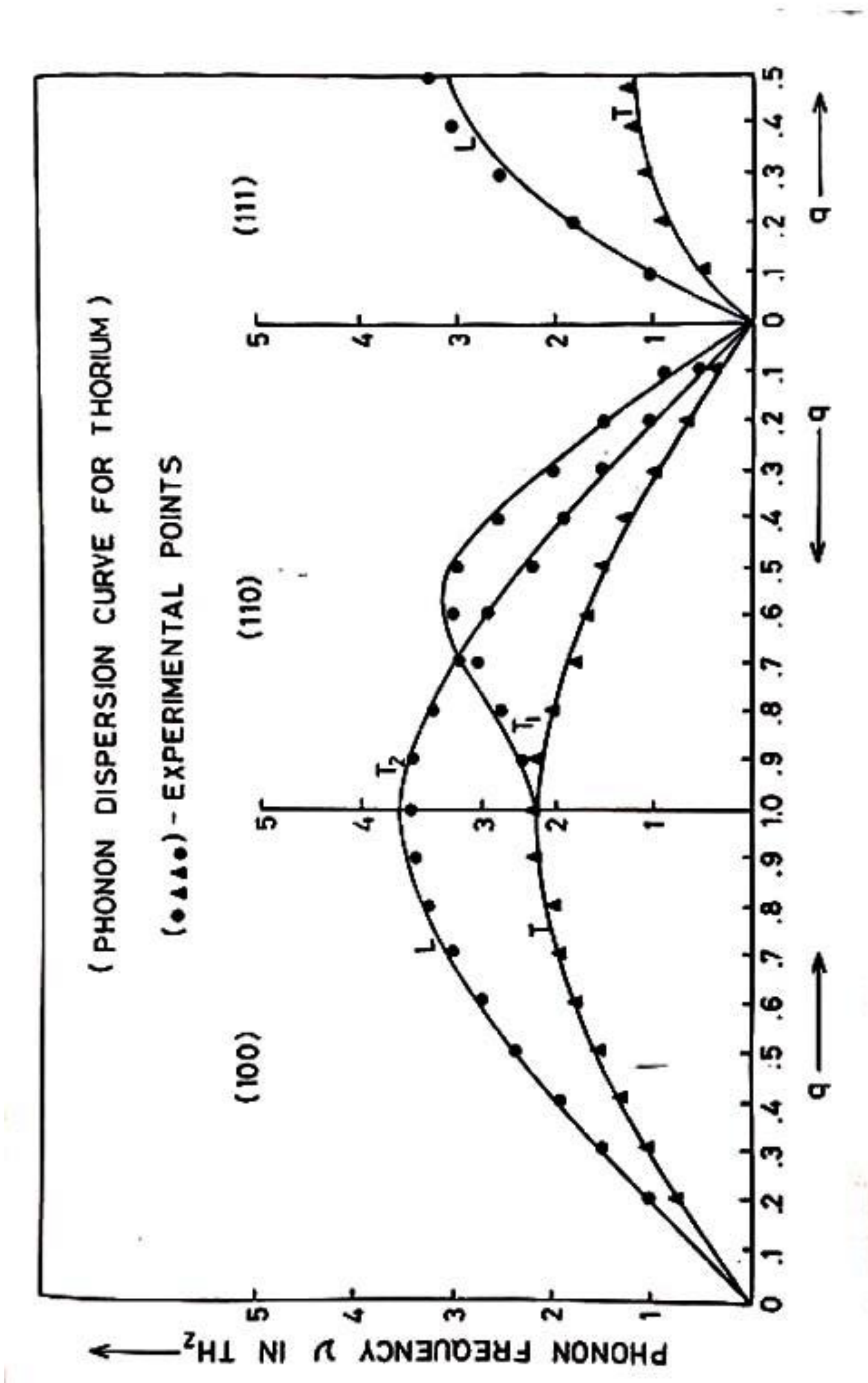
The Predicted TOEC ($\times 10^{-12}$ dyne-cm^{-2})

Sr. No.	Solid	C_{111}			C_{112}			C_{123}		
		Two Body	Three Body	Total	Two Body	Three Body	Total	Two Body	Three Body	Total
1	Th	-5.970	-0.094	-6.064	-2.216	+0.089	-2.127	0.097	+0.017	0.114

TABLE – 3

The Pressure derivatives of SOEC

Sr. No.	Solid	$\partial C_e/\partial P$			$\partial K/\partial P$			∂C_s-∂P		
		Two Body	Three Body	Total	Two Body	Three Body	Total	Two Body	Three Body	Total
1	Th	0.794	0.219	1.013	3.786	3.209	6.995	1.241	1.735	2.976


(PHONON DISPERSION CURVE FOR THORIUM)
(●▲▲●) - EXPERIMENTAL POINTS
(100)
(110)
(111)
PHONON FREQUENCY ν IN TH$_z$
q
L
T
T$_1$
T$_2$

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