Three Body Forces and New Approach to the Lattice Dynamical Study of Pb, Pd and Pt.

Anil Kumar Bajpai
Department of Physics
Bipin Bihari College, Jhansi (India)

Sunil Bhatia
Department of chemistry
Bipin Bihari College, Jhansi (India) Email-anilbajpai333@mail.com

Abstract

New approach to the lattice dynamical study of metals based on Morse potential has been considered. This study finds better agreement between experimental and theoretical results.

Key Words

Morse Potential Lattice dynamics Phonon dispersion of diagonal and off diagonal Dynamical Matrix

Introduction

Recently Singh and Rathore[1] have studied the lattice dynamics of some cubic metals based on generalised Morse potential. According to this study, cohesive energy, lattice constant and compressibility are the input data for empirical Morse potential[2].

Calculation

As we know that compressibility and co-hesive energy are the sum of ionic interaction and interaction due to electrons. Mishra and Rathore[3-4] have seperated two and three body part for compressibility on the lines of the Mohammad et al[5] and then used Morse potential for lattice dynamical study of some metals. The Morse potential comprising of two and three body part coupling the atom (l,k) with two common nearest neighbours (1', k') and (1", k"), may be written as,

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

where A(k) is the three body parameter, r_1, and r_2, are separations of the atoms (l', k') and (1", k") from the atom (1, k) respectively and α, β are the usual parameter of the two body Morse potential. The prime on first summation means

l', K' ≠ l'', k''

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

$$D_{\alpha'\alpha}(\vec{q}) = 4(\beta_1 + 2\alpha_1) - 2(\beta_1 + \alpha_1)C_{\alpha'}(C_{\beta'} + C_{r'}) - 4\alpha_1 C_{\beta'}C_{r'} + 4\beta_2 S^2_{\alpha'} + 4\alpha_2(S^2_{\beta'} + S^2_{r'}) + 4\beta_3[4 - 2C_{2\alpha'}(C_{\beta'} + C_{r'})] \quad \text{-------- (2)}$$

$$D_{\alpha'\beta'}(\vec{q}) = 2(\beta_1 - \alpha_1)S_{\alpha'}S_{\beta'} + 4\beta_3[(C_{\alpha'} + C_{r'}) - 2] \quad \text{-------- (3)}$$

Where, $C_{\alpha'} = Cos\left(\frac{aq_{\alpha'}}{2}\right); D_{\alpha'} = Sin\left(\frac{aq_{\alpha'}}{2}\right)$

α_1, α_2 are the first and β_1, β_2, are the second derivatives of the potential $\phi^{(2)}_{(rj)}$ while β_3 is second derivative of $\phi^{(3)}(r_1, r_2,)$. The Phonon dispersion based on this model is well predicted by Mishra and Rathore[3] for complicated metal Pb.

In this present communication I am going to elaborate the paired and unpaired part in terms of co-hesive energy. Following procedure has been adopted for the same purpose i.e.

$\phi = \phi_i + \phi_e$ where ϕ → total cohesive energy

ϕ_i → energy due to ions

ϕ_e → energy due to electrons

Further,

$\phi_e = E_f + E_x + E_c$ --------- (4)

Where E_f (The Fermi energy) = $\frac{2.21}{r^2}$ Rydberg

E_x (Exchange energy) = $-\frac{0.916}{r}$ Rydberg

E_c (Correlation energy) = $[0.0622\, L_n r - 0.096]$ Rydberg

while l Rydberg = $13.0 \times 1.6 \times 10^{-24}$ ergs.

Hence energy due to electrons

$$\phi_e = \left\{\frac{2.21}{r^2} - \frac{0.916}{r} + [0.0622 L_n r - 0.096]\right\} \text{ Rydberg} \quad \text{-------- (5)}$$

Here r is the dimension less quantity and may be true as 2, 3, 4 or 5.

Result and Discussion

From the above facts we reached on the conclusion that input parameters should be purely ionic for the study of Singh and Rathore[1] and of Mishra and Rathore[3-4]. This was the main drawback in the above studies[1,3,4,5]. These studies[1,3,4,5] were predicting that whole of the co-hesion comes from the two body interaction only while it is contradictory to the basic concept of parameters evaluation. We have developed three body Morse potential on the lines of Mishra and Rathore[3-4] and predicted dispersion relations for fcc solids i.e. Pb, Pd and Pt.

The experimental data[6] on the Pb have been compared with our results and also with the theoretical findings of Mohammed et al.[5] and sarkar et al.[10] The neutron scattering data[7] on Pd in better agreement with our results than that of other theoretical findings of Mohammed et al[5] and Vrati[9]. Our results in the Pt are very close to the experimental findings of Duttan et al[8]. The theoretical results of Rajput[11] deviates upwardly while that of Vrati[9] deviates down wardly with the excperimental findings[8].

Conclusion

The results shown in the curves, confirm my consideration in terms of co-hesive energy. Fig. 1,2,3 represents the phonon frequencies of the fcc solids Pb, Pd and Pt. Table shows the computed force constants of the same metals.

Table 1 : The Computed Force Constants [$\times 10^4$ dynes/cm]

Solids	α_1	α_2	β_1	β_2	β_3
Pb	0.051	+0.005	0.391	–0.020	0.054
Pd	-0.179	0.029	1.779	0.008	0.175
Pt	-0.247	0.030	2.032	0.075	0.282

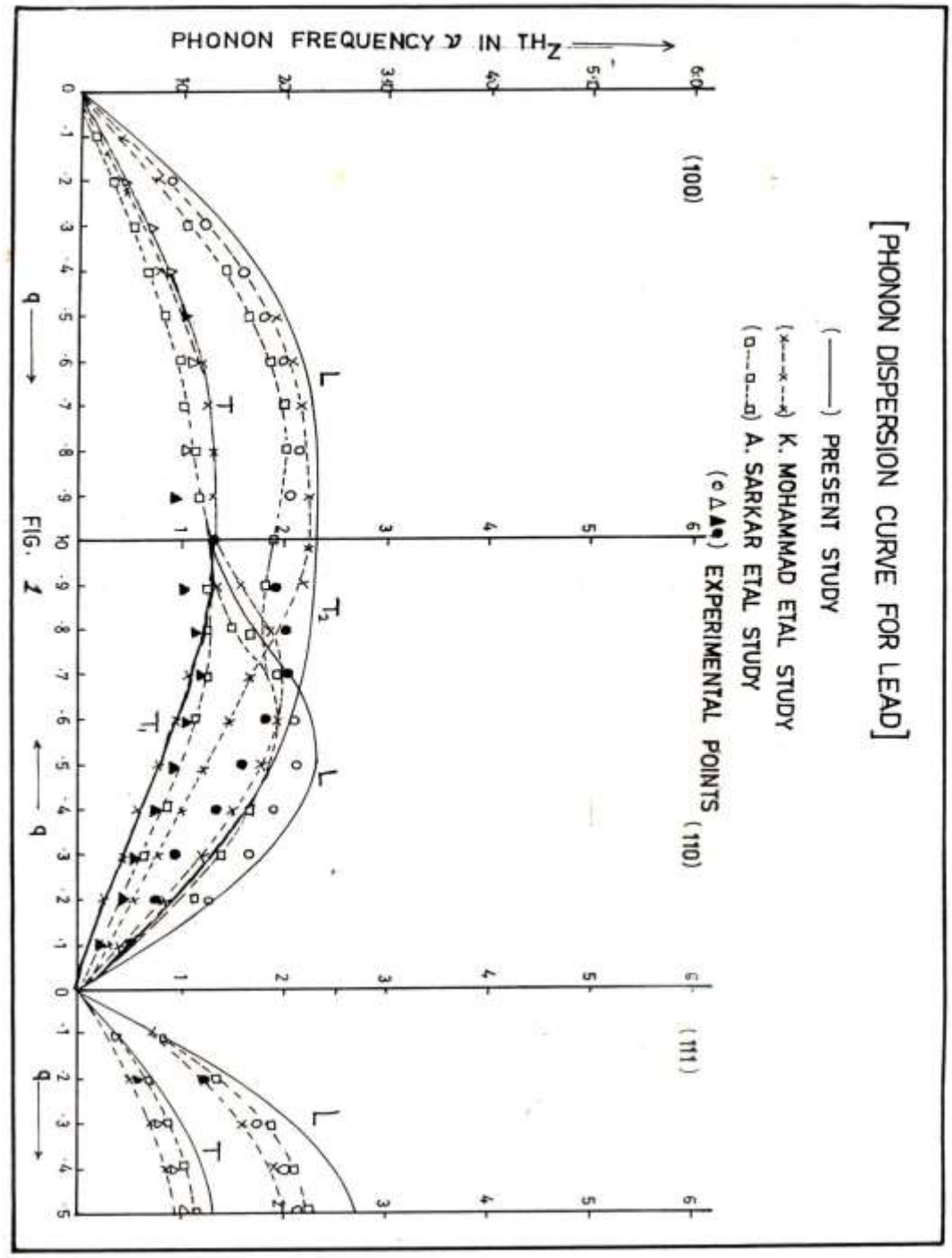
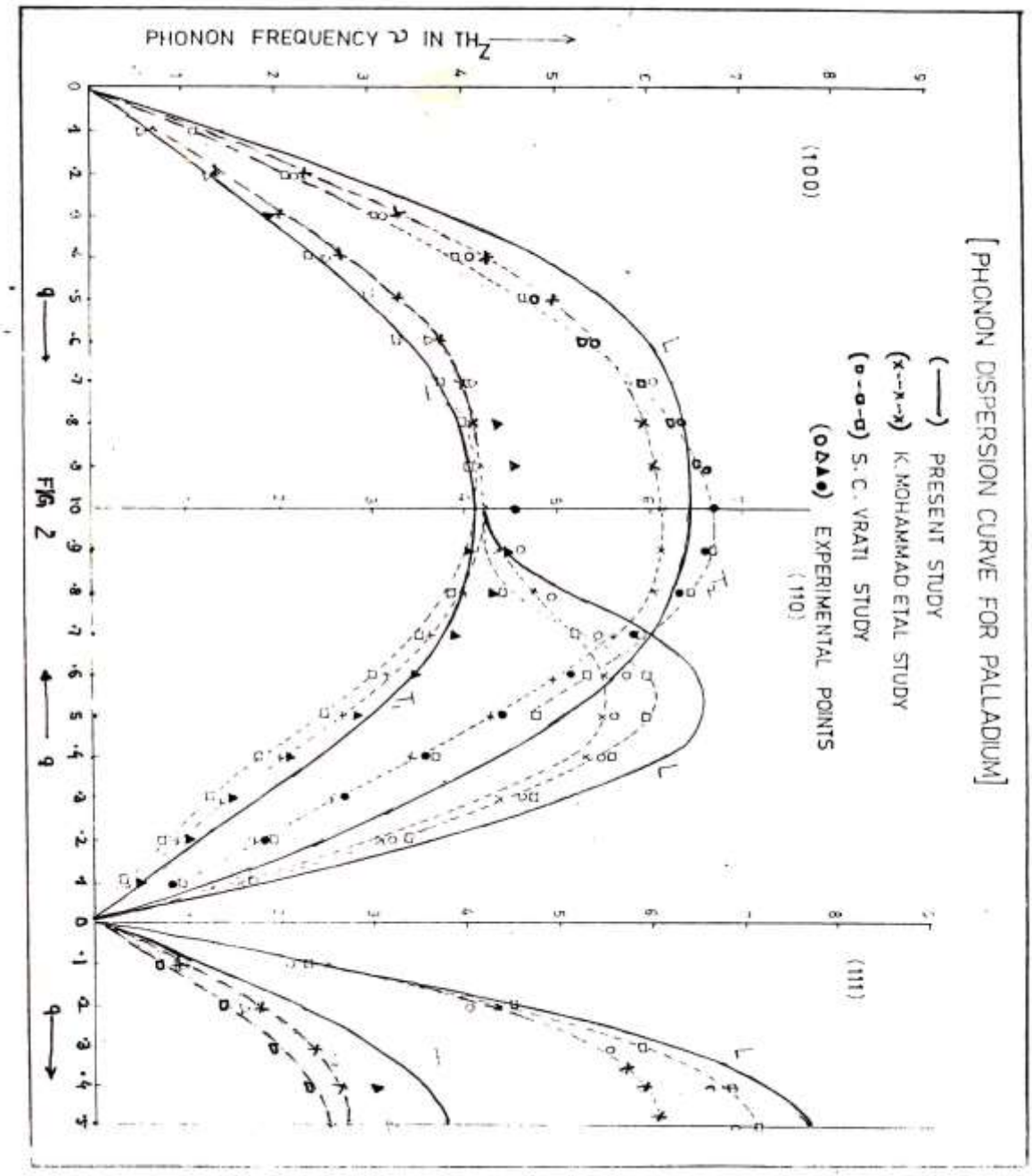
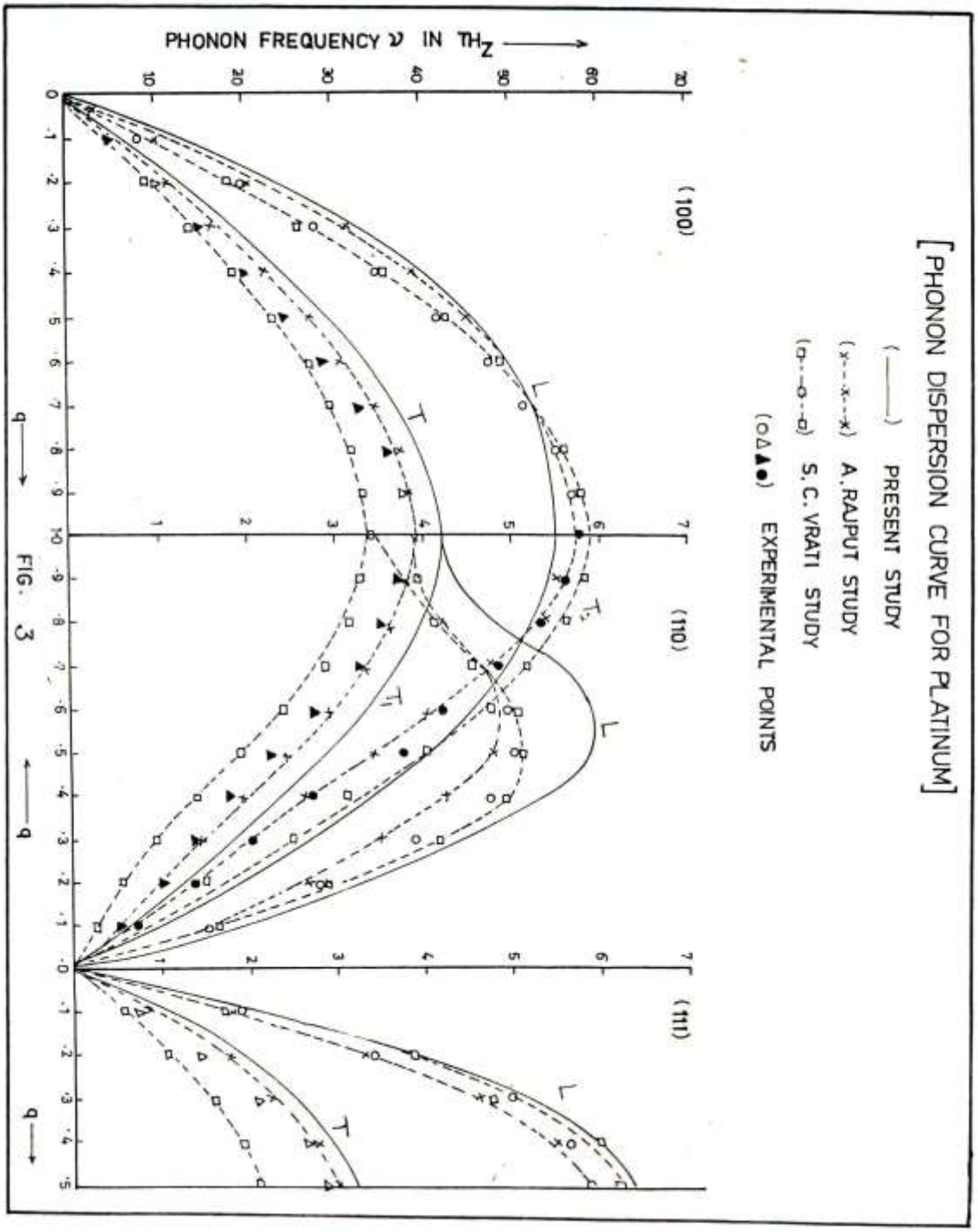

PHONON FREQUENCY ν IN THz
(100)
(110)
(111)
L
T
T2
T1
q
[PHONON DISPERSION CURVE FOR LEAD]
(——) PRESENT STUDY
(x---x---x) K. MOHAMMAD ETAL STUDY
(□---□---□) A. SARKAR ETAL STUDY
(○△▲●) EXPERIMENTAL POINTS

FIG. 1


PHONON FREQUENCY ν IN THz
[PHONON DISPERSION CURVE FOR PALLADIUM]
(——) PRESENT STUDY
(x--x--x) K. MOHAMMAD ETAL STUDY
(□-□-□) S. C. VRATI STUDY
(○△●) EXPERIMENTAL POINTS
(100)
(110)
(111)
q
FIG. 2



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