CHAPTER VI

THE CONCLUSIONS AND FOLLOW-UPS

6.1 Introduction

6.2 The Conclusions

6.3 The Follow-ups
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The Conclusions and Follow-Ups.

6.1 Introduction:

This chapter draws the attendant conclusions from the investigations given in preceding chapters. The follow ups demanded herein are also given for future modification of the present work. The special points of the present work are thus:

(a) the two body ion ion interaction is presented in a known mathematical form - the Morse potential,
(b) none of the experimental frequencies are employed to determine the model parameters,
(c) the bulk modulus \( (K_e) \) of the electron gas has been assigned the physically meaningful value corresponding to the Cauchy's discrepancy \( (C_{12} - C_{44}) \),
(d) the cohesive energy has been separated into two and three body parts.

6.2 The Conclusions:

The careful review of the inferences given at the end of the preceding chapters, one may draw the following conclusions:

1. The attractive and repulsive part of the original Morse potential represent in general the main dominant interactions responsible for the cohesion in metal. The lattice dynamical behaviour of the metals may qualitatively be predicted by the potential. The potential is more effective in describing the
phonon dispersion of those metals for which Cauchy's discrepancy is relatively insignificant.

2. The average elastic behaviour of the metals finds its explanation through the interactions stated by the original potential. The Cauchy's discrepancy in all the orders of the elastic behaviour is however not given by the potential.

3. The inclusion of the three body forces developed and derived in the present dissertation does improve the slope of the phonon dispersion substantially.

4. The Cauchy's discrepancy contained in the SOEC, TOEC and FOEC are satisfactorily explained by the three body forces formulated during the present course of study. The reliable and fairly accurate prediction of the elastic behaviour is ensured through the two and three body interactions considered here in.

5. The separation of two and three body parts in the terms of cohesive energy explains excellently phonon dispersion curve for the some fcc metals.

6. The elastic and thermophysical behaviour are also very near to the experimental findings. Thus this study is better than others to explain lattice as well as elastic and thermophysical behaviour of the fcc solids.

The subject matter of present thesis is important and uses minimal member of parameters for expressing two and three body forces.
6.3 The Follow-ups:

The depiction of the lattice dynamical and elastic behaviour of the fcc metals in general and comparison of the former behaviour with the neutron scattering data in particular lead to following lines for future follow ups.

(1) More versatile and effective form of the three body potential depending on the spatial and angular separations may be attempted to improve the elastic and thermophysical behaviour of the metals.

(2) The long range electron-ion interactions incorporating (a) the volume dependence of the dielectric screening, (b) the effective Umklapp terms, (c) the volume dependence of conduction electrons and (d) the statical and dynamical field factors, may be developed for explaining the better agreement of Phonons, especially in the proximity of the zone boundaries.
Your paper "Lattice dynamical study of some FCC metals" has been accepted for publication in Acta Physica Hungarica and will appear in Vol. 71.

Yours sincerely,

Prof. I. Kovács
Editor
Three-body forces and new approach to the lattice dynamical study of Pb, Pd and Pt

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Received 31 August 1990; revised received 18 January 1991

A new approach to the lattice dynamical study of metals based on Morse potential, has been considered. This potential is modified to determine the two- and three-body forces in a consistent manner. These forces are employed to build up the dynamical matrix, which predicts the qualitative features of phonon dispersion in some of the face centered cubic (FCC) metals, i.e. Pb, Pd and Pt.

Theory—Singh and Rathore have recently 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. Compressibility and cohesive energy are, respectively, the sums of ionic interactions and interactions due to electrons. Mishra and Rathore have separated two and three-body parts for compressibility on the lines of the Mohammad et al. and then used Morse potential for lattice dynamical study of some metals. The Morse potential comprising two- and three-body part coupling the atom \((l,k)\) with two common nearest neighbours \((l',k')\) and \((l'',k'')\), may be written as:

\[
\phi^{(3)}(r_1\cdot r_2)=\sum_{l'k'}\sum_{l''k''}\sum\frac{A(k)}{2}\beta^2\exp\left(-2\alpha(r_1+r_2)\right) -\beta\exp\left(-\alpha(r_1+r_2)\right)
\]

where \(A(k)\) is the three-body parameter, \(r_1\) and \(r_2\) are separations of the atoms \((l',k')\) and \((l'',k'')\) from the atom \((l,k)\), respectively, and \(\alpha, \beta\) are the usual parameters of the two-body Morse potential. The prime on first summation in Eq. (1) means \(l', k' \neq l'', k''\).

The three-body potential \(\phi^{(3)}(r_1\cdot r_2)\) is first used to build up the dynamical matrix. The usual procedure leads to the following diagonal and off-diagonal elements of the matrix, i.e.

\[
D_{aa}(q) = 4\beta^2(4-2C_2a - C_a(C_\beta + C_\gamma))
\]

\[
D_{ab}(q) = 4\beta_3[C_a(C_\beta + C_\gamma) - 2]
\]

where \(\beta_3\) is the second derivative of \(\phi^{(3)}(r_1\cdot r_2)\), \(C_a = \cos(aqa')/2\) and \(C_2a = \cos(aqa')\). The two-body potential \(\phi^{(2)}(r)\) describes the following contribution to the dynamical matrix, i.e.

\[
D_{aa}(q) = 4(\beta_i + 2\alpha_1) - 2(\beta_i + \alpha_1)C_a(C_\beta + C_\gamma)
\]

\[
-4\alpha_1C_\beta C_\gamma + 4\beta_2S_a^2 + 4\alpha_2(S_a^2 + S_\beta^2)
\]

\[
D_{ab}(q) = 2(\beta_i - \alpha_1)S_aS_\beta
\]

where \(S_a = \sin(aqa'/2)\), \(\alpha_1\) and \(\alpha_2\) are the first derivatives of the potential coupling the first and second neighbours, and \(\beta_i\) and \(\beta_2\) the second derivatives.

The phonon frequencies \(\nu\) are obtained by solving the usual secular equation, i.e.

\[
D_{aa}(q) - 4\pi^2\nu^2 mI = 0
\]

where \(m\) is the mass of atom. \(I\) is the unit matrix of \(3 \times 3\) order and \(D_{aa}\) is the total dynamical matrix.

The most significant contribution to the binding energy which arises from the interaction between the metal ions and the electrons is not included in the potential, even though the potential is fitted to the total cohesive energy. In this note the following procedure has been adopted to separate the ionic interaction and interaction due to the electrons in terms of cohesive energy, i.e.

\[
\phi = \phi_i + \phi_e
\]

where \(\phi\) is the total cohesive energy; \(\phi_i\), energy due to ions; and \(\phi_e\), energy due to electrons. Further,

\[
\phi_e = E_f + E_x + E_c
\]

where

- \(E_f\) (fermi energy) = \(- 2.21/r^2\) Rydberg
- \(E_x\) (exchange energy) = \(- 0.916/r\) Rydberg
- \(E_c\) (correlation energy) = \([0.0622 \ln r - 0.096]\) Rydberg,

while 1 Rydberg = \(13.0 \times 1.6 \times 10^{-24}\) ergs.

Hence, energy due to electrons

\[
\phi_e = \left[\frac{2.21}{r^2} - \frac{0.916}{r} + [0.0622 \ln r - 0.096]\right] \text{Rydberg}
\]

... (6)
NOTES

(---) PRESENT STUDY
(---) K. MOHAMMAD et al. STUDY
(---) A. SARKAR et al. STUDY
(••••) EXPERIMENTAL POINTS

Fig. 1—Phonon dispersion curve for lead

(---) Present study
(---) K. Mohammed et al. study
(••••) S. C. Vrati study
(••••) Experimental points

Fig. 2—Phonon dispersion curve for palladium

(---) Present study
(••••) A. Rajput study
(••••) S. C. Vrati study
(••••) Experimental points

Fig. 3—Phonon dispersion curve for platinum
Here $r$ is the dimensionless quantity and may be varied like 2, 3, 4 or 5 while ln is the natural log.

Discussion—In their recent studies, Singh and Rathore employ the composite compressibility of solids to evaluate the paired parameters of the general potential on the one hand while they make use of Cauchy’s discrepancy (compressibility of electrons) to determine the three-body parameters of the potential on the other hand. It is evident that the compressibility of electrons enters in both the paired and three-body parameters. The generalised potential studies are inconsistent with respect to (a) electron’s contribution towards the parameters and (b) symmetry requirements. Mishra and Rathore have separated two- and three-body parts for compressibility on the lines of Mohammad et al. These studies also ignore the most significant contribution to the binding energy which arises from the interaction between the metal ions and the electrons, even though the potential is fitted to the total cohesive energy. In the present work we have developed three-body morse potential to get their input data from both ionic compressibility and cohesive energy.

The experimental data on Pb have been compared with our results and also with the theoretical findings of Mohammad et al.; and Sarkar et al. Our results include directions near the zone boundary along the direction [110]. The neutron scattering data on Pd are in better agreement with our results than with those of other theoretical findings of Mohammad et al. and Vrati.

Our results in the Pt are very close to the experimental findings of Dutton et al. The theoretical results of Rajput deviates upwardly, while that of Vrati deviates downwardly with the experimental findings. The deviations particularly at zone boundaries may be attributed to (i) spin-orbit coupling, (ii) superconductivity and other electronic properties associated with electron phonon interactions and (iii) Friedel oscillations associated with Fermi surfaces.

Figs 1, 2 and 3 represent the phonon frequencies of the fcc solids Pb, Pd and Pt. Table 1 shows the computed force constants of the same metals.

<table>
<thead>
<tr>
<th>Solid</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\beta_1$</th>
<th>$\beta_3$</th>
<th>$\beta_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb</td>
<td>0.051</td>
<td>0.005</td>
<td>0.391</td>
<td>-0.020</td>
<td>0.054</td>
</tr>
<tr>
<td>Pd</td>
<td>-0.179</td>
<td>0.029</td>
<td>1.779</td>
<td>0.008</td>
<td>0.175</td>
</tr>
<tr>
<td>Pt</td>
<td>-0.247</td>
<td>0.030</td>
<td>2.032</td>
<td>0.075</td>
<td>0.282</td>
</tr>
</tbody>
</table>

Table 1—The computed force constants ($\times 10^4$ dynes/cm)

References
1. REF. NO. P-509 1927-73
2. Title of the Paper: "Three Body...""Pd, and Pb"
4. Address of the Authors: D.A.V. College, Dept. of Physics, Kanpur.
5. Estimated STATUS: ACCEPTED/REJECTED
6. Estimated Time of Publication, if page charges are honoured:
   Vol. 5 No. 1
   Jan. 1993
7. Estimated Time of Publication, if page charges are not honoured:
   Vol. 6 No. 1
   Jan. 1994
8. Estimated number of printed pages: -20-
9. Estimated printing charges at the rate of Rs. 75/- per printed page with 10 free reprints.
10. Draft/Cheque to be issued in favour of "School of Optics, Hyderabad"
(please add Rs. 5/- extra for clearance of out-station cheques).
11. Deadline date for sending page charges:
   November 30, 1992
12. Please inform if you want to withdraw your paper.

* Thank you very much for your kind help and co-operation *

(K. Surender)
Assistant Editor, J.P.A.P.