NON-CENTRAL INTERACTIONS IN NON-CUBIC METALS

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PREFACE

The present investigations deal with the non-entral interactions in non-cubic metals. Non-central orces have been invoked to explain the Cauchy discrepancy in the case of metals. There are two ways in which these non-central interactions have been expressed, in one as a combinations of central and volume forces and in the second as the sum of central plus angular forces. The volume forces according to Fuchs[1] owe their origin to the presence of the free conduction electrons in metals. In the case of bcc and fcc metals de-Launay[2] by resolving each plane wave into a dilatal and shear part found that the Cauchy discrepancy must be equal to the bulk modulus of the free electron gas. In their paper 'on elastic and force constants of a simple tetragonal crystal' Mitra and Gokhale[3] have applied a similar approach in

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1. K. Fuchs. Proc. Roy. Soc. <u>A153</u>, 622 (1936).
2. J. deLaunay J. Chem. Phys. <u>21</u>, 1975 (1953).
3. G.B. Mitra and V.B. Gokhale J. Chem. Phys. <u>26</u>, 1655 (1957).

which the equations of motion are expressed in terms of a dilational strain and shearing strain and the effect of the electron-gas is introduced in the former. Their results demand the equality of $(C_{12} + C_{44})$ and $(C_{13} + C_{66})$ which is not supported by the experiments. In the present investigations, it was therefore decided to reexamine the inconsistency on the basis of the non-central forces. The angular forces have been introduced in two different ways one by Clark, Gazis and Wallis[4] (CGW) and the other by de-Launay[2]. The former presents some difficulties therefore the latter approach was adopted for the body centred tetragonal indium. A new secular determinant was set up by considering one-two-three neighbour non-central angular interactions. This determinant when compared in the long-wave length limit with the elastic determinant makes C_{13} and C_{44} double valued. This apparent double valuedness disappears on the applications of the well known Huang's condition of equilibrium.

4. B.C. Clark, D.C. Gazis and R.F. Wallis: Phys. Rev. 134A, 1486 (1964).

The failure of the above approach made it abundantly clear that the angular forces in themselves cannot account for the inequality observed in the case of Cauchy discrepancies for indium. Therefore an alternative approach in which the electron-ion interaction can exhibit anisotropy becomes necessary. Electron-ion interactions have been treated in different ways by various authors (de-Launay[2], Bhatia[5] Leibfried and Brenig[6], Sharma and Joshi[7] and Krebs[8]) in the field. The introduction of anisotropy in the electron-ion interactions seemed possible only in Joshi's[7] model developed for cubic metals. In this model, the electronic contribution to the force constants is obtained by averaging the electron displacement in an atomic polyhedron and by approximating this polyhedron by a sphere of an equivalent volume. The same was used by Gupta and Dayal[9] in the lattice dynamics

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5. A.B. Bhatia, Phys. Rev. 97, 363 (1955).
6. G. Leibfried and W. Brenig, Z. Phys. 134, 451(1953).
7. P.K. Sharma and S.K. Joshi, J. Chem. Phys. 39, 2633 (1963).
8. K. Krebs Phys. Rev. 138A, 143 (1965).
9. R.P. Gupta and B. Dayal Phys. Stat. Soli. 8, 115 (1965).

of hexagonal metals. The replacement of atomic polyhedron in cases where the axial ratio $\frac{c}{a} \neq 1$ is clearly unreasonable. In the present investigation therefore it was thought more appropriate to consider the electron ion interactions by replacing the atomic polyhedron by an ellipsoid of an equivalent volume. The deduction of the expressions for the electron-ion interactions by approximating atomic polyhedron by an ellipsoid of an equivalent volume and application of these expressions for the study of the lattice dynamics of nine non-cubic metals (two tetragonal and seven hexagonal) namely, indium, white-tin, beryllium, magnesium, thallium, zirconium, hafnium, titanium and yttrium, form the subject matter of the entire present investigation. The three important features of the new electron-ion interaction expressions are:

(i) They pass the test of degenerating into Joshi's[7] expression for the cubic case as the axial ratio $\frac{c}{a}$ becomes unity.

(ii) With five neighbour central interaction in the case of indium the two Cauchy discrepancies

$C_{13} - C_{44}$ and $C_{12} - C_{66}$ in conformity with the experiment turn out to be different.

(iii) The ratio $\frac{C_{13} - C_{44}}{C_{12} - C_{66}}$ is found to be a function of the axial ratio, giving a close agreement between the calculated and the observed values.

In the presentation of the results availability of the experimental data has remained one of the chief considerations. For example, low temperature Θ-T curves for all the metals are drawn and are compared with the experimental curves. Dispersion relations have been plotted along symmetry directions for all of them whereas comparisons with experiment have been done only for beryllium and magnesium for which data were available. The results of the present investigations are completely new and have been carried out for the first time. The essential details about all the present investigations are presented in the form of a thesis comprising of five chapters and three appendices. First two appendices are thought necessary for giving details about some preliminary and supplementary work carried out along with the present investigations. Part of the work has been published, the details of which are given at the end. The papers appear in the joint name of the supervisor (Dr. B. Sharan) and the author (R.P. Bajpai). It may be noted that the supervisor was mainly responsible for suggesting the problems and valuable discussions whereas the rest was done entirely by the author himself.

The following is the chapterwise summary of the thesis.

CHAPTER I INTRODUCTION

This Chapter gives chronological description of the development work done by the previous workers in the field.

CHAPTER II

Non Cubic Structures their reciprocal lattice and the allowed wave vectors.

It deals with the description of lattice, Brillouin zone and the enumeration of the phase points. It has been shown that the Brillouinzone is divided into 10x10x10 points, they reduce to 84 and 110 non equivalent points in the case of hcp and tetragonal indium respectively, under symmetry operations.

CHAPTER III Secular determinant for different elastic force model.

It deals with the deduction of the electron- ion interaction expressions for the non-cubic metals by approximating the atomic polyhedron by an ellipsoid of an equivalent volume. The secular determinant for non-central interaction consisting of central and electron-ion part for tetragonal and hexagonal metals have been set up. Essential features of expressions and results about Cauchy discrepancy have been discussed. A new secular equation for one-two-three neighbour non-central angular interactions in indium is also discussed.

CHAPTER IV Dispersion Relation and heat capacities of hexagonal metals.

It presents dispersion relations along [0001] and [01$\bar{1}$0] directions and Θ-T curves for most of the hexagonal metals. For magnesium and beryllium dispersion relations are compared with the results of neutron scattering data while for other metals comparison for dispersion relations is not made due to lack of experimental data on it. θ-T curves for all other metals are compared with the experimental curves. All of them are in good agreement with the experimental results.

CHAPTER V Heat Capacities of tetragonal indium.

It gives the heat capacities of tetragonal indium based on new non-central electron force model. Results show good agreement with the experimental θ-T curves.

APPENDIX 1 Dispersion relations of white-tin along [100] direction.

It gives dispersion relations of white tin along [100] directions using the new electron force model. The results show fair agreement.

APPENDIX 2 Dispersion relations and heat capacities of Silver.

It gives lattice dynamics of Silver based on Sharma and Dayal's model. The present dispersion curves along symmetry directions and low temperature θ-T curves show good agreement with the theoretical dispersion curves of Singh and experimental Θ-T curves.

APPENDIX 3.

It gives deduction of the electron-ion interaction part in the ellipsoidal approximation.

LIST OF PUBLISHED PAPERS

1. Electron-Ion Interaction in Non-cubic Metals:
   B. Sharan and R.P. Bajpai.
   Phys. Letters. 31A, 120 (1970).

2. Lattice Dynamics of Hexagonal Metals Based on a New Electron-Ion Interaction:
   B. Sharan and R.P. Bajpai.
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3. Elastic and Force constants of Body Centred Tetragonal Crystals for one-two-three Neighbours Non-Central Interactions.
   B. Sharan and R.P. Bajpai.
   J. Phys. Soc. (Japan) 26, 1359 (1969).

4. Lattice Dynamics and Heat Capacities of Indium.
   B. Sharan and R.P. Bajpai.
   Ind. J. Pure & Applied Phys. Vol. 8, (1970).

5. Lattice dynamics of zirconium and hafnium.
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7. Lattice specific heats of beryllium, magnesium and thallium.
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8. Lattice Dynamics of Silver based on the models of Dayal and Sharma; B. Sharan and R.P. Bajpai.
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9. Lattice dynamics of white-tin.
B. Sharan and R.P. Bajpai.
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10. Lattice dynamical study of cobalt.
B. Sharan, R.P. Bajpai and Ashok Kumar.
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