NON-CENTRAL INTERACTIONS IN METALS

ASHOK KUMAR

Thesis submitted to Indian Institute of Technology, Delhi
in partial fulfilment for the Degree of
Doctor of Philosophy
1973

PREFACE

Although a lot of theoretical work has been done[1] in lattice dynamics to interpret the thermal properties, phonon dispersion curves and Cauchy discrepancies in metals, still there are at least two areas which need further considerations and refinements. One is that of Cauchy discrepancies. It is well known[2] that if the lattice structure is such that every lattice particle occupies a centre of symmetry and if the particles interact with central forces, then there would exist a few relations between the elastic constants. These are known as the Cauchy relations.

These relations are almost satisfied by the experimental values of the elastic constants in case of ionic solids, and it may thereby be concluded that the interaction in ionic solids is central. In the case of covalent solids, however, the Cauchy relations are not satisfied. This discrepancy demands the incorporation of angular interaction besides the central one. In case of metals also, these relations are not satisfied. Since metals have free electrons, the volume forces should also be invoked along with the central and angular forces. Thus the total interaction in metals is divided into three parts, (i) central, (ii) angular, and (iii) volume.

---

1. S.K.Joshi and A.K.Rajagopal, Solid State Physics, 22, 159 (1968).

2. M.Born and K.Huang, Dynamical Theory of Crystal Lattices, Oxford University Press (1954).

The volume forces owe their origin to the interaction of the conduction electrons with the ions. Mostly they have been incorporated in either phenomenological or semi-phenomenological manner. The many-body notion of the problem makes its explicit theoretical evaluation rather difficult. One of the approaches that is relevant to the present discussion is by Sharma and Joshi[3]. They visualized the metallic crystal as a lattice of bare ions imbedded in a uniform cloud of electrons. The expression for the volume dependent potential energy was obtained by averaging the compressive strain over the Wigner-Seitz sphere. The replacement of Wigner-Seitz polyhedron by a sphere, according to Wilson[4], 'makes the energy a function of volume only and not of the type of the crystal structure'. A better approach to the problem is due to Sharan and Bajpai[5], who averaged the compressive strain over an ellipsoid of equivalent volume. The approach is still approximate, besides the fact that the determination of the semi-axes of the ellipsoid is questionable.

In the present investigation five cubic metals viz. lithium, sodium, potassium and copper have been studied. There is only one Cauchy relation viz. $C_{12} = C_{44}$ in the case of cubic structure. The unknown parameters (force constants and the bulk modulus of electron gas) appearing in the process of

---

3. P.K.Sharma and S.K.Joshi, J.Chem.Phys., 39, 2633 (1963).

4. A.H.Wilson, Theory of Metals, Cambridge University Press (1953).

5. B.Sharan and R.P.Bajpai, Phys.Letters, 31A, 120 (1970).

incorporating the three types of interactions are evaluated from the experimental values of three elastic constants and zone boundary frequencies. In addition to cubic metals, the tetragonal indium has also been studied. This, being tetragonal, is less symmetrical than the cubic metals and therefore contains more number of elastic constants and force constants. Also, it has two Cauchy relations viz. $C_{12} = C_{66}$ and $C_{13} = C_{44}$. Further, the experimental values of frequencies are not available, and this presents some difficulty in evaluating the force constants.

The entire work has been divided into six chapters.

In the first chapter of the thesis the chronological developments in the field of lattice dynamics of metals with special reference to force constant model approach have been discussed.

In the second chapter the structure of b.c.c., f.c.c. and body-centred tetragonal (b.c.t.) lattices in direct and wavenumber spaces have been described. In addition, it deals with the construction of the Brillouin zone of b.c.t. lattice.

In the third chapter the equations of motion have been developed for b.c.c., f.c.c. and b.c.t. lattices. The angular force interaction is considered in two ways viz., (i) the de Launay model[6], and (ii) the CGW model[7]. (This is the first time that the CGW model has been extended to the tetragonal structure).

---

6. J. de Launay, Solid State Phys., 2, 219 (1956).

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

In the fourth chapter the volume forces have been discussed. The compressive strain of the conduction electrons has been averaged over the actual shape of the Wigner-Seitz polyhedron.

In the fifth chapter the unknown parameters, viz. the central and angular force constants and the bulk modulus of the electron gas, have been evaluated. In the case of tetragonal indium where the experimental values of frequencies are not available, the bulk modulus of electron gas has been evaluated by making use of the virial theorem.

In the sixth chapter specific heats, frequency distribution, θ_D- T and dispersion curves have been obtained. The anomaly, observed experimentally[8], in the [100] direction of the dispersion curves in lithium has been explained.

The entire work has resulted into the following papers by the present author:-

1. Lattice dynamical study of indium, Phys.Rev. B7, 1362 (1973).
2. Bulk modulus of the electron gas, Physica, 63, 626 (1973).
3. Lattice dynamics of lithium,- J.Phys.F: Metal Phys.
4. Electron-ion interaction in metals, Solid State Commun., 11, 1223 (1972).
5. Lattice dynamics and the heat capacity of indium, J.Phys.C: Solid State Phys. 5,3161 (1972).
6. Lattice dynamics of copper, communicated.
7. Lattice dynamics of sodium and potassium, communicated.

---

8. H.G.Smith et al., Neutron Inelastic Scattering, Proc. of Symposium, Vienna, 1, 149 (1968).

ACKNOWLEDGEMENTS

I wish to express my sincerest gratefulness and profound sense of gratitude to Professor B.Sharan for the valuable guidance, kind encouragement and inspiration without which the present work would not have been possible. I take this opportunity to express my deep sense of gratitude to Dr. V.Rama Murthy also whose guidance, encouragement and inspiration can never be forgotten.

I would also like to express my indebtness to Prof. M.S.Sodha and Prof. K.L.Chopra for providing all the essential facilities in the Department.

With great pleasure, I express my thanks to Dr. L.M.Tiwari, Dr. R.P.Bajpai, Mr. K.Neelakandan and other colleagues for stimulating discussions. Thanks are also due to Mr. T.N.Gupta, for the efficient typing, and Mr. N.S.Gupta, for drawing the figures.

Finally, the financial assistance provided by the Council of Scientific and Industrial Research is most gratefully acknowledged.

Ashok Kumar

(Ashok Kumar)

CONTENTS