LATTICE DYNAMICAL STUDY OF TETRAGONAL METALS

by

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Thesis submitted to Indian Institute of Technology, Delhi in partial fulfilment for the degree of

DOCTOR OF PHILOSOPHY

DEPARTMENT OF PHYSICS

INDIAN INSTITUTE OF TECHNOLOGY, DELHI

1982

PREFACE

Many physical properties of solids are directly dependent upon their atomic arrangement and the corresponding crystal structure. The unusual properties possessed by metallic glasses, amorphous semiconductors and composite materials are a consequence of the modifications in their atomic arrangement. In order to develop new materials for specific purposes, it is essential to understand the relation between the interatomic forces which hold the atoms together and the macroscopic properties exhibited by the solids. However, the nature of these interatomic forces has eluded exact description. One of the ways to probe into their nature is to disturb the equilibrium configuration of atoms in the solid and to study the reaction of the unbalanced forces to this disturbance. This takes us to the field of lattice dynamics which deals with the coupled vibrations of atoms that are arranged on the lattice sites of a crystal. Information regarding the nature and range of interatomic forces is obtained by comparing the theoretically deduced spectrum of permissible frequencies of solids and the vibrational frequency dependence on its wave vector with the corresponding experimental data.

The phonon frequencies of metals are calculated either by a force constant method or by a pseudopotential approach. The atomic interactions are split into short-range ion-ion interactions and long-range electron-ion interactions in the former whereas they are expressed in terms of an appropriate

pseudopotential in the latter. A variety of force constant models in which the ion-ion interactions are expressed interms of tensor, central and angular forces and the electron-ion interactions in terms of volume forces as well as a large number of pseudopotentials have been developed for the lattice dynamical study of metals. However, the cubic metals in general and alkali metals in particular have received most of the theoretical attention so far and their experimental data could be fitted as well as predicted rather well by many theoretical models.

Among the noncubic metals the lattice dynamical study of hexagonal close packed metals has received sufficient attention but the theoretical models suffer from many serious deficiencies. On the contrary, the tetragonal metals have received hardly any theoretical attention in the past. Monatomic indium and diatomic white tin are the only metals which have tetragonal structure. Both of them exhibit superconducting properties at low temperatures. Diamond cubic (DC) grey tin undergoes marteneitic transformation to body centred tetregonal (BCT) white tin. Besides, the misinterpretation of the crystallographic equivalence between face centred and body centred tetragonal structures has led to many serious errors in the lattice dynamical studies of indium. Above all, certain aspects of interatomic forces which are completely obscured by the high degree of symmetry associated with the cubic structures manifest themselves in these structures leading to the elastic inconsistency of the force constant models.

All force constant models that have been developed for the lattice dynamical study of tetragonal metals suffer from serious inadequacies. For instance, some of these neglect the electron-ion

interactions altogether while others do not satisfy the symmetry requirements of the lattice. In the present investigation, the contributions from umklapp processes to the electron-ion interactions, summed over several reciprocal lattice vectors, are included in order to restore the translational symmetry to these models. Further,the elastic inconsistency of these models gives rise to two different expressions for C_{44}. The author has analysed a variety of force constant models to establish that this deficiency is associated with the neglect of contributions from "three-body forces" to the ion-ion interactions of noncubic metals. Besides, phonon frequencies, phonon distribution function and the specific heat of indium and tin have been calculated using models which are free from above mentioned deficiencies and treating the atomic arrangement as face centred tetragonal (FCT) as well as body centred tetragonal (BCT) inorder to arrive at the correct interpretation for their crystallographic equivalence.

The entire work has been divided into eight chapters.

The first chapter deals with the chronological developments in the field of lattice dynamics of tetragonal metals and the scope of the present work. Second chapter deals with the construction of Brillouin zones of these metals and the enumeration of phase points. Variety of force constant models developed for the lattice dynamical study of these metals are described and their deficiencies are discussed in chapter three. Volume forces due to presence of conduction electrons and the importance of umklapp processes are described in chapter four. Fifth chapter deals with the evaluation of force constants of all models using requisite number of experimental elastic constants and zone boundary frequencies.

Sixth chapter describes a fundamental analysis of various force constant models which reveals the origin of the elastic inconsistency of the models. In seventh chapter the results of the present investigations are presented and compared with others. The conclusions based on the present work and suggestions for the future work are included in the last chapter.

The following papers deal with the work done by the author on indium, other papers dealing with the work on tin are under preparation.

1. Phonon dispersion curves of indium
   J. Phys. F: Metal Phys. 11, 2275(1981).

2. Lattice dynamical study of body centred tetragonal indium
   Pramana 19(1982) ~~(In Press)~~. 435

3. Lattice dynamical study of face centred tetragonal indium
   Canad. J. Phys. 60(1982) (In Press). 58

4. Elastic inconsistency of force constant models for tetragonal indium
   (Communicated to Physica B)

5. Role of three-body forces in the lattice dynamics of noncubic metals
   (Communicated to Phys. Stat. Solidi (b))

Besides, the author has investigated the homology of rare gas solids, which resulted in two papers. These are enclosed at the end of the thesis.

This work was done by the author 1978-1982 at the Physics Department, Indian Institute of Technology, Delhi, under the supervision of Dr. V.Ramamurthy.

ACKNOWLEDGEMENTS

It is my privilege to express my heartfelt gratitude and reverence to Dr. V.Ramamurthy, Assistant Professor of Physics, I.I.T.Delhi for his excellent guidance, keen interest and constant encouragement throughout the course of research work.

I am highly grateful to Dr. J.C. Swihart for sending the phonon frequencies of indium and to Dr. H.G. Smith for kind permission to use the data.

My thanks and regards to Prof. P.K.C.Pillai and Prof. B.B.Tripathi, the successive Heads of the Department of Physics for providing necessary facilities. I am thankful to the authorities of Computer Centre for their help in using the computer.

I am greatly indebted to my colleague Dr. Satish Kumar Mahna for many stimulating discussions and kind co-operation. My sincere thanks are also to all my friends whose timely help and encouragement can never be forgotten. To mention here are Mr. N.S.T. Sai, Mr. A.K. Saraswat, Mr. M.V.N. Ambika Prasad and Mr. A. Thayumanavan. Thanks to Mr. Malik for his pains taking typing the manuscript.

Finally, the financial assistance provided by I.I.T.Delhi and C.S.I.R., New Delhi are gratefully acknowledged.

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