LATTICE DYNAMICS OF METALS AND SEMICONDUCTORS

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To My Parents

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ABSTRACT

The present work has been devoted mainly to the theoretical studies of the lattice dynamics of metals and semiconductors. Two distinct approaches have been followed to investigate the problem.

The first part deals with the elastic force approach and is based on the Born-von-Karman theory of lattice dynamics. The total interatomic force has been divided into three parts: central, angular and volume. The scheme has been used to study some of the lattice dynamical and thermodynamical properties of a few body centered cubic, face centered cubic and hexagonal close packed metals and semiconductors having the diamond structure (including diamond).

The second part deals with the pseudopotential approach. A model potential has been developed to investigate the elemental semiconductors and has been used to study some of the electronic properties of silicon, germanium and grey-tin. The scheme, with a different model potential, has also been applied to investigate the band structure of five simple metals.

The work has resulted in the following publications:-

1. "A Model Pseudopotential for Semiconductors", Phys. Lett. 36A, 65 (1971).
2. "Noncentral Forces in the study of Lattice Dynamics of Metals", J.Phys.F. 2, 426 (1972).

3. "Calculation of Electronic Band Structure of Aluminium, Lead, Lithium, Sodium and Potassium", Ind. J.Pure App. Phys. 10, 768 (1972).

4. "The Lattice Dynamics of Hexagonal Close Packed Metals", J.Phys.Soc.Japan 34, 1006 (1973).

5. "Phonon Dispersion in Scandium", Phys.Lett. 43A, 365 (1973).

6. "Phonon Dispersion in Diamond", Presented in the Indo Soviet Conference on Solid State Materials, I.I.Sc., Bangalore, India, (1972, To be published in the Proceedings).

7. "Pseudopotential Approach in the study of Lattice Dynamics of Semiconductors", Presented in the Indo Soviet Conference on Solid State Materials, I.I.Sc., Bangalore, India (1972, To be published in the Proceedings).

8. "Angular Forces in the Lattice Dynamics of Diamond Crystal Lattices", J.Phys.Chem.Solids, (1973, In Press).

9. "The Resistivity and Thermoelectric Power of Molten Semiconductors", J.Phys.Chem.Solids, (1973, In Press).

10. "CGW Angular Force Model for Hexagonal Close Packed Metals: An Application to Be, Mg and Zn", (1973, Communicated).

CONTENTS

PART II