

A Study of Lattice Dynamics and Other Physical Properties of Some Semiconducting Crystals of II, -VI, III-V and IV-IV Compounds



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ABSTRACT

The dynamical behaviour of constituent atoms in solid phase plays a very important role in the study of cohesive forces in solid and it provides promising means for adequate description of a large number of solid state phenomena like phonon dispersion curves, thermal and elastic properties diffuse scattering of X-rays, neutron scattering, spin-lattice relaxation etc. In order to understand any of these phenomenon, it is necessary to develop the theory of vibration of atoms which is the theory of lattice dynamics.

INTRODUCTION

With the availability of high intensity thermo-neutron beams from nuclear reactors, it became possible to study the frequency distribution function and phonon dispersion relation. This stimulated a lot of dynamics of crystal lattices. Various models regarding the nature of inter atomic interaction in solids has been proposed to describe the nature of vibration of atoms in solids. Different theoretical model of lattice dynamic provide an understanding of the vibrational, thermo-dynamical, elastic, optical and other physical properties. A reliable theoretical model for the lattice dynamic of perfect crystal help in predicating the physical properties of imperfect crystals. The influence of vibration of atoms in crystals on the thermo dynamic properties of solids, and the relation of elastic property of a crystal with the atomic force constants which determine the scale of lattice vibration at a given temperature have been the subjects of considerable study these days.

Various theoretical models for the lattice dynamics of tetrahedral crystals having Zinc-Blende structure have been proposed by different workers. Such crystals are formed mainly from the elements of II, III, IV and V group of periodic table. These crystals which have two interpenetrating face centred crystals lattices are II-VI, III-V, IV-IV compounds. These compound are partially covalent and ionic in bonding except the crystals of diamond structure. The lattice dynamical models employed to describe different interactions inside the crystals of these compounds should be physically consistent with the nature of bonding manifested by them.

We were motivated to develop a new theoretical model for the lattice dynamics of Zinc Blende crystals due to simplicity of their structure and the use of some of the solids of this structure as binary semiconductor. This has

drawn the attention of a large number of theoretical and experimental workers to study the lattice dynamics of this structure. An exact knowledge of a perfect lattice provides a basis for the study of perturbed lattice. The theory of lattice dynamics for semiconductors has been discussed with the phenomenological rigid ion and shell models. In the shell model calculation the polarizability of ions is accounted by considering both core and shell interaction between respective ions. The shell model though it gives a reasonable agreement with neutron scattering experiment, requires heavy computation and involves a large number of parameters. Further, the shell model loses its significances when one studies the land effects of narrow.

Basically the dynamical theory of crystals is a many body problem which involves a large number of electrons interacting with the ions constituting the lattice and can not be solved explicitly. Hence it is therefore, imperative to adopt certain approximations in solving the problems. The approximations adopted in developing the general theory of lattice dynamics are the adiabatic approximation and the harmonic approximation.

In adiabatic approximation, electrons in metallic crystals are treated to responds to quickly to the motion of ions, that their state is always just a function of the ionic co-ordinates. Hence adiabatic principles allow to separate the ionic motion from electronic motion leaving only a residual interaction between the electron and phonons.

A simple and practical method is presented for analysing the vibrational symmetries in any perfect crystal. It takes the space spanned by the complete set of normal modes of wave vector q , and factorizes it into a 'cell space' SC, and a 'complex Euclidean space' SE. Two simple equations describe the effect of the crystal symmetry operations in each of these factor spaces, so that the symmetry of all the normal modes can readily be determined. This formalism makes it easy to understand several qualitative features of vibrational spectra: for example, if the unit cell contains only two atoms and they are dissimilar, the irreducible representations inside the Brillouin zone always appear doubled. Similarly, it is shown that the number of different types of atom vibrating in any mode cannot exceed the number of times that modes of the same symmetry appear in the vibrational spectrum: so that if a mode has a unique symmetry, only one type of atom is vibrating in that mode, and all other atoms are stationary. Vibrations in the perovskite structure are discussed briefly by way of an example, and this is followed by a fuller treatment of the zineblende and diamond structures.

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