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Various Theoretical Models to Study Crystal Structures

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ABSTRACT

Crystals are considered due to periodicity of atoms in it. The study of nature of interatomic forces in crystals is of great importance as it is the way to understand the physical properties of the solids.The dynamics of atoms in crystals is known as Lattice Dynamics.All physical properties of crystals depend upon their constituent atoms which can be obtained with the help of theoretical models of lattice dynamics. The quanta of energy in an elasticwave travelling through solid is called phonon. As phonons are elementary particles for excitation of solids, they provide complete information about interatomic forces in solids. The physical properties of solids including thermal, optical and electronic properties are directly dependent upon the frequency-wave vector relationship called phonon dispersion relation. Thus, phonon dispersion relation is an essential feature for lattice dynamics.

Keywords: Lattice dynamics, interatomic forces, force constant, dispersion relation.

I INTRODUCTION

Various Models

Some of widely used models in lattice dynamics are briefly discussed below:-

Conventional Force Constant Model

In conventional force constant model [1], [2], the motion of the nucleus is determined by the effective potential which depends only on nuclear coordinates. The electrons are assumed as a medium for exerting inter nuclear force. The wave function of the electrons is taken to be same as if the nuclei are occupying their instantaneous positions. This model was modified by considering general interactions out to third-nearest neighbours in the plane and second-nearest neighbours in adjacent planes.This model gives an exact fit to all five elastic constants and a good fit to phonon dispersion data.

Born-Von Karman Model

In Born-Von Karman model [3], [4], the vibration of particles follows Hooke's force law and condition of equilibrium for equation of motion is used. It is a basic model to describe movements of atoms in a crystal lattice. The model is based on Born-Oppenheimer approximation. This proximity means that vibrations of atoms in a lattice is described as a mass, the line between two springs is fixed which swings back and forth. Diamond was the first crystal structure investigated by Born using this model.

Shell Model

In this model [5], every ion is divided into a rigid spherical shell of a portion of nucleus and rest of electron cloud. The two are coupled together by an isotropic spring and have a common centre in equilibrium configuration. This model permits a better description of dielectric polarization in ionic crystals, it does not go beyond the rigid-ion model with respect to elastic behaviour of these solids. It is an extension of the Born-Karman model in which each atom is no longer rigid but regarded as charged core consisting of nucleus and inner electrons and an oppositely charges shell representing other electrons. This model allows an atom to have the property of polaizability in electric field and of distortion polarizability under the influence of short range forces acting through both core and shell.

Rigid Ion Model

In rigid ion model [6], the forces in crystal arise from two contributions: one belongs to long range or coulombian interaction between effective charges on ions and other is short range central and non-central interactions. In ionic or semi-ionic solids like silicates, it appears that coulombian terms are most important component of cohesive energy. Ions are obviously not point charges as assumed when calculating coulombian energy, but instead are composed of a nucleus and an associated electron cloud of finite size. It is therefore, necessary to include a term in the potential which represents energetic effect of overlap of electron clouds which results in a short range repulsion strongly felt by nearest neighbour ions.

Ab-Initio Calculation Model

The basic idea of this model [7] is to determine force constants via total energy of crystal under investigation. Within adiabatic approximation, total energy is a function of only position of ions. There are two approaches for the calculations of total energy: firstly direct approach and secondly linear approach. In this model, there is replacement of analytic model by a full quantum mechanical electronic structure calculation of a super cell of N atoms. This can be done by making a series of small displacements of atoms and evaluating forces exerted on other atoms. Each such calculation provides 3N elements of force constant matrix and symmetry can be used to deduce these elements. This reduces the number of electronic structure calculations required.

de Launay Angular Force (DAF) Model

In DAF model [8], the relative displacement of reference atom and one of its neighbours is considered. In one dimensional lattice dynamics, the interatomic force acts only along the line joining two neighbours called central force. In more than one dimensional lattice, an additional force comes into play called angular or non-central force which depends on the angle which the line joining moving atoms make with the equilibrium position of the line. The restoring force is the vector sum of both central and angular force. Different force constants are used for various types of neighbours. The net force on the reference atom is obtained by summing over the contribution from all the neighbours.

Density Functional Theory(DFT)

DFT [9] has long been the mainstay of electronic structure calculations in physics and chemistry. It is a quantum mechanical modelling method. It became quite popular due to its useful balance between accuracy and computational cost. Functional is the function of another function. In this model, spatially dependent electron density is used as functional. So, it was given the name density functional theory. This model became quite popular in 1990s when approximations used were further refined to better model the exchange and correlation interactions.It is a completely different way of approaching any interacting problem by converting it exactly into a non-interacting problem Here, a problem of N-electrons in a material can be studied as a set of N one-electron equations which are known as Kohn-Sham equations.

CONCLUSION

DFT allows larger system to be treated with high accuracy which was not possible with traditional methods. Computational costs are relatively low as compared to other models.This model is much easier to solve. It is applicable to large variety of fields with ground state electronic problem being the most common.

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