CHAPTER 1

GENERAL INTRODUCTION

1.1 Lattice dynamics and neutron scattering

Most of the solids with which physicists or material scientists are concerned are crystalline. For a complete understanding of the crystalline solid, on the one hand one has to study the static atomic arrangement and consequent crystal symmetry manifested by real solids, on the other hand studies are to be made for the excitations that the crystal lattices can experience and their relation with the various physical properties of the solid. The present investigation is concerned with the lattice vibrations that play a dominant role in many solid state phenomena. Hence the subject of the lattice dynamics of metals has been one of fundamental importance for the study of the thermodynamical, elastic, electrical and other physical properties of solids. All those physical properties of a crystal which depend on the heat motion of the constituent particles require for their detailed explanation a knowledge of the actual form of phonon spectrum, which is studied both theoretically and experimentally.

The progress made in about the last two decades in the field of slow neutron inelastic scattering [1-6] has caused renewed interest in the subject of lattice dynamics which is the oldest branch of or rather which has started modern solid

state Physics. Inelastic neutron scattering is now a well established technique for the experimental study of the dynamical properties of condensed matter at the atomic level. Neutrons serve as an excellent probe for lattice dynamical studies of solids on account of the fact that neutrons interact with both nuclei and magnetic, or unpaired electrons, and that slow neutrons have energies and wavelengths that match those of excitations and collective modes, e.g., rotational energy levels in molecules and acoustic and optic phonons.

From the point of view of crystal dynamics, the most useful scattering processes are those involving one phonon - scattering; subject to the existence of coupling mechanism, the single phonons produce significant scattering and the measurement of this yields valuable and direct information on the phonon spectrum. While the incoherent scattering gives information about the frequency distribution function, the one-phonon coherent scattering is used for finding the phonon wave vector ($\vec{q}$) vs frequency (ν) dispersion relations. The one-phonon scattering process follows the two conservation conditions[3], those of energy and crystal momentum:

$$E_o - E \equiv \frac{\hbar}{2m}(k_o^2 - k^2) = + h\nu, \qquad (1.1.1)$$

$$\vec{k}_o - \vec{k} \equiv Q = 2\pi \vec{\tau} \pm \vec{q}, \qquad (1.1.2)$$

where E_o, E are the initial and final energies $\vec{k}_o$, $\vec{k}$

the corresponding neutron wave vectors, m the neutron mass, $\vec{Q}$ the momentum transfer vector and $\vec{\tau}$ any reciprocal vector. The + (-) sign corresponds to energy loss (gain) processes related to phonon creation (annihilation).

To determine the phonon dispersion relations using (1.1.1) and (1.1.2) , it is necessary in the experiment to find the energy gain or loss of the scattered neutrons as a function of the scattering direction.

1.2 Theoretical studies

The dynamical theory of metallic crystals is a many body problem of a number of electrons interacting with the constituent ions besides the interaction amongst themselves. The close proximity of atoms that contain many electrons inevitably leads to highly complex wave functions. The atoms of each element have distinct electronic structures and hence there are many different highly complex systems. Due to this variety of problems, which have no rigorous solutions, one is forced to make certain approximations that render the system tractable to study.

Theoretically, this problem is attempted in two distinct ways. The first one is the Born-Von Karman[7] (BVK) approach which is a phenomenological one and is correct within well defined and reasonably good approximations. The second one uses

theories which are more closely linked with the theory of metals. In the second approach, Toya[8] has discussed in a fundamental way the phonon dispersion curves in metals by the extension of the Hartree-Fock method to take into account the effect of correlation as well as exchange interactions between the electrons on their self-consistent shielding field. In the last few years, several workers have studied the lattice dynamics of metals based on the idea of a 'pseudopotential'.[9] This is introduced into the Schrodinger equation and then certain approximations are made to localise the pseudopotential to the ion sites. Wallace[10] has made a detailed lattice dynamical calculation for sodium and potassium using the local pseudopotential theory. Animalu[11] has studied the lattice dynamics of transition metals in the pseudopotential approximation based on a new transition metal model potential (TMMP) of Heine - Abarenkov[12,13] type. Fielek[14] has proposed a simple model for the noble and transition metals using the screened pseudopotential for the conduction electrons response. Very recently, the model potential method of Heine and Abarenkov[13] has been used by Oli[15] to develop a microscopic theory of the lattice dynamics of the acitinide metal thorium.

In spite of this progress made in the pseudopotential models, even to-day the task remains formidable. The pseudopotential models involve approximations which, although are well defined, and whose effects are difficult to estimate. On the other hand, the phenomenological analysis on the lines of BVK theory leads to the occurrence of the interatomic force constants which have

a direct intuitive significance and are therefore of interest. The phenomenological models are important as they allow the calculation of the properties related to the phonon - density of states in a very simple way.

The theoretical study of the lattice dynamics of metals is generally made on the basis of the harmonic and the adiabatic approximations. By harmonic approximation, we mean that in the expansion of the potential energy in terms of the atomic displacement, all terms past those which are quadratic in the displacement are neglected. This implies that the amplitudes of vibration are sufficiently small so that Hook's law is obeyed. There is no phonon-phonon interaction in this case and hence these quasi particles have an infinite life time which in turn means that the energy of the phonons is exactly defined. The neglect of higher order terms in the potential energy expansion in fact prevents us from discussing the anharmonic effects.

The adiabatic approximation means that the eigen functions of the electrons adjust themselves to the nuclear positions in the perturbed crystal almost instantaneously. It is assumed that the core electrons are rigidly bound to the neuclei and the valence electrons respond easily to smooth out the changes in the electrostatic field of the disturbed ions. This approximation allows us to consider the motion of electrons and that of ions separately[4,16].