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A Short Review of Phonon Physics

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Abstract— In this article the phonon physics has been summarized shortly based on different articles. As the field of phonon physics is already far advanced so some salient features are shortly reviewed such as generation of phonon, uses and importance of phonon physics.

Index Terms— Collective Excitation, Phonon Physics, Pseudopotential Theory, MD simulation, First principle method.

1. Introduction

There is a collective excitation in periodic elastic arrangements of atoms or molecules. Melting transition crystal turns into liquid and it loses long range transitional order and liquid appears to be disordered from crystalline state. Collective dynamics dispersion in transition materials is mostly studied with a view to existing collective modes of motions, which include longitudinal and transverse modes of vibrational motions of the constituent atoms. The dispersion exhibits the existence of collective motions of atoms. This has led us to undertake the study of dynamics properties of different transitional metals. However, this collective excitation is known as phonon. In this article phonon physics is shortly reviewed.

2. GENERATION AND PROPERTIES OF PHONON

Generally, over some mean positions the atoms in the crystal tries to vibrate. Even in a perfect crystal maximum amount of phonons are unstable. As they are unstable after some time of period they come to on the object surface and enters into a sensor. It can produce a signal and finally it leaves the target object. In other word, each atom is coupled with the neighboring atoms and makes vibration and as a result phonon can be found [1].

Phonon participates in physical properties of materials. Phonon is called bosons when it is treated as particles. It is some of kinetic energy and potential energy. Photon causes polarizing, electric, magnetic vibrations and it can be known as phonon if it is quasi particle. It can be described as wave packets as it shows both particle and wave properties [11].

Coherent movements of atoms of the lattice of their equilibrium position are known as acoustic phonon. Acoustic phonons can be longitudinal or transverse. If the wavelength of acoustic phonon becomes infinity this may cost zero deformation energy. Pump and probe is an important effect using for generation of coherent acoustic phonons. Velocity and attenuation of high-frequency phonons can be studied from this method where mean free path is very small [7]. Optical phonon exhibits no dispersion to the long wavelength as it has non zero frequency.

Acoustic phonon travels in straight line for long time when temperature is low and it has less scattering. Considering out of phase movement of atoms optical phonon can be found. Optical phonons have no zero frequency and it doesn't show no dispersion near long wavelength limit.

3. COMPUTATIONAL DETAILS

So far many difficult theories have been developed to approximate the Hamiltonian for real metallic systems for approaching phonon physics. For example, density functional theory, pseudopotential theory and semi-empirical methods etc. Pseudo potential is applicable for simple metals. In Pseudo potential core electrons can be eliminated as its effective potential plays important role by the effect on the valences state and sometimes the core electrons are nearly bound to the nucleus [13]. The assumptions are included in pseudo potential concept are

- In one electron Hamiltonian in metals the interaction between electrons can be expressed by potentials. Coulombs repulsion and states are the two important factors for this method. Poisson equation and Pauli's principles help to determine this concept.
- D shell should be tiny and valance and core level can be separated.
- Pseudo potential is weak and small and the equation can be written as,

$$\left[-\frac{\hbar}{2m}+V(r)\right] l\, \psi^{\gamma} >= E\, l\, \psi^{\Upsilon} >$$

$V(r)$ is the one electron real potential. Ψ is state function, ϒ indicates valance state. [9]

MD simulation has been a powerful method for many body problems. To apply this method precise input parameters are needed. Analytical solution cannot be applied when the body is more than two. Precise input can be found either from theoretical or experimental data. Molecular dynamics established relationship between molecular structure and their movements [10]. In Addition, a theoretical study of their condensed states cannot be determined by simple models.
Computer simulation of physical movements of atoms and molecules is called Molecular dynamics. Atoms and molecules are allowed to interact for a span of time. Approximation of phonon physics can give an idea of the motion of the atoms. Generally molecular systems normally have an enormous number of particles and it is impossible to find the properties of such complex system analytically. When the number of body is more than two no result can be reached to a specific destination [4].MD simulation solves this problem by using numerical methods. Microscopic interaction also can be found by this method. MD simulation can be done by this major steps:

- Study the initial parameters such as density, initial temperature, no of particles etc.
- Initialization of the system.
- Calculate particles' forces by periodic boundary conditions.
- Integrate Newton's equation of motion. [4]
  Harmonic approximation, mean square atomic displacements, quasi-harmonic approximation are the methods used for first principles phonon calculations. These calculations can be applied

In material sciences and condensed matter physics [3]. When considering low temperature, the harmonic approximation is useful for solid state physics and it is also good for strong covalent bonding like carbon systems at room temperature [13].
Phonon hydrodynamic is easier than the first principle method calculations though first principle method is more popular these days [6].

4. APPLICATION

For crystalline structure phonon is very valuable for considering various properties and behavior. For example, thermal properties, mechanical properties, phase transition, and superconductivity. There are some examples of applications of the first principles phonon calculations [3].
One of the main excitations of particles is phonon in solid for electrical and sound properties respectively. Phonon dynamics in condensed matter physics has very important impact on modern technology. Such as, now a day's devices are becoming smaller which generates heat. This generated heat makes some unusual parametric changes and to avoid it full dynamics of both electrons and phonon to be needed [5]. Phonon structure is also related to the thermodynamic properties of a solid.

Sensing of phonon which is not equilibrium is very important for the development of dark matter detector. The object may be insulator, semiconductor or superconductor at below transition temperature. As temperature is below transition temperature free electron is very small. As particles scatter off a nucleus of the object phonons can be found at different points on the surface are detected by sensors. It is stored as a function of time [1].
In semiconductor and dielectric solid phonon helps to transport heat. In thermal conductivity scattering at crystal surfaces is detected [8]. Phonon also important for having a clear idea on micro and nanotechnology [6].

Phonons also play an important role in superconductivity. Such as by some processes some specific metals loses all electrical resistance at absolute temperature. At low temperature electrons attract each other slightly by intermediate effect of phonons in superconductor when it is already known electrons repel each other in normal cases. In fact, for many materials phonons are the major conveyors of heat. It is used in thermoelectric devices as well as in computer chips. For quantum mechanics it also can be used as carrier of information.

Another different application of phonon is found in insulators. Phonons are interacted with other carriers and as a result there is an extra voltage in the system [2,12].

5. CONCLUTION:

As we all know two major excitations in solid are phonon and electron. So the main intension of this article was to get a better idea about phonon physics with the help of its limited background. In conclusion it can be said that, as electrical and thermal conductivity are the physical properties of condensed matter so phonon physics has crucial impact in every aspect of solid state physics.

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