Lattice Vibrations – Phonons in Solid State

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Abstract—**Phonons are quanta of lattice vibrations. They play an important role in various phenomena seen in solid state. The physics of phonons and phenomena associated with them are explored.**

Index Terms—Phonons, Lattice Vibration, Solid State, Dispersion Relation

I. INTRODUCTION

THE term phonon is used to draw an analogy between photon representing a quantum of electromagnetic radiation and quanta of lattice vibration. Theory of phonons explains most solid state phenomena which cannot be explained with static lattice theory [1].

II. MECHANICS OF PHONONS

The energy of a phonon can be derived by considering the lattice as a collection of oscillators. There can be many kinds of interaction between atoms. The potential energy of an atom can be expressed as

$$U = U_0 + \sum_{n,\alpha} u_\alpha^n x_\alpha^n + \frac{1}{2} \sum_{n,m,\alpha,\beta} u_{\alpha\beta}^{mn} x_\alpha^n x_\beta^m + O(x^3) \qquad (1)$$

where U_0 is the potential energy in equilibrium, α and β can be x, y or z. u represents the interaction between atoms, x is the position and m and n are labels of atoms in m^{th} and n^{th} position. The total kinetic energy of the crystal can be written as the sum of kinetic energies of the constituent unit cells.

$$K = \frac{1}{2} \sum_{n,\alpha} m^n {v_\alpha^n}^2 \qquad (2)$$

The Hamiltonian for this model can be written as

$$H = \frac{1}{2} u_{\alpha\beta}^{mn} x_\alpha^n x_\beta^m + \frac{1}{2} m^n v_\alpha^n v_\alpha^n \qquad (3)$$

$$m \frac{\partial^2 x}{\partial t^2} = -\frac{\partial U}{\partial x} \qquad (4)$$

A solution to the equation representing harmonic potential maybe written as $U = Ae^{i(kna-\omega t)}$

This yields the relationship between ω and k.

$$\omega(k) = 2\sqrt{\frac{K}{m}} \, |\sin \frac{1}{2} ka| \qquad (5)$$

where K is the second derivative of the interaction energy u and a the separation between the ions.

This relationship is called the dispersion relation [2].
Proceeding in a similar way, the dispersion relation for a solid consisting of unit cells with two ions can be derived. The relation between ω and k in this case is

$$\omega^2 = \frac{K+G}{m} \pm \frac{1}{m} \sqrt{K^2 + G^2 + 2KG \cos ka} \qquad (6)$$

where K and G are quantities analogous to spring constant representing interaction between the atoms in a unit cell and that between unit cells.
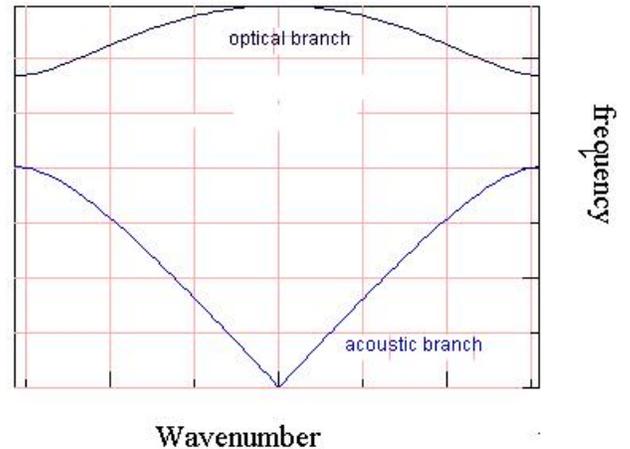
The two solutions are shown in Figure 1.

Fig. 1. Dispersion curves [1].

The lower branch is called acoustic branch because the dispersion curve when k is small is of the form $\omega = vk$, which is the frequency-k relationship of sound waves. The upper branch is called optical branch. This branch is responsible for most optical behavior of solids. Most ionic crystals are easily excited by radiation leading to a vibrational state in which negative and positive ions oscillate out of phase with each

other.

III. PHONON STATISTICS

When a solid absorbs energy, the number of phonons changes. Macroscopic properties like thermal energy can be described by suitable statistical models. If a solid is viewed as a collection of distinguishable oscillating atoms, they would obey Maxwell-Boltzmann distribution [3]. Since phonons are indistinguishable particles like photons, they follow Bose-Einstein distribution. There is no limit on the number of particles a boson state can occupy. The mean occupation number of phonons at a temperature T is

$$\overline{n(kj)} = (e^{\hbar\omega(kj)/k_B T} - 1)^{-1} \qquad (7)$$

This equation gives the number of phonons occupying an energy state with frequency ω(**k**j). The total vibrational energy is

$$E = \sum_{kj} \hbar\omega(kj)[\overline{n(kj)} + \frac{1}{2}] \qquad (8)$$

IV. PHONONS AND SOLID STATE PROPERTIES

The theory of phonons is required to explain many solid state properties, some of which are listed below.

A. Specific Heat

Static model of lattice fails to give a mathematical description of the temperature dependence of specific heat of solids. It assumes that all contributions to specific heat come from electronic degrees of freedom. At low temperatures specific heat varies as T^3. The additional contribution to specific heat comes from phonons. T^3 dependence of specific heat at low temperatures can be explained by looking at phonons from a quantum mechanical point of view. Debye specific heat gives a reasonably good formula for specific heat over the full range of temperatures [4]. Figure 1 shows the agreement of specific heat as obtained from the formula and experimental values for silver (Debye temperature, TD = 215K) [5].Debye specific heat is derived by linking specific heat to total vibrational energy.
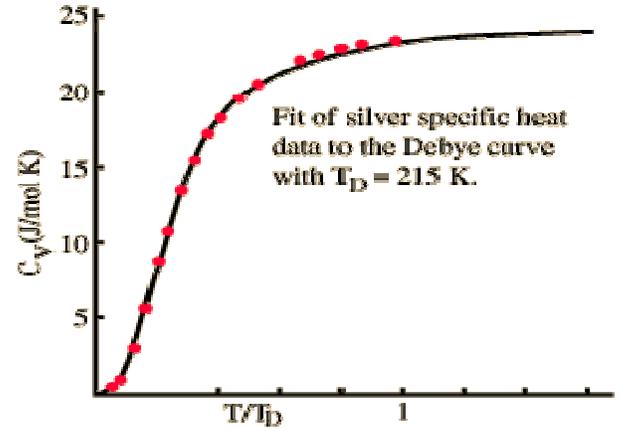

Fig .2. Low Temperatures Specific Heat of Silver [5].

B. Melting

Phonon amplitude increases with increasing temperature. Hence there is a strong dependence of melting on phonon amplitude.

C. Thermal and Electrical Conductivity

In a perfect periodic potential, electrons experience no collision. This would lead to infinite thermal and electrical conductivity. A major source of scattering is lattice vibration. Phonon theory explains the deviation of thermal conductivity from electrical conductivity in non-metals. In most metals, thermal conductivity characteristics and electrical conductivity characteristics are correlated. However, phonons as heat carriers are relatively more important in non-metals. In pure crystalline structures, thermal conductivities are different along different axis due to differences in phonon coupling. Electron-phonon plays an important role in electrical conductivity of certain materials [6].

D. Superconductivity

BCS theory of superconductivity models Type I semiconductors. A key element in this theory is the pairing of electrons into Cooper pair. This pairing is a result of coupling with phonons.

E. Transmission of Sound

If there are no phonons, all materials would be acoustic insulators.

F. Reflectivity of Ionic Crystals

In ionic crystals reflectivity maximum occurs at frequencies below their energy gap. This can be explained by the generation of optical phonons, when radiation forces out-of-phase vibration of ions in a unit cell.

G.   Interaction of Phonons with other particles

Typical phonon energies are comparable with infrared radiation. This makes this region of electromagnetic spectrum particularly important in the context of phonons. In all interactions momentum is conserved. The coupling between lattice vibration and photons involves two phonons in crystals such as germanium and silicon. Lax and Burstein have proposed two mechanisms for this coupling. [7]

Mechanism 1 – A transverse optical phonon created by the photon decays into two phonons.

Mechanism 2 – Direct coupling between photon and phonon. A dipole moment results when an atom displaced by a phonon distorts the charge distribution of neighboring atoms.

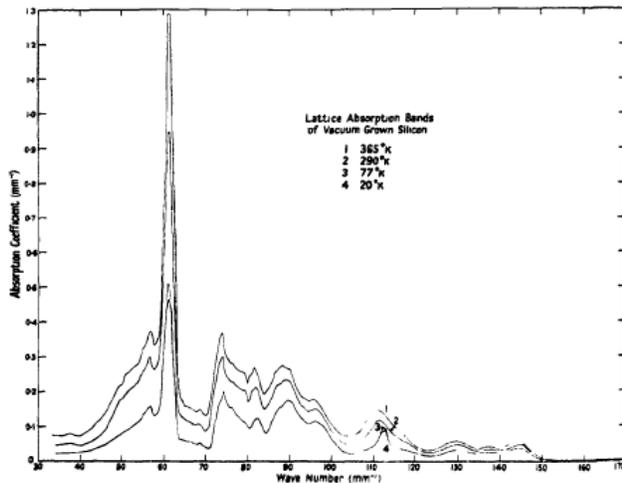Figure 3 shows phonon generation in Silicon [8].

Fig. 3. Lattice Absorption in Silicon [8].

Scattering mechanism with higher energies, 1eV to 10 eV also provides information on phonon spectra. Brillouin and Raman scattering are two important spectroscopic tools. They involve inelastic scattering of photons by a solid. The resulting shifts in frequency can be explained by creation or annihilation of phonons. Raman scattering involves optical phonon whereas Brillouin scattering involves acoustic phonons.

X-rays can be scattered by phonons [9]. This effect must be taken into account when calculating peak intensities. Bragg peaks predicted by static lattice model is incorrect. Neutron scattering is a powerful tool in analyzing crystals. Scattered electrons lose energy in discrete amounts. This phenomenon can easily be explained by quantum theory of phonons.

V.   CONCLUSION

The concept of phonons is a key element in solid state physics. Phonon theory gives a satisfactory explanation of most solid state phenomenon.

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