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Out lines:-

Lattice Vibrations

1. Vibration modes of linear monoatomic lattice .

2. Vibration modes of linear diatomic lattice.

Introduction:-

- When studying the bonding energy between atoms, the state of the lattice is shown in equilibrium, where each atom is positioned in its place.

- Atomic vibrations are a spontaneous process in the lattice of solid materials at a temperature T, where the average energy of each atom of the crystal is (K_BT), Where K stands for Boltzmann's constant, this energy leads to vibration of the atom around its places of stability, the higher the temperature, the wider the range of these vibrations, which are called vibrations of the lattice.

- all the forces between atoms are electrical forces which work to put the atom or molecule in equilibrium state .

- The thermal, Optical and Electrical properties of the solid materials depend on lattice vibration.

1. Vibration modes of linear monoatomic lattice:

The figure (1) shows a series consisting of one type of atom, the mass of each atom is(m), and the distance between each two adjacent atoms is (a), so when a wave passes, it causes a small displacement of each atom

(u) from its original position. The motion made by the displaced atom is a simple harmonic motion, and the force that tries to return the atoms to their equilibrium position is known as the returning force and is expressed by Hooke's law F= - k x,

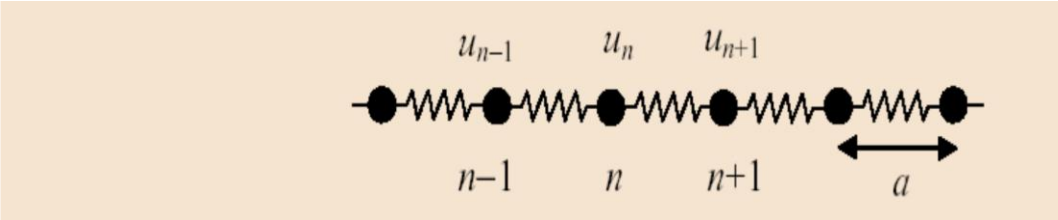


fig.1

We notice from Figure (1) that the force acting on the atom n is the sum of two forces, the first in the positive direction by the atom n + 1, and is given by the relationship:

$$\mathbf{F_1 = -C\,(u_n - u_{n+1})} \quad \ldots\ldots 1$$

And the second force acting on the atom n by the atom n-1 in the negative direction is given by the relationship:

$$\mathbf{F_2 = C\,(u_n - u_{n-1})} \quad \ldots\ldots 2$$

The net force acting on the atom n is the sum of the two previous relations:

$$\mathbf{F_n = F_1 - F_2 = -C\,(2u_n - u_{n+1} - u_{n-1})} \quad \ldots\ldots 3$$

By applying Newton's second law of motion to equation No. 3, we get a second-order differential equation, and by solving this differential equation we get the following relations:

$$\omega = \pm 2\sqrt{\frac{c}{m}}\left|\sin\frac{qa}{2}\right| \quad \ldots\ldots 4$$

Equation No. 4 is called the scattering relationship, and it relates the frequency of vibration (w) and the wave vector (q), and The two signs indicate the direction of the wave's transmission, whether it is to the right or left.

This dispersion relation have a number of important properties :

1. Most of the information is available in it by studying it in the first Brillouin region.

2. Phase velocity and group velocity : The phase velocity relationship, which represents the velocity of the plane wave propagation, is given by the following relationship :

$$v_p = \frac{\omega}{q}$$

3. The group velocity is given, which is the velocity of energy in the medium.

$$v_g = \frac{\partial \omega}{\partial q}$$

2. Vibration modes of linear diatomic lattice:

Suppose we have a linear lattice that includes the presence of two types of atoms, the mass of the first atom is denoted by the symbol M_1, and the mass of the second atom is denoted by the symbol M_2, as shown in Figure 2:-

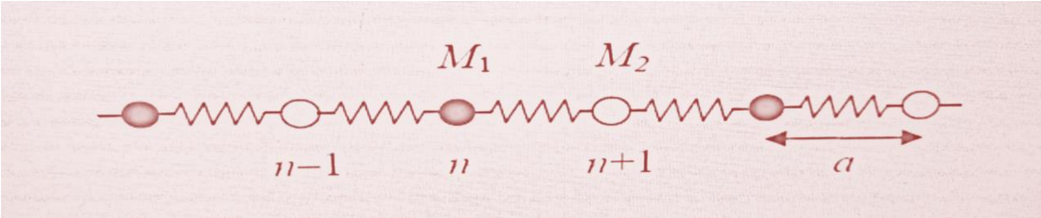


fig.2

We can treat the motion of this lattice in a similar fashion as for monoatomic lattice. However, in this case because we have two different kinds of atoms, we should write two equations of motion:

$$F_n = -C\,(2u_n - u_{n+1} - u_{n-1}) \quad \text{....5}$$

$$F_{n+1} = -C\,(2u_{n+1} - u_{n+2} - u_n) \quad \text{...6}$$

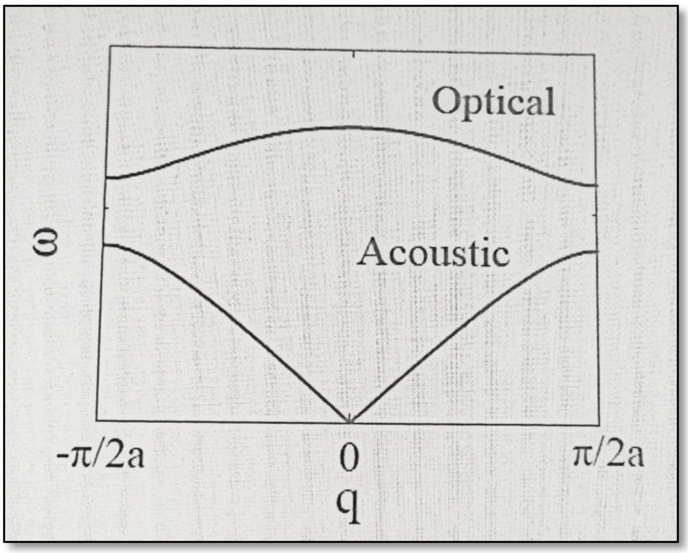
After solving these equations using the matrix, a second-order equation was reached and it is as follows :

$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 qa}{M_1M_2}} \quad \text{.....7}$$

Equation 7 represents the scattering relationship of wave propagation in a diatomic linear lattice.

Depending on sign in this formula there are two different solutions corresponding to two different dispersion curves, as shown in figure 3:-

fig.3



The lower curve is called the acoustic branch, while the upper curve is called the optical branch. The optical branch begins at q=0 and w=0.

The reason for this name is due to the oscillation phase of the atoms, where the oscillation of different atoms of the Acoustic branch is in one phase, while the phase difference between the oscillations of the atoms of the optical branch is equal to π