UNIT - III

Phonons and Lattice Vibrations

* Vibrations of a Mono atomic Lattices :- Derive the dispersion relation for one-dimensional infinite Mono atomic Lattices :-

Let us consider one dimensional infinite Mono atomic lattice with atoms at rest. Let "a" be the inter atomic spacing. Let "m" be the mass of the each atom. In this theory force of interaction will be between nearest neighbouring atoms only & also HOOK's law is obeyed.

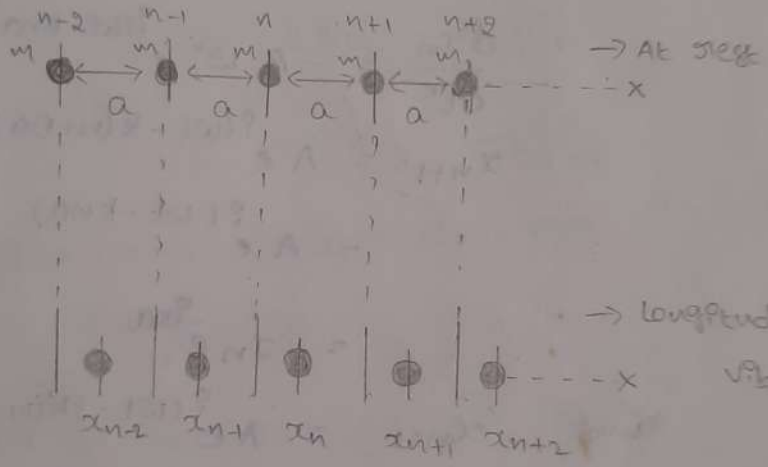


Fig: Geometry of the Mono atomic lattice.

Let us suppose a wave Propagated along x-direction of a Mono atomic lattice & this Problem is in Longitudinal only.

Under the Equilibrium Position of all the atoms remains at rest with equal spacing. When wave is Propagating Vibrational motion is Excited. So the atoms Excute Simple harmonic motion about their mean Position. So, the displacements are not equal. Let "x_n" be the displacement of the n^{th} atom.

Force of interaction on one atom due to an another atom is directly Proportional to difference of their displacements. Force of interaction on n^{th} atom will be

due to $(n+1)$ atom & $(n-1)^{th}$ atom only.

$$F = \beta(x_{n+1} - x_n) - \beta(x_n - x_{n-1})$$

$$F = \beta[x_{n+1} - x_n - x_n + x_{n-1}]$$

$$\Rightarrow m\frac{d^2x_n}{dt^2} = \beta[x_{n+1} + x_{n-1} - 2x_n] \quad -(1)$$

Let $x_n = A.e^{i(\omega t - kna)}$ be the soln of Eqn (1). where na = x coordinate of n^{th} atom differentiating w.r.t to "t" we get

$$\frac{dx_n}{dt} = Ae^{i(\omega t - kna)}(i\omega)$$

again differentiating w.r.t to "t".

$$\frac{d^2x_n}{dt^2} = -A\omega^2 e^{i(\omega t - kna)}$$

$$x_{n+1} = Ae^{i(\omega t - k(n+1)a)}$$

$$= Ae^{i(\omega t - kna)}.e^{-ika}$$

$$= x_n e^{-ika}$$

and $x_{n-1} = Ae^{i(\omega t - (k(n-1)a)}$

$$= Ae^{i(\omega t - kna)}e^{ika}$$

$$= x_n e^{ika}$$

Substituting the above values in Eqn (1). we get

$$-m\omega^2 A e^{i(\omega t - kna)} = \beta[x_n e^{ika} + x_n e^{-ika} - 2x_n]$$

$$-m\omega^2 x_n = \beta x_n[e^{ika} + e^{-ika} - 2]$$

$$-m\omega^2 = \beta[e^{ika} + e^{-ika} - 2]$$

$$-m\omega^2 = \beta[2(\cos ka) - 2]$$

$$-\omega^2 = \frac{2\beta}{m}[\cos ka - 1]$$

$$\omega^2 = \frac{2\beta}{m}[1 - \cos ka]$$

$$\omega^2 = \frac{2\beta}{m}\left[2\sin^2\frac{ka}{2}\right]$$

$$\omega^2 = \frac{4\beta}{m}\left[\sin^2\frac{ka}{2}\right]$$

$$\boxed{\omega = 2\sqrt{\frac{\beta}{m}}\sin\left(\frac{ka}{2}\right)} \quad \text{---(2)}$$

This is called the Dispersion relation for one dimensional infinite mono atomic lattice

Case i:- This mono atomic lattice acts as a low pass filter. It allows the waves whose, frequency less than the critical frequency "ν_n".

For maximum frequency $\sin\frac{ka}{2} = 1$

Eq^n 2. becomes $\omega = 2\sqrt{\frac{\beta}{m}}$

$$\Rightarrow 2\pi\nu_n = 2\sqrt{\beta/m}$$

$$\nu_n = \frac{1}{\pi}\sqrt{\frac{\beta}{m}}$$

Case ii:- If "λ" very much greater than ka ($\lambda >> ka$) then

$$\sin\frac{ka}{2} = \frac{ka}{2}$$

Now Eq^n (2) becomes $\omega = 2\sqrt{\frac{\beta}{m}}\sin\frac{ka}{2}$

$$\omega = 2\sqrt{\frac{\beta}{m}}\frac{ka}{2}$$

$$\boxed{\omega = \sqrt{\frac{\beta}{m}}\,ka}$$

Case iii:- At higher frequencies, Phase & group velocities are differe & are obtained from Eq^n (2)

$$\omega = 2\sqrt{\frac{\beta}{m}}\sin\frac{ka}{2}.$$

$$\omega = \frac{2}{a}v_s\left|\sin\frac{ka}{2}\right| \quad \text{---(3)}$$

Where $v_s = \sqrt{\frac{c}{\rho}}$ is a constant for given lattice & has dimensions of velocities. $c = \beta a$ & $\rho = \frac{m}{a}$. It is normally referred to as the velocity of sound waves in solids.

$$v_p = \frac{\omega}{k} = \frac{2v_s}{ka}\left|\sin\frac{ka}{2}\right| \quad [\because \text{From Eq}^{n}(3)]$$

$$v_g = \frac{d\omega}{dk} = v_s \cos\frac{ka}{2} \quad [\because \text{From Eq}^{n}(3)]$$

Thus both v_p & v_g are functions of frequency. This is refered to as the phenomenon of dispersion & the medium is called dispersion medium.

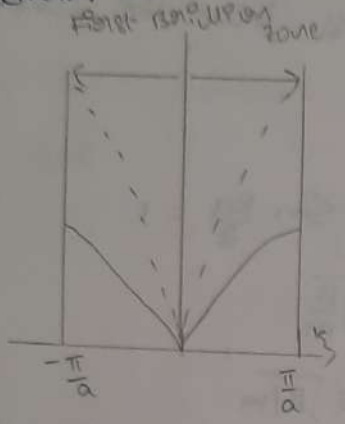


Fig 2. Dispersion relation for a 1-D mono atomic lattice.

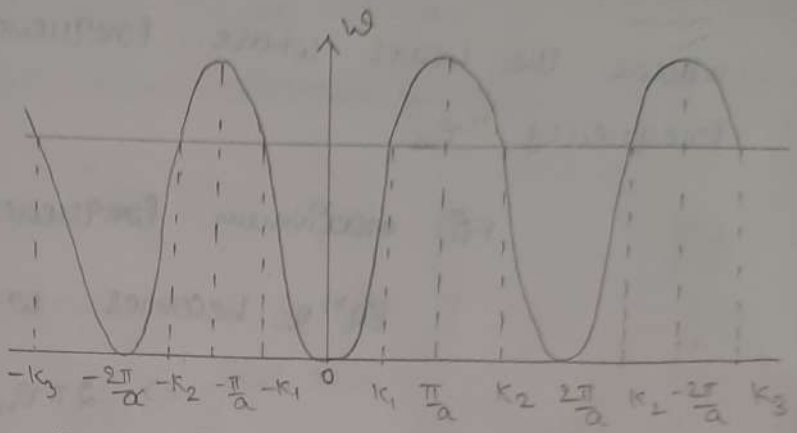


Fig: 3) Dispersion relation for a range of k-values along with the Brillouin zone.

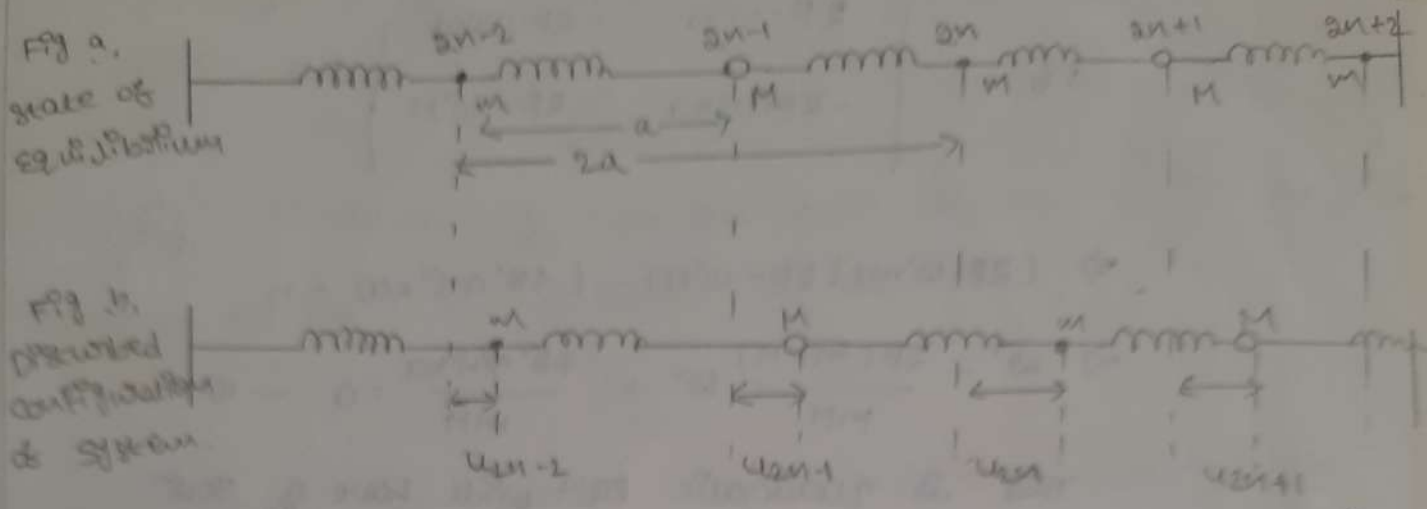
* A Linear diatomic lattice for Primitive cell &. lattice with two atoms per Primitive cell &. Derive the dispersion relation for Linear diatomic lattice :-

Consider a one dimensional (Linear) Primitive lattice with containing of two atoms of masses m, M (m<M) which are placed alternatively along the X-axis with an inter atomic distance equal to "a" in a state of equilibrium but the atoms be located at sites represented by $0 \cdots 2n-2, 2n-1, 2n, 2n+1, 2n+2, \cdots$ as shown in the fig ①.

Let "u_{2n}" be the displacement of an atom corresponding to the $2n^{th}$ site at any time during the vibratily motion of atoms.

In this theory force of interaction will be btw nearest neighbouring atoms only & Hooke's law is obeyed.

Force of interaction on one atom due to an another atom is directly proportional to difference of their displacements.



We obtained the following different eqns of motion one for lighter atoms & other for heavier atoms.

$$F_{2n} = m\frac{d^2u_{2n}}{dt^2} = \beta(u_{2n+1} + u_{2n-1} - 2u_{2n})$$
$$F_{2n+1} = M\frac{d^2u_{2n+1}}{dt^2} = \beta(u_{2n+2} + u_{2n} - 2u_{2n+1}) \quad \Big\} - (1)$$

The soln of the eqn (1) are given by

$$u_{2n} = Ae^{i(\omega t - 2kna)}$$
$$u_{2n+1} = Be^{i(\omega t - (2n+1)ka} \quad \Big\} - (2)$$

Where 'k' is the wave vector & A, B are different amplitudes of different masses m, M respectively. writing similar expressions for u_{2n-1} & u_{2n+2} substituting eq(2) into eq(1) we get

$$-m\omega^2 A = \beta B(e^{ika} + e^{-ika}) - 2\beta A$$
$$-M\omega^2 B = \beta A(e^{ika} + e^{-ika}) - 2\beta B \quad \Big\} - (3)$$

since $e^{ika} + e^{-ika} = 2\cos ka$

$$(2\beta - \omega^2 m)A - (2\beta\cos ka)B = 0$$
$$2\beta(\cos ka)A - (2\beta - \omega^2 M)B = 0 \quad \Big\} - (4)$$

This set of Homogeneous linear Eqns would gives rise to Non-zero soln for A & B only.

$$\text{If} \quad \begin{vmatrix} 2\beta - \omega^2 m & -2\beta\cos ka \\ -2\beta\cos ka & 2\beta - \omega^2 M \end{vmatrix} = 0$$

$$\Rightarrow (2\beta - \omega^2 m)(2\beta - \omega^2 M) - (4\beta^2 \cos^2 ka) = 0$$

$$\Rightarrow \omega^4 - \frac{2\beta(m+M)}{mM}\omega^2 + \frac{4\beta^2 \sin^2 ka}{mM} = 0 \quad \text{— (5)}$$

This is quadratic eqn will have a soln.

$$\omega^2 = \beta\left(\frac{1}{m} + \frac{1}{M}\right) \pm \beta\sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4\sin^2 ka}{mM}} \quad \text{— (6)}$$

In this case these are two values of "ω". These two values are written as

$$\omega_+^2 = \beta\left(\frac{1}{m} + \frac{1}{M}\right) + \beta\sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4\sin^2 ka}{mM}} \quad \text{— (7)}$$

$$\omega_-^2 = \beta\left(\frac{1}{m} + \frac{1}{M}\right) - \beta\sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4\sin^2 ka}{mM}} \quad \text{— (8)}$$

Case i: Consider the expression for ω_+ (Dose find that $k \to 0$ $\sin ka$ is negligible, we get

$$\omega_+ = \sqrt{2\beta\left(\frac{1}{m} + \frac{1}{M}\right)}$$

(ii) For $k \to \frac{\pi}{2a}$, $\sin ka \to 1$

$$\omega_+^2 = \beta\left(\frac{1}{m} + \frac{1}{M}\right) + \beta\sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4}{mM}}$$

$$\omega_+^2 = \beta\left(\frac{1}{m} + \frac{1}{M}\right) + \beta\left(\frac{1}{m} - \frac{1}{M}\right)$$

$$\omega_+ = \sqrt{\frac{2\beta}{m}} \quad \text{— (9)}$$

Case ii: Now consider the expression for ω_-

(i) For $k \to 0$, $\sin ka \cong ka$

$$\omega_-^2 = \beta\left(\frac{1}{m}+\frac{1}{M}\right) - \beta\left(\frac{1}{m}+\frac{1}{M}\right)\sqrt{1-4K^2a^2\left(\frac{mM}{m+M}\right)^2}$$

$$\omega_-^2 \cong \frac{2\beta}{m+M}(K^2a^2) \qquad \text{[using binomial theorem]}$$

$$\omega_- = Ka\sqrt{\frac{2\beta}{m+M}} \qquad -(10)$$

(ii) For $K \to \frac{\pi}{2a}$, we get eqn similar to eqn (9) with replaced by the "m" replaced by the "M".

$$\omega_- = \sqrt{\frac{2\beta}{M}} \qquad -(11)$$

* The larger mass ratio $\frac{M}{m}$, greater the width of the forbidden band. i.e width of the forbidden band depends on the differences of masses. If two masses are equal then the two branches become degenerate (join) at $K = \frac{\pi}{2a}$.

* The physical difference btw acoustical & optical branch at $K = 0$ we find that

$A = B$ for acoustical branch

$\frac{A}{B} = \frac{-M}{m}$ for optical branch

In acoustical branch all the particle moves in same direction while in optical branch the two type of particle move in opposite direction as shown in the figure (3).

Fig (a) Acoustical branch.

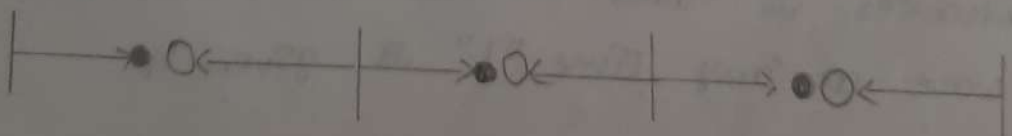


Fig. b : Optical branch.

Displacement of Particles in Acoustical & optical branch.

* Group velocity & Phase velocity :-

Phase velocity :- It is denoted by "v_p" & defined as the ratio of angular frequency "ω" to wave propagation vector "k".

→ The velocity with which planes of waves of constant phase move in a medium is called "**phase velocity**".

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

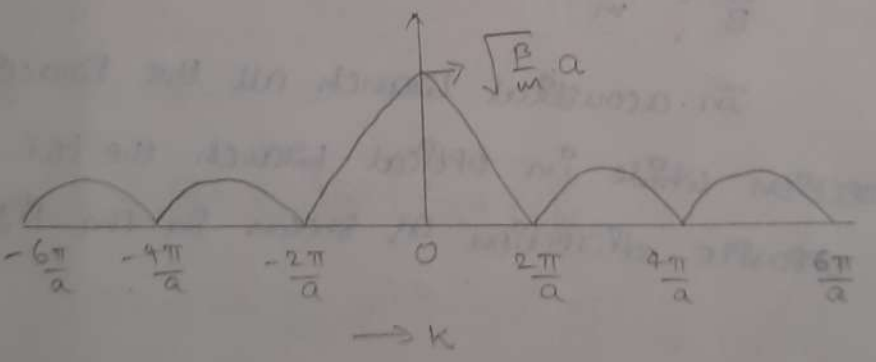
$$= \frac{2\sqrt{\frac{\beta}{m}} \sin\frac{ka}{2}}{k}$$

$$= \frac{2\sqrt{\frac{\beta}{m}} \cdot \frac{ka}{2}}{k}$$

(since if $\lambda >> ka$ then $\sin\frac{ka}{2} = \frac{ka}{2}$)

$$\therefore v_p = \sqrt{\left(\frac{\beta}{m}\right)}a = \text{constant}$$

The below graph shows phase velocity as a function of propagation constant "k".



Let us consider a monochromatic wave having a fixed frequency & wave length, the velocity with which the wave advances is called "phase velocity". Equation of motion of the wave at any time "t" is given by

$$y = A\sin(\omega t - kx)$$

Where $\omega t - kx$ is called the phase of wave motion for constant phase, $\omega t - kx$ = constant.

difference w.r.t to "t".

$$\omega - k\frac{dx}{dt} = 0.$$

$$\omega = k\frac{dx}{dt}$$

$$\frac{dx}{dt} = \frac{\omega}{k}$$

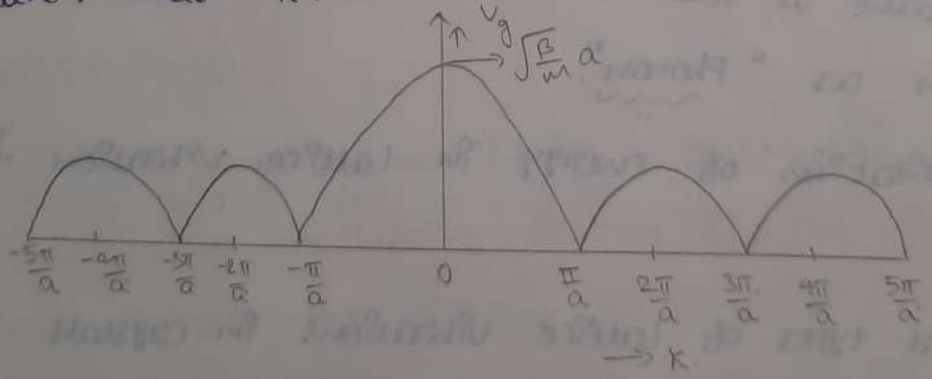
$$\boxed{v_p = \frac{dx}{dt} = \frac{\omega}{k}}$$

Group velocity :- It is denoted by "v_g" & defined as the ratio of change in angular frequency $d\omega$ with respect to change in wave propagation dk. i.e

$$v_g = \frac{d\omega}{dk}$$

→ Let us consider a no. of waves with slightly difference frequencies, then these waves travelled in the same direction their superimposed different components will have different phase velocities. The velocities with which maximum amplitude travells is called "Group velocity".

→ The below fig. shows group velocity as a function of wave propagation vector "k".



$$v_g = \frac{d\omega}{dk} = \frac{d}{dk}\left(2\sqrt{\frac{\beta}{m}}\sin\frac{ka}{2}\right)$$

$$= \frac{d}{dk}\left(2\sqrt{\frac{\beta}{m}}\frac{ka}{2}\right)$$

$$= \sqrt{\frac{\beta}{m}}\cdot a \qquad \left[\because \lambda >> 2a \ \sin\frac{ka}{2} \cong \frac{ka}{2}\right]$$

$$v_g = \left(\sqrt{\frac{\beta}{m}}\right)a = \text{Constant}.$$

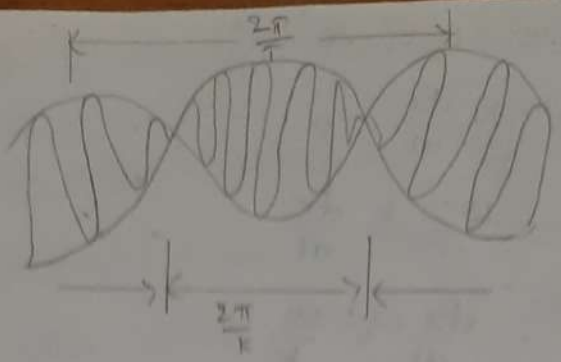


Fig shows the resultant wave formed due to super position of two wave trains.

For long wavelengths the medium behaviour as continuous & homogeneous medium. The phase velocity is nearly equal to group velocity.

$$v_p = v_g = \sqrt{\frac{\beta}{m}}\, a = \text{Constant.}$$

Quantization of lattice vibrations & Phonons :- &

Explain Phonons and give an evidence for existance of Phonon?

We know that the energy of an electromagnetic wave is quantized and this quantum of energy is called "Photons". similarly the energy of a lattice vibration or an elastic wave is also quantized & a quantum of this energy is known as "Phonon".

→ "Quantization of energy in lattice vibration is called Phonon"

All types of lattice vibrations in crystals comprise Phonons.

→ Thermal vibrations are thermally excited Phonons.

→ The vibration of optical branch results in optical Phonons.

→ Sound waves are acoustical Phonons.

Most of the concepts which apply to Photons are also valid for Phonons. For ex, the concept of wave Particle duality holds good for Phonons. The Vibrational spectrum of Phonon waves occupy a wide range from 10^{12} to 10^{13} cycles / sec. The Low frequency Path in vibrational spectrum is in acoustical branch & high frequency path in IR range.

Properties of Phonons:-

* Phonons will have wave Particle duality.
* Phonons are Elastic waves in solids, they travells with the velocity of sound in solids.
* The energy of Phonons is the thermal Energy of the solids.
* Phonons are indistinguishable Particles, the Bose - Einstein distribution function must be used to describe their distribution.

$$\bar{n} = \frac{1}{\exp\left(\frac{\hbar\omega}{K_B T}\right) - 1}$$

Where K_B → Boltzmann Constant

T → Absolute temperature.

* The interaction btw two Phonons is //er to the scattering of two Particles.

There is no direct Experimental avidence of the quantigation of Lattice Energy but the following Experimental facts suggest the Existance of Phonons.

* Lattice heat capacity approaches zero as the temperature approaches to zero. In this the temperature decreased, Lattice Vibration Contribution to the heat capacity also decreased.

Energy & momentum changes are observed.

In this Experiment are due to action of, absorption of Phonons.

This process is called inelastic scattering of X-ray Photons by the crystal. This can be explained only if lattice vibration is quantized.

Momentum of Phonons :, Crystal Momentum :, Elastic, Inelastic scattering of Photons by Phonons :-

Physically, a Lattice Phonon does not carry any momentum, but it interacts with other Particles & Fields as if it has a momentum "$\hbar k$", where k - represents wave vector of the Phonon from De Broglie relation.

$$P = \frac{\hbar}{\lambda}$$

$$= \frac{\hbar}{2\pi} \cdot \frac{2\pi}{\lambda}$$

$$P = \hbar \cdot k.$$

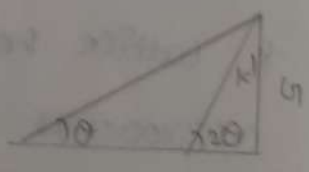
The quantity "$\hbar k$" is sometimes called the crystal momentum. The physical significance of $\hbar k$ (Phonon momentum) is provided by the momentum conservation laws in crystals.

These laws must be followed elastic & inelastic scattering of Photons.

Elastic scattering of Photons :

* The wave vector conservation law for elastic scattering of the Braggs diffraction of X-ray Photons from crystals is given by

$$k' = k + G \quad \text{— (1)}$$

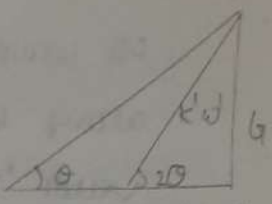


Where k' & k represents the wave vectors for the scattered & incident Photons respectively & G is the Reciprocal Lattice vectors. [Equals scattering]

The Conservation of momentum & Energy are given by

$$\hbar k' = \hbar k + \hbar G \quad -(2)$$

and $$\hbar \omega_{ph} = \hbar \omega'_{ph} \quad -(3)$$



Where ω_{ph} & ω'_{ph} are the frequencies of incident & scattered photons respectively.

Ewalds scattering

In this process the crystal as a whole recoils with a momentum $\hbar G$ & Frequency of incident photons remains unchanged. i.e.,

$$\omega_{ph} = \omega'_{ph} \quad -(4)$$

This is also follows from the relation.

$$|k'| = |k| \quad -(5)$$

Such a process in which the frequency of the incident photon is the same the scattered photon, is called normal (or) N-Process.

Inelastic scattering of Photons :

Now, consider the case of inelastic scattering of the photon which proceeds with the emission of phonon of wave vector "k" (or) absorption of a phonon of wave vector "K". As shown in figure below.

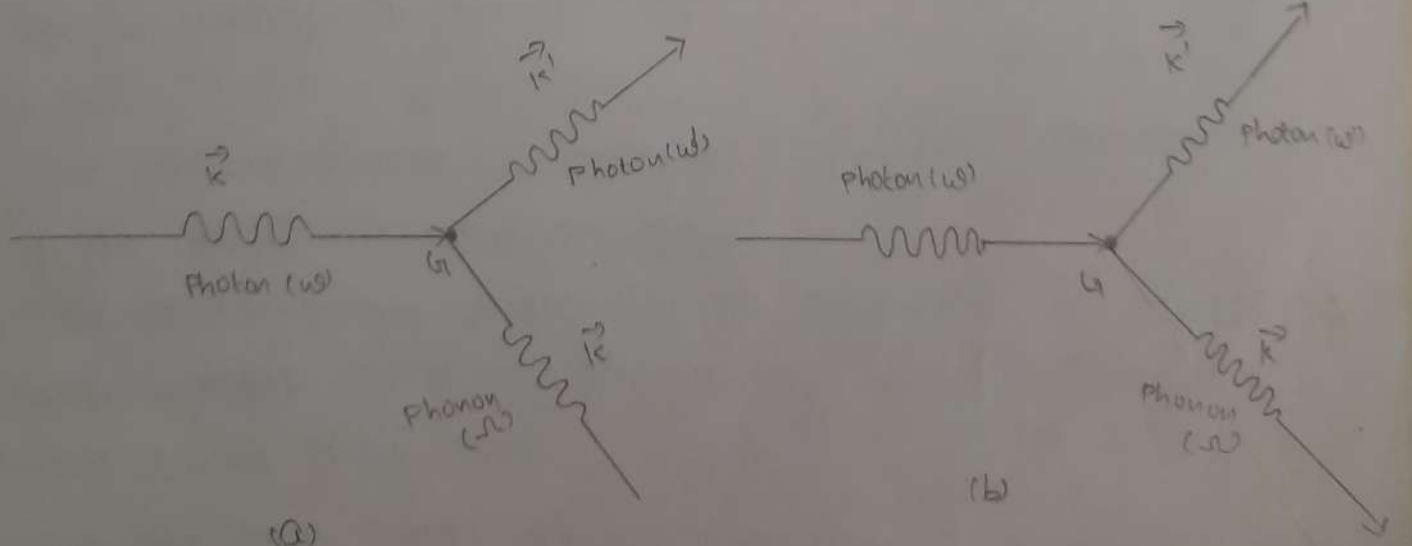


Fig shows in elastic scattering of incident Photon of wave vector k to produce scattered photon of wave vector k' along with the emission (a) absorption (b) of a Phonon of wave vector "K".

The wave vector conservation law then takes the form

$$k' + k = k + G \quad \text{— (6) (a) emission of Phonons}$$

and the momentum & Energy conservation laws can be written as

$$\hbar k' + \hbar k = \hbar k + \hbar G \quad \text{— (7)}$$

$$\hbar \omega'_{ph} + \hbar(-\Omega) = \hbar \omega_{ph} \quad \text{— (8)}$$

Where "Ω" is frequency of Phonon generated.

b. absorption of Phonon.

The wave vector conservation law gives & the momentum & Energy conservation laws becomes.

$$\hbar k' = \hbar k + \hbar k + \hbar G \quad \text{— (10)}$$

$$\hbar \omega'_{ph} = \hbar \omega_{ph} + \hbar \Omega \quad \text{— (11)}$$

It is clear that $\omega'_{ph} \neq \omega_{ph}$ since from Eqn (8) & Eqn (11) such a process in which the frequency of the photon changes is called "unclapp Process (or) U-Process".

* Geometrical structure Factor (S) :- Unit cells having the atoms only at the corners i.e Primitive cells. Now we shall study the characteristics of radiation diffracts from crystals and it having complex unit cells containing more than one atom such as cubic cells for the BCC & FCC structures. In such situation we will have to account for the interaction of beams which are diffracted by the various atoms with in the unit cell.

Let us consider the reflection h', k', l'

we denote the ratio of the amplitude of the radiation scattered by entire unit cell to that scattered by a point electron at the origin by

$$F(h'k'l') = \sum_j f_j e^{i\phi_j} = \sum_j f_j e^{\frac{2\pi}{\lambda}(r_j \cdot N)i} \quad \text{— (1)}$$

$$\left[\because \phi_j = \frac{2\pi}{\lambda}(r \cdot N) \right]$$

Where f_j is the atomic scattering factor for the j^{th} atom of the unit cell.

ϕ_j is the phase difference btw the radiation scattered at the origin & the radiation scattered at the j^{th} atom of unit cell.

The sum is extended over all the atoms belonging to the unit cell.

r_j is a vector from the origin to j^{th} atom of the unit cell.

It can be expressed as $r_j = x_j a + y_j b + z_j c$

$$r_j \cdot N = \lambda (h'x_j + k'y_j + l'z_j) \quad \text{— (2)}$$

substituting eqn (2) in eqn (1), we get

$$F(h'k'l') = \sum_j f_j e^{2\pi i [\lambda (h'x_j + k'y_j + l'z_j)]}$$

$$F(h'k'l') = \sum_j f_j e^{2\pi i (h'x_j + k'y_j + l'z_j)} \quad -(3)$$

* When all the atoms are identical eqn (3) can be written in a particular simple form.

$$F(h'k'l') = f_j S = f.S \quad -(4)$$

Where $S = \sum_j e^{2\pi i (h'x_j + k'y_j + l'z_j)}$ $-(5)$

From eqn (4) it is clear that the total scattering amplitude is the product the atomic scattering factor "f" & "S" which represents the geometric arrangement of atoms with in the unit cell. and which is called "geometrical structure factor" given by eqn (5)

* For crystal in which all atoms are different i.e contain more than one type of atoms; no such separation is possible & total scattered amplitude is defined by eqn (3).

The intensity of diffracted beam I is proportional to square of the total scattering amplitude F. Since F is complex & therefore we can define more accurately. The intensity of diffracted beam which is proportional to absolute value of F. If $F(h', k'l')$ is expressed as complex number $\alpha + i\beta$ then $F^* = (\alpha - i\beta)$ is conjugate of F.

$$I = |F|^2 = FF^* = \alpha^2 + \beta^2 \quad -(6)$$

where $\alpha = Re(F) = \sum_j f_j \cos 2\pi (h'x_j + k'y_j + l'z_j)$

$$\beta = \text{Im}(F) = \sum_j f_j \sin 2\pi (h'x_j + k'y_j + l'z_j) \quad -(8)$$

using (7) & (8), eqn (6) becomes

$$I = |F|^2 = F \times F^* = \sum_j f_j^2 [\cos 2\pi (h'x_j + k'y_j + l'z_j) + \sin 2\pi (h'x_j + k'y_j + l'z_j)]$$

Ex:- Simple cubic crystal.

In simple cubic crystal there is one atom per unit cell. From eqn (3) diffraction amplitude for $h'k'l'$ becomes $F(h'k'l') = f$

It is evident that the atomic scattering factor is large enough so that the intensity peaks can be scan.