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B.Sc (PS) Chemistry VI Sem
Solid State Physics

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(100), (300), (111), (221) etc are missign from spectrum while lines corresponding (200) (110) (220) planes are present in spectrum.
The absence of lines can be understood by considering that the beam from these planes are out of phase by π and hence not contributing. However the other planes are contributing in diffracted beam.

Elementary lattice dynamics

Lattice vibrations

The elastic vibration of the atom in a solid are influenced or are due to thermal / heat energy which is provided to solid. The heat energy increases the internal energy of solid and is manifested mainly as:

1 Increase in vibration of atom about their mean position usually called lattice vibration and increasing the K.E of free e's-
Lattice vibration can be thought of as series of superimposed sound / strain waves / lattice waves with a frequency spectrum determined by elastic properties of crystal and quanta of elastic wave of energy is called Phonon. (In analogy with photon). All the concepts such as wave particle duality which apply to photon apply equally on phonon. Similar to photons, phonons are bosons and are

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not conserved and can be created or destroyed in collisions.

Energy of phonon = $h\nu$

There is no strong evidence of quantaization of phonon but some indirect evidence are there to support eg lattice contribution to specific heats of solid can only be explained if phonons are supposed to be quantaised.

-08-2017

Debye considered solid to be continuous medium and obtained expression for density of vibrational modes using relation $\omega = v \times q$ where ω and q are frequency & wave vector of elastic wave (phonon) & v is velocity of wave. He assumed that the assumption that medium is continuous is not quite valid because solid is composed of large no of atoms arranged in lattice with specific spacing (however small) b/w the atoms. So on microscopic scale, medium is actually always descrete. Descreteness of medium becomes more significant when one considers high frequency vibrational modes because wavelengths of those modes will be of order of interatomic spacing. Such high frequency modes see the descreteness of medium and hence it becomes necessary to consider the lattice vibrations as vibration of individual atom in a force constant governed by

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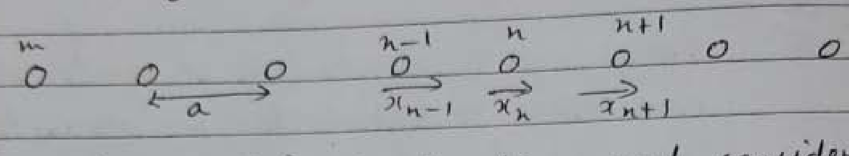
interaction of nearest neighbour atom.

Infinite one-D lattice of identical atoms

Consider one D lattice of identical atoms of mass m with interatomic spacing 'a' as shown. The lattice is considered to be extending infinitely in x direction.



Consider motion of nth atom and considering only nearest neighbour interaction i.e interaction b/w n and (n+1) th atom and n and (n-1) th atom.
Let force constant of interaction b/w two nearest neighbour be K then eq of motion of n^{th} atom will be given by

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

where x_n, x_{n+1} & x_{n-1} are displacement of n^{th}, $(n+1)^{th}$ & $(n-1)^{th}$ atoms respectively w.r.t origin at any time.
First term of eq(1) is displacement of nth atom w.r.t (n+1) th & second term is displacement of nth atom w.r.t (n-1) th atom.

dispersion relation → relation b/w frequency and wavelength

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~~Periodic~~ Solution of eq ① is given by

eq of travelling wave → $x_n(t) = A e^{+i(\omega t - qna)}$ —②

for $(n+1)$th atom

$x_{n+1}(t) = A e^{+i(\omega t - q(n+1)a)}$ —③

for $(n-1)$th atom

$x_{n-1}(t) = A e^{+i(\omega t - q(n-1)a)}$ —④

using ②, ③, ④ in ①

$$\boxed{\omega^2 = \frac{4K}{m}\sin^2\left(\frac{qa}{2}\right)} \quad —⑤$$

$$\boxed{\omega = \omega_{max}\left|\sin\left(\frac{qa}{2}\right)\right|} \quad —⑥ \quad \rightarrow \text{dispersion relation}$$

where $\omega_{max} = \sqrt{\frac{4K}{m}}$

$$W = \sqrt{\frac{4K}{m}}\left|\sin\left(\frac{qa}{2}\right)\right| \quad —⑦$$

eq ⑥ shows that in descrete medium, the frequency is a periodic function of wave vector unlike in continuous medium where ω is directly proportion to q or related as $\omega = vq$. However it can be shown that eq ⑥ can reduce to continuous case for long wavelength phonon $(\lambda >>> a)$

$q = \frac{2\pi}{\lambda}$

$q \cdot a = \frac{2\pi}{\lambda} a = \frac{2\pi}{\lambda a}$

$q \cdot a << 1$

$\omega = \omega_{max}\left(\frac{qa}{2}\right)$ → neglected.

$\omega \propto q$ as in case of continuous medium.

For continuous medium, approximation holds for long wavelength or low frequency phonon

where $v_s = \sqrt{\frac{c}{\rho}}$ and is refered to as velocity of Sound waves in solid.

Since freq. is always +ve hence

$$\omega = +\sqrt{4K/m}\,\sin\left(\frac{qa}{2}\right) = +\frac{2}{a} v_s \sin\left(\frac{qa}{2}\right) \quad —⑧$$

$-m\omega^2 = K(e^{iqa} - 2 + e^{-iqa})$

$= K[e^{iqa/2} - e^{-iqa/2}]^2$

$\because \sin x = \frac{e^{ix} - e^{-ix}}{2i}$

and $\sin^2 x = -\frac{1}{4}[e^{ix} - e^{-ix}]^2$

hence $-m\omega^2 = -4K\sin^2\left(\frac{qa}{2}\right)$

or $\omega = \pm\sqrt{\frac{4K}{m}}\sin\left(\frac{qa}{2}\right)$ —⑤

If C & ρ denote longitudinal stiffness and mass per unit length resp. then

$C = Ka$

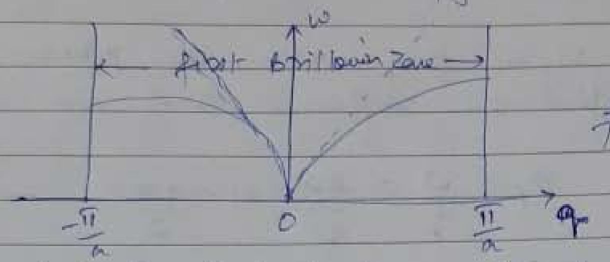
& $\rho = m/a$

hence eq. ⑤ can be written as

$\omega = \pm\frac{2}{a}\sqrt{\frac{C}{\rho}}\sin\left(\frac{qa}{2}\right)$

$= \pm\frac{2}{a} v_s \sin\left(\frac{qa}{2}\right)$

The relation b/w ω & q is called Dispersion relation and is plotted in figure below:



fig(1)

The following important results can be obtained from this relation:-

(i) At low frequencies, $q \to 0$

$$\sin\left(\frac{qa}{2}\right) \to \frac{qa}{2}$$

and eq. 7 gives

$$\omega = \frac{2}{a} v_s \frac{qa}{2} = v_s q \quad \text{--- (9)}$$

We introduce here the terms phase velocity and group velocity. The phase velocity of wave is defined as the rate of advance of a point of constant phase along the direction of wave propagation and is given by

$$v_p = \omega/q \quad \text{--- (10)}$$

The group velocity is defined as the velocity of a group of waves or its envelope and represents the velocity with which the waves transmit energy along the direction of propagation. It is expressed as

$$v_g = \frac{d\omega}{dq} \quad \text{--- (11)}$$

It is now obvious from eq. (9) that, in the long wavelength limit or low frequency, the phase velocity is same as group velocity, each being equal to v_s. An exactly similar result is obtained for a homogeneous and continuous line.

(ii) At higher frequencies, the phase and group velocities are different and are obtained as:

$$v_p = \frac{\omega}{q} = \frac{2v_s}{qa} \sin\frac{qa}{2} \quad \text{— (12)}$$

$$v_g = \frac{d\omega}{dq} = v_s \cos\frac{qa}{2} \quad \text{— (13)}$$

Thus both v_p & v_g are functions of frequency. This is referred to as the phenomenon of dispersion and the medium is called dispersive medium. A similar phenomenon of dispersion is encountered when light passes through a medium whose refractive index is a function of frequency. For very long wavelength, eq (10) and (11) obviously give $v_p = v_g = v_s$ i.e dispersion effects are negligible and medium behaves like a homogeneous continuous medium. The dotted curve in fig (1) represents the dispersion relation for a continuous string.

$\omega = \sqrt{4K/m}$

At freq. ω_m, which represents the maximum angular frequency of of vibrations. Eq. 7 gives us

$$q = \frac{\pi}{a} \text{ or } \lambda = 2a. \quad \text{— (14)}$$

and from eq. (12) & (13) we obtain

$$v_p = \frac{2v_s}{\pi} ; \; v_g = 0 \quad \text{— (15)}$$

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It follows that there is no transfer of signal or energy corresponding to this freq. limit and hence the waves behave like a standing wave. The situation is analogous to the Bragg's reflection of x-vibrations from successive atomic planes in the crystal. The condition to be satisfied for the Bragg's ~~normal~~ ~~incidence~~ reflection to occur is $2d\sin\theta = n\lambda$, or $\lambda = 2d$ for the first order reflection with normal incidence. Thus the condition eq. (14) is equivalent to the condition for the Bragg's reflection. ~~The detailed physical character of the propagation of the wave (condition of standing wave) is depicted by~~

Thus it follows from the above description that only the vibrations of freq. $\omega < \sqrt{\frac{4K}{m}}$ $\left(\text{or } \frac{2v_s}{a}\right)$ can propagate through the lattice. Hence the lattice behaves as a low-pass filter which transmits only if the freq. lies between zero and $2v_s/a$. Using typical values of $a = 10^{-10}\,m$ and $v_s = 10^4\,m/s$, the max freq. which can be transmitted is $= 10^{14}/s$

~~(iii) Now consider the vibrational system of the lattice corresponding to any freq. $\omega_0 < \sqrt{\frac{4\beta}{m}}$, which lies in the vibrational range. A plot of this~~