Lecture 14

4-2 Vibrations of crystals with diatomic basis

Now we consider a one-dimensional lattice with two non-equivalent per primitive basis of masses m and M with the distance between two neighboring atoms a (see Fig.28) .

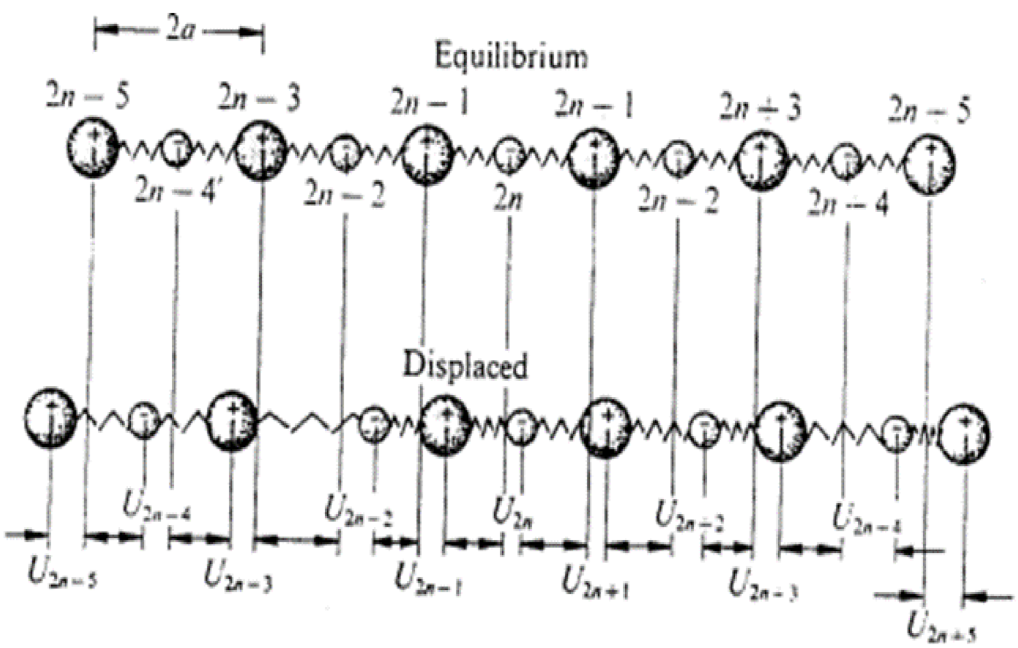

Fig. 3.10 Linear diatomic lattice of lattice constant 2a. As in the monatomic case, only nearest neighbor interactions need be considered.

The displacements of the two kinds of atom will usually have <u>different amplitudes</u>:

$$\left.\begin{aligned} U_{2n} &= A\exp[i(k(2n)a\text{-}wt)] \\ U_{2n+1} &= B\exp[i(k(2n+1)a\text{-}wt)] \end{aligned}\right\} \quad \ldots\ldots 1$$

If we suppose that displacements are in the elastic range of Hooke's law, then the force equations can be written in the same fashion with a monatomic chain:

$$\left.\begin{aligned} -mw^2 U_{2n} &= A\,[U_{2n+1} + U_{2n-1} - 2U_{2n}] \\ -Mw^2 U_{2n+1} &= B\,[U_{2n+2} + U_{2n} - 2U_{2n+1}] \end{aligned}\right\} \quad \ldots\ldots 2$$

Substitution of the two portions of Eq.1 into Eq.2 produces the two simultaneous equations.

$$\left.\begin{aligned} -mw^2 A &= CB\,[exp(ika) + exp(-ika)] - 2CA] \\ -Mw^2 B &= CA\,[exp(ika) + exp(-ika)] - 2CB] \end{aligned}\right\} \quad \ldots.3$$

But $exp(ika) + exp(-ika) = 2coska$ so the Eq. 3 becomes:

$$\left.\begin{aligned} (mw^2 - 2C)A + 2CB\,coska &= 0 \\ (Mw^2 - 2C)B + 2CA\,coska &= 0 \end{aligned}\right\} \quad \ldots\ldots.4$$

$$\left| \begin{matrix} mw^2-2C & 2C\,coska \\ 2C\,coska & Mw^2-2C \end{matrix} \;\middle|\; \begin{matrix} A \\ B \end{matrix} \right| = 0$$

Now by solving the matrix and use the law $\frac{-b\pm\sqrt{b^2-4ac}}{2a}$ we get :

$$w^2 = C\left[\frac{1}{m} + \frac{1}{M}\right] \pm C\left[\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4\ sin^2(ka)}{mM}\right]^{½} \quad \ldots\ldots 5$$

This relation is called the dispersion relationship between w and k for the propagation of a longitudinal wave in a linear diatomic lattice. The spectrum of the result for w as a double-valued function of k is shown in Fig.29.

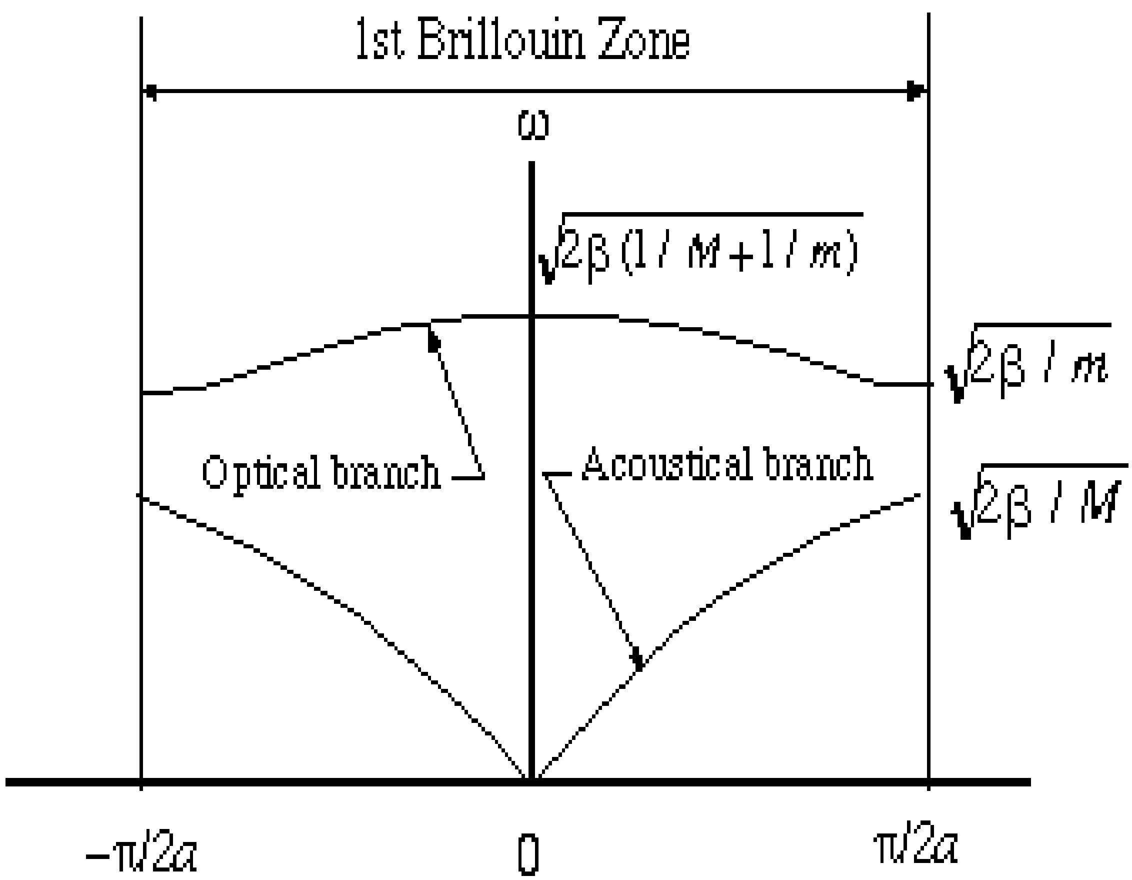

Fig.29

There are two values of w for a given k

1-For $k \to 0$ Eq.5 become

w_1^2=$C(\frac{1}{m}+\frac{1}{M}) \pm C\ (\frac{1}{m}+\frac{1}{M})$ 6

In the case of negative signal we get:

$w_1^- = 0$

and positive signal we get:

$$w_1^+ = \sqrt{2C(\frac{1}{m}+\frac{1}{M})}$$

2- For $k = \frac{n\pi}{2a}$ where n=1,3,5,7... Eq.5 become

w_2^2=$C[\frac{1}{m}+\frac{1}{M}] \pm C\ [\ (\frac{1}{m}+\frac{1}{M})^2 - \frac{4}{mM}]^{1/2}$ 7

In the case of negative signal we get: $w_2^- = (\frac{2C}{M})^{1/2}$

and positive signal we get: w_2^+=$(\frac{2C}{m})^{1/2}$

Referring to Fig. 29 , the lower branch (which may be compared with that of Fig.27) is the acoustic branch, and the new upper branch is usually called the optical branch of the vibrational spectrum.

The question now is why the first branch is called acoustical branch?, and why the second branch is called optical branch?.

The reason for the first one can be understood if we look into the amplitudes of the two types of atoms as a function of frequency.

Eq.4 can be arranged as:

$$\left.\begin{aligned} \frac{B}{A} &= \frac{2C-mw^2}{2C\, coska} \\ \frac{B}{A} &= \frac{2C\, coska}{2C-Mw^2} \end{aligned}\right\} \quad \ldots\ldots.8$$

in the long wavelength (k→ o) and for the acoustic phonon branch, we have, $coska = 1$ and $w = 0$, so $\frac{B}{A}$=1 (which demonstrates that, the vibrations of the two atoms in one primitive unit cell have exactly the same amplitude and phase (i.e. direction, as shown in Fig.30), for this called the acoustic branch.

in the long wavelength (k→ o) and for the optical phonon branch, we have, $w_1^+ = \sqrt{2C(\frac{1}{m} + \frac{1}{M})}$, therefore, by substituting into Eq. 8 we get $\frac{B}{A}$= - $\frac{m}{M}$

which shows that, in the long wavelength of the optical branch, the vibrations of the two atoms in one primitive unit cell have a specific amplitude ratio and opposite phases (i.e. directions), as shown in Fig. 30, for this called the optical branch.

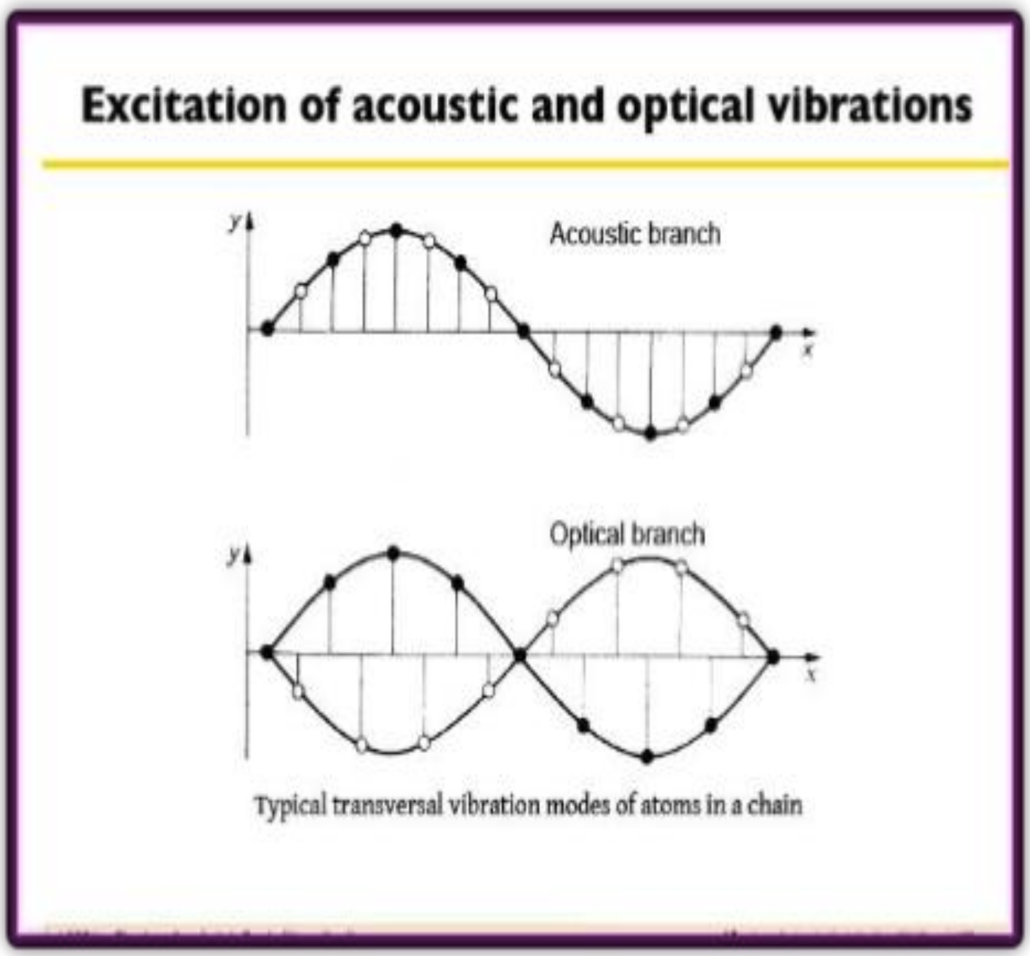

Fig.30