Chapter 4.

Phonon Ⅰ, Crytical Vibrations.

Vibration of crystals with monatomic basis.

First Brillouin Zone.

group velocity.

long wavelength limit.

Derivation of force const.[constant] from exp.[experiment].

Two atoms per primitive Basis.

Quantization of elastic waves.

phonon momentum.

Inelastic scattering by phonon.

	Name	Field
——→	Electron	—
∿∿→	Photon	Electromagnetic wave
—∿∿—→	Phonon	Elastic wave
—‖—→	Plasmon	Collective electron wave
—ℓℓℓ—→	Magnon	Magnetization wave
–	Polaron	Electron + elastic deform
–	Exciton	Polarization wave

1-D vibration, one atom in the primitive cell,

freq. of an elastic wave in terms of wave vector.

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

M:mass of an atom.

$$\therefore \; -Mw^2u_s = C(u_{s+1} + u_{s-1} - 2u_s)$$

$$u_{s\pm1} = u\exp[i(s\pm1)Ka]$$

$$-Mw^2u\exp(isKa) = C\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\}$$

$$+Mw^2 = -C[\exp(iKa) + \exp(-iKa) - 2]$$

$$w^2 = \frac{2C}{M}(1 - \cos Ka)$$

At the Brillouin Zone $K = \pm\frac{\pi}{a}$

$$\frac{dw^2}{dK} = (2Ca/M)\sin Ka = 0$$

$$K = \pm\frac{\pi}{a}$$

$$w^2 = \frac{2C}{M}(1-\cos Ka)$$
$$= \frac{2C}{M} \cdot 2 \cdot \sin^2\frac{Ka}{2}$$
$$\therefore w = \sqrt{\frac{4C}{M}}\left|\sin\frac{Ka}{2}\right|$$

First Brillouin Zone.

$$\frac{u_{s+1}}{u_s} = \frac{u \exp iK(s+1)a}{u \exp iKsa} = \exp iKa$$

out of phase at zone boundary.

The range of independent values of K.

$$-\pi \le Ka \le \pi$$
$$\text{or } -\frac{\pi}{a} \le K \le \frac{\pi}{a}$$

만약 outside에 있다면 $K' = K - \frac{2n\pi}{a}$.

$$\frac{u_{s+1}}{u_s} = \exp iKa = \exp 12\pi n \cdot \exp i(Ka - 2n\pi)$$
$$= \exp iK'a$$

따라서 zone boundary 내부의 K로 기술이 가능.

$K_{\max} = \pm\frac{\pi}{a}$ 인데, 이 때 $u \cdot \exp(isKa)$는 trveling wave가 아니고 standing wave이다.

zone boundary에서 $sK_{\max}a = \pm s\pi$

$$u_s = u\exp(\pm is\pi)$$
$$= u \cdot (-1)^s$$
오른쪽으로도 왼쪽으로도 안간다.

group velocity:

$v_g = dw/dK$ or $v_g = \nabla_K w$

위식에서 $v_g = \sqrt{\frac{Ca^2}{M}} \cos\frac{1}{2}Ka$

Long wavelength limit.

Ka $\ll 1$, $\cos Ka \simeq 1 - \frac{1}{2}(Ka)^2$

따라서 dispersion에서 $w^2 = \frac{C}{M}K^2a^2$

$\therefore v = w/K$ velocity of sound는 frequency에 무관하다.

Derivation of force constants from experiment.

거의 20plane 까지 interaction이 있는 경우도 있다.

$$w^2 = \frac{2}{M} \sum_{p>0} C_p (1 - \cos pKa)$$

$\cos rKa$를 곱하자.

$$M \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK \omega^2 \cos rKa = 2 \sum_{p>0} C_p \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK (1 - \cos pKa) \cos rKa.$$

$$= -2\pi C_r / a$$

the integral vanishes except for p=r.

$$\text{Thus} \quad C_p = \frac{-Ma}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK \ w_k^2 \cos pKa$$

Two atoms per primitive cell.

dispersion relation : LA, TA mode

LO,TO mode.

p개의 atom이 있으면 3p개의 dispersion relations.

3 acoustical branches,

3p-3 optical branches.

p개의 atom이 primitive cell 속에 있고, n개의 primitive cell이 있으면,

3np개의 degrees of freedom이 있고,

(3p-1)N개의 optical mode,

3N개의 acoustic mode. [2N:transverse, N:Longitudinal mode]

$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s)$$
$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$

different amplitude.

$$u_s = u \exp(isKa) \exp(-i\omega t)$$
$$v_s = v \exp(isKa) \exp(-i\omega t)$$

substitute!

$$-M_1 \omega^2 u = Cv[1 + \exp(-iKa)] - 2Cu$$
$$-M_2 \omega^2 v = Cu[1 + \exp(-iKa)] - 2Cv$$

$$0 = \begin{vmatrix} 2C - M_1\omega^2, & -C[1 + \exp(-iKa)] \\ -C[1 + \exp(iKa)], & 2C - M_2\omega^2 \end{vmatrix}$$

$$\therefore M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 + 2C^2(1 - \cos Ka) = 0$$

$|Ka| < 1$

$$0 = M_1 M_2 \omega^4 - 2C(M_1+M_2)\omega^2 + 2C^2 \cdot \frac{1}{2} K^2 a^2$$

$|Ka| \ll 1$

$$\omega^2 = \frac{C(M_1+M_2) \pm \sqrt{C^2(M_1+M_2)^2 - K^2a^2C^2M_1M_2}}{M_1M_2}$$

$$\Rightarrow \approx 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right)$$ optical branch

$$\omega^2 = \frac{C(M_1+M_2) \pm C(M_1+M_2)\cdot\left[1 - \frac{1}{2}\frac{K^2a^2C^2M_1M_2}{C^2(M_1+M_2)^2}\right]}{M_1M_2}$$

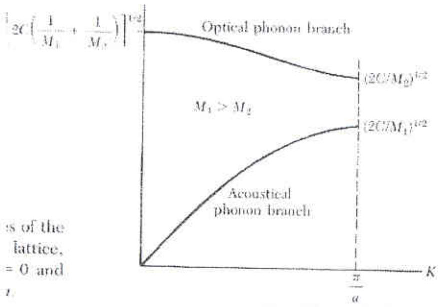
$$= \frac{K^2a^2C^2}{2C^2(M_1+M_2)^2} \cdot C(M_1+M_2) = \frac{K^2a^2C}{2(M_1+M_2)}$$

$$\therefore \omega^2 = \frac{\frac{1}{2}C}{M_1+M_2} K^2a^2$$ Acoustic branch

near the zone.

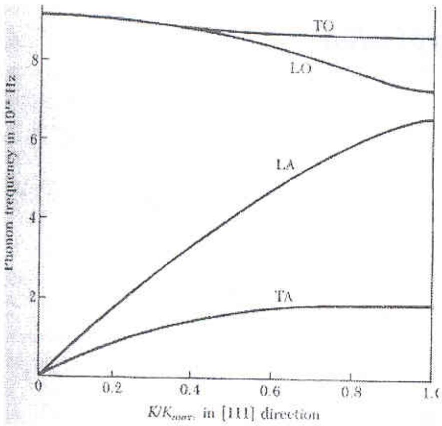
$$Ka = \pm\pi,$$

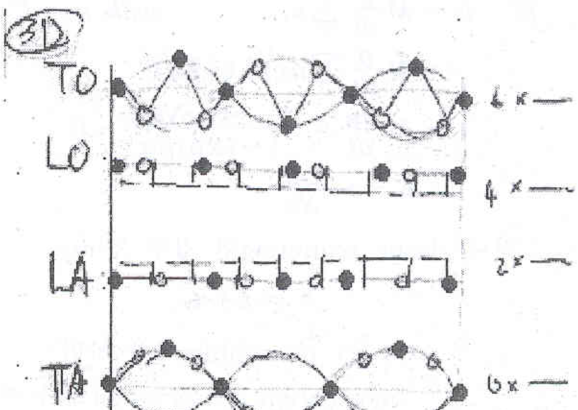
$$0 = M_1M_2\omega^4 - 2C(M_1+M_2)\omega^2 + 2C^2(1+1)$$
$$= M_1M_2\omega^4 - 2C(M_1+M_2)\omega^2 + 4C^2$$
$$= (M_1\omega^2 - 2C)(M_2\omega^2 - 2C)$$
$$\therefore \omega^2 = \frac{2C}{M_1} \text{ or } \frac{2C}{M_2}$$



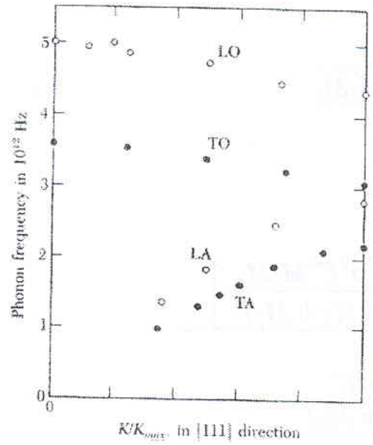
s of the
lattice,
= 0 and

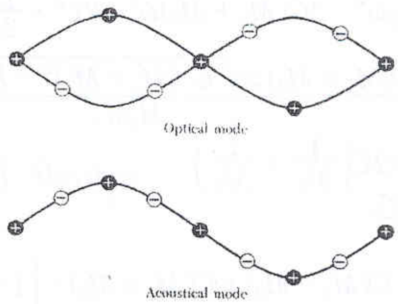
For diatomic linear lattice.





Phonon dispersion relation





Transerse and optical mode.

Quantization of Elastic wave.

lattice vibration의 quantization.

phonon이라 부른다.

elastic mode of angular frequency ω

$$\varepsilon = (n + \frac{1}{2})\hbar\omega$$

mean square phonon amplitude.

$$u = u_0 \cos Kx \cdot \cos \omega t$$

The time average Kinetic Energy.

$$\frac{1}{2}\ \rho V \omega^2 u_0^2 = \frac{1}{2}(n + \frac{1}{2})\hbar\omega$$

$$u_0^2 = \frac{4(n + \frac{1}{2})\hbar}{\rho V \omega}$$

Phonon momentum.

phonon은 momentum을 운반하지 않는다. [except for K=0]

$$pf.\quad p = M\frac{d}{dt}\sum u_s \qquad with\ u_s = C\exp(isKa)$$

$$= M\frac{d}{dt}\sum u \exp(isKa)$$

$$= M\frac{du}{dt}\cdot\frac{1-\exp iNKa}{1-\exp iKa} = 0$$

$$\therefore K = \pm\frac{2\pi r}{Na}$$

그러나 elastic scattering인 경우 X-ray.

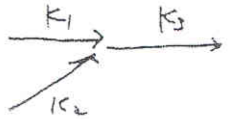
$$\vec{k}' = \vec{k} + \vec{G}$$

$\therefore \hbar\vec{k}$를 momentum이라 하면

momentum conservation law 만족.

만약 inelastic이면 wave vector selection rule은

$$\vec{k}' + \vec{K} = \vec{k} + \vec{G}$$
$$\vec{k}' = \vec{k} + \vec{K} + \vec{G}$$ [아래의 $\vec{K}$는 absorbed phonon!]



probability of collision

= product of the three phonon wave amplitude.

$$\sum_n \exp(-i\vec{k_1}\cdot\vec{r_n})\exp(-i\vec{k_2}\cdot\vec{r_n})\exp(i\vec{k_3}\cdot\vec{r_n})$$
$$= \sum_n \exp[i(\vec{k_3} - \vec{k_1} - \vec{k_2})\cdot\vec{r_n}]$$

Inelastic scattering by phonon.

$\omega(K)$는 inelastic scattering으로 결정한다.

$$\vec{k} + \vec{G} = \vec{k}' \pm \vec{K}$$

$\vec{G}$와 $\vec{K}$는 1st Brillouin zone에 있다.

$$\frac{\hbar^2 k^2}{2M_n} = \frac{\hbar^2 k'^2}{2M_n} \pm \hbar\omega$$

$+$ Creation of phonon.
$-$ Anhilation of phonon.
M_n Neutron mass

Mirror symmetry

A^+B^-와 A^-B^+는 dispersion relation이 거의 비슷.

KF와 NaCl은 매우 비슷.

K^+, Cl^-는 isoelectronic
F^-, Na^+는 isoelectronic

mass는 다르지만 dispersion relation은 비슷하다