- Overview

Mechanical property

- $U_{tot}(R)$; $B \equiv -V\left(\frac{\partial P}{\partial V}\right)_T = V\left(\frac{\partial^2 U_{tot}}{\partial V^2}\right)_P \rightarrow \overset{\partial}{V} = nv$
  $v \propto R$

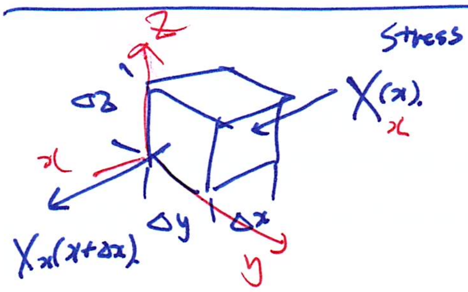
- C_{ij} : $U = \frac{1}{2}\sum_{i=1}^{j}\sum_{j=1}^{6} C_{ij} e_i e_j$

  $\downarrow$ $e_1 = e_2 = e_3 = \frac{1}{3}\delta$.

  $U \equiv \frac{1}{2}B\delta^2$; $B = \frac{1}{3}(C_{11} + 2C_{12})$ cubic case.

- C_{ij} ?

· Elastic waves in crystals



mass $= \rho \cdot V$

$= \rho \cdot \Delta x \Delta y \Delta z$

acceleration $\partial^2 u / \partial t^2$

net Force btw x & $x + \Delta x$

$$\left(\frac{\partial X_x}{\partial x}\Delta x\right)\underbrace{\Delta y \cdot \Delta z}_{\text{area}}$$

similarly

$$\left(\frac{\partial X_y}{\partial y}\Delta x\right)\Delta y \cdot \Delta z \quad , \quad \left(\frac{\partial X_z}{\partial z}\Delta x\right)\Delta y \cdot \Delta z$$

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ & C_{22} & C_{11} \\ & & C_{11}C_{44} \dots \end{bmatrix}$$

$ma = F$

$$\rho \cdot \frac{\partial^2 u}{\partial t^2} \cdot \Delta x \Delta y \Delta z = \left(\frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z}\right)\Delta x \Delta y \Delta z .$$

$$\rho \cdot \frac{\partial^2 u}{\partial t^2} = \frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z}$$

$$X_x = \boxed{C_{11}} e_{xx} + \boxed{C_{12}} e_{yy} + \boxed{\cancel{C_{13}}} e_{zz} + \cancel{C_{14}} e_{yz} + \cancel{C_{15}} e_{zx} + \cancel{C_{16}} e_{xy}$$

C_{12}, C_{12}

cubic sym.

$$= C_{11}\frac{\partial e_{xx}}{\partial x} + C_{12}\left(\frac{\partial e_{yy}}{\partial x} + \frac{\partial e_{zz}}{\partial x}\right)$$

$$+ C_{44}\left(\frac{\partial e_{xy}}{\partial y} + \frac{\partial e_{zx}}{\partial z}\right)$$

$$X_y = \boxed{C_{66}} e_{xy} \Rightarrow \cancel{C_{61}} e_{xx} + \cancel{C_{62}} e_{yy} + \cancel{C_{63}} e_{zz} + C_{64} e_{yz} + C_{65} e_{zx}$$

C_{44}

~~$X_z = Z_x = C_{11}$~~

$e_{xx} = \frac{\partial u}{\partial x}$

$e_{yy} = \frac{\partial v}{\partial y}$

$e_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}$ $\quad$ $e_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}$

$\boxed{\text{u, v, w. displacement component}}$ ⇒

(1)
$$\rho \cdot \frac{\partial^2 u}{\partial t^2} = C_{11}\frac{\partial^2 u}{\partial x^2} + C_{44}\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) + (C_{12} + C_{44})\left(\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 w}{\partial x \partial y}\right)$$

$$X_z = Z_x = \cancel{C_{51}} e_{xx} + \cancel{C_{52}} e_{yy} + \cancel{C_{53}} \dots$$
$$\cancel{C_{54}} e_{yz} + \boxed{\cancel{C_{55}}} e_{zx} + \cancel{C_{56}} e_{xy}$$

C_{44}

(2)
$$\rho \cdot \frac{\partial^2 v}{\partial t^2} = C_{11}\frac{\partial^2 v}{\partial y^2} + C_{44}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial z^2}\right) + $$
$$+ (C_{12} + C_{44})\left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 w}{\partial y \partial z}\right);$$

(3)
$$\rho \cdot \frac{\partial^2 w}{\partial t^2} = C_{11}\frac{\partial^2 w}{\partial z^2} + C_{44}\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right) + (C_{12} + C_{44})\left(\frac{\partial^2 u}{\partial x \partial z} + \frac{\partial^2 v}{\partial y \partial z}\right)$$

· Waves in the [100] direction.

$$\begin{cases} e^{ix} = \cos x + i\sin x \\ e^{-ix} = \cos x - i\sin x \end{cases}$$

②

one solution (longitudinal wave)

$$u = u_0 \exp[i(Kx - \omega t)]$$
$$= u_0 e^{iKx} e^{-i\omega t}$$

; $K = \frac{2\pi}{\lambda}$ wavevector, $\omega = 2\pi\nu$ angular frequency

velocity $\frac{\omega}{K} = \nu \cdot \lambda$.

substitution in (1)

$$\rho \cdot \cancel{u_0 e^{-ikx - i\omega t}} (-i\omega)^2 = C_{11} \cdot \cancel{u_0 e^{ikx} e^{-i\omega t}} \cdot (-iK)^2.$$

$$\omega^2 \rho = C_{11} K^2$$

· velocity $\frac{\omega}{K}$ of a longitudinal wave in [100] direction.

$$v_s = (C_{11}/\rho)^{1/2}$$

· transverse or shear wave

$$v = v_0 \exp[iKx - \omega t]$$

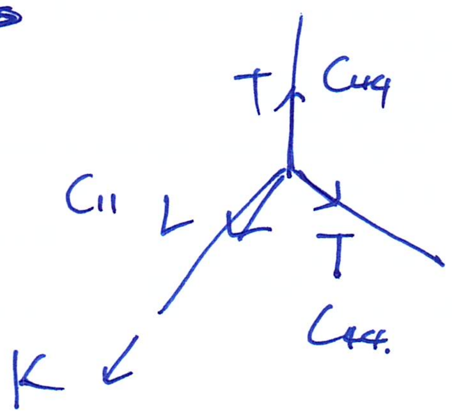
substitution in (2)

$$\rightarrow \omega^2 \rho = C_{44} K^2, \quad v_s = (C_{44}/\rho)^{1/2}$$

$$w = w_0 \exp[iKx - \omega t]$$

substitution in (3) same result. $v_s = (C_{44}/\rho)^{1/2}$.

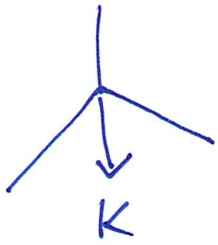
~~$\omega^2 \rho$~~



Wave in [100] direction

	v_s (velocity)
L	$(C_{11}/\rho)^{1/2}$
T	$(C_{44}/\rho)^{1/2}$

· Waves in [110] direction.



$$u = u_0 \exp[i(K_x x + K_y y - \omega t)]$$

$$v = v_0 \exp[i(K_x x + K_y y - \omega t)]$$

$$w = w_0 \exp[i(K_x x + K_y y - \omega t)] \rightarrow \omega^2 \rho = C_{44}(K_x^2 + K_y^2)$$

↳ shear wave 1 (T_1)

(4) $$\omega^2 \rho u = (C_{11} K_x^2 + C_{44} K_y^2) u + (C_{12} + C_{44}) K_x K_y v \,;$$

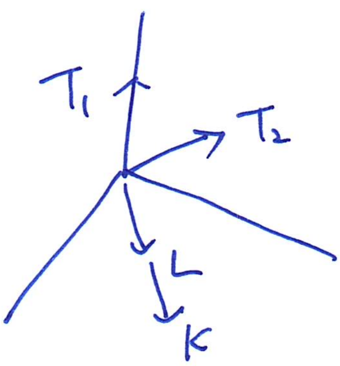
(5) $$\omega^2 \rho v = (C_{11} K_y^2 + C_{44} K_x^2) v + (C_{12} + C_{44}) K_x K_y u \,;$$

pair solution $K_x = K_y = K/\sqrt{2}$. $\longrightarrow \omega^2 \rho = C_{44} K^2$

$$\begin{vmatrix} -\omega^2 \rho + \frac{1}{2}(C_{11} + C_{44}) K^2 & \frac{1}{2}(C_{12} + C_{44}) K^2 \\ \frac{1}{2}(C_{12} + C_{44}) K^2 & -\omega^2 \rho + \frac{1}{2}(C_{11} + C_{44}) K^2 \end{vmatrix} = 0$$

$\rightarrow \omega^2 \rho = \frac{1}{2}(C_{11} + C_{12} + 2C_{44}) K^2$ → longitudinal wave (L)

$\omega^2 \rho = \frac{1}{2}(C_{11} - C_{12}) K^2$ → shear wave 2. (T_2)



wave in [110] direction.

	V_s (velocity)
L	$\{(C_{11} + C_{12} + 2C_{44})/2\rho\}^{1/2}$
T_1	$\{(C_{44}/\rho)\}^{1/2}$
T_2	$\{(C_{11} - C_{12})/2\rho\}^{1/2}$

2 solutions. $\begin{cases} \omega^2\rho = \frac{1}{2}(C_{11}+C_{12}+2C_{44})K^2 & \rightarrow (4) \\ \omega^2\rho = \frac{1}{2}(C_{11}-C_{12})K^2 & \rightarrow (5) \end{cases}$

수정

$\rightarrow (4) \quad \frac{1}{2}(C_{11}+C_{12}+2C_{44})K^2u = \frac{1}{2}(C_{11}K_x^2+C_{44}K_y^2)u + \frac{1}{2}(C_{12}+C_{44})K^2v$

$= \frac{1}{2}(C_{11}+C_{44})K^2u. \quad + \quad$ 〃

$\Rightarrow u = v \rightarrow$ longitudinal wave. [110] direction.
paralleled to K. vector

$\rightarrow (5) \quad \frac{1}{2}(C_{11}-C_{12})K^2\cancel{u}\,v = \frac{1}{2}(C_{11}+C_{44})K^2\cancel{u}\,v + \frac{1}{2}(C_{12}+C_{44})K^2\cancel{v}\,u$

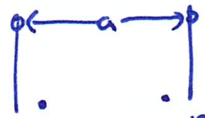
$\Rightarrow u = -v \rightarrow$ transverse wave [$\bar{1}$10] ~~[1$\bar{1}$0]~~ direction
perpendicular to K vector

· Sounds in Crystals.

· Established the frequency of elastic waves in terms of wavevector (K) that describes the wave using elastic constants (C_{ij})

· Each wavevector has three modes. as solution for u (longitudinal, two transverse)

· Allow small deviations in atoms vibration.



$R_i + u_i$

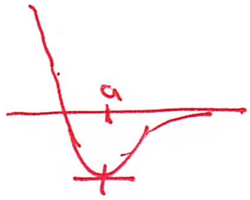
at Equilibrium $\rightarrow \frac{1}{2}\sum_{i\neq j}\phi(R_i - R_j) = U_{eq.}$

$$U_{total} = \frac{1}{2}\sum_{i\neq j}\phi(R_i - R_j + u_i - u_j)$$

Taylor series
$f(x_0+\delta)$
$\cong f(x_0) + \delta\left(\frac{df}{dx}\right)_{x=x_0}$
$+\frac{1}{2}\delta^2\left(\frac{d^2f}{dx^2}\right)_{x=x_0} \cdots$

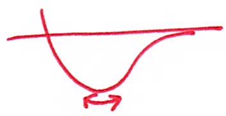
$$= \frac{1}{2}\sum_{i\neq j}\phi(R_i - R_j) + \frac{1}{2}\sum(u_i - u_j)\cancel{\left(\frac{d\phi}{d(R_i - R_j)}\right)}_{R_i - R_j = a} \rightarrow 0$$

at equilibrium condition



$$+ \frac{1}{4}\sum(u_i - u_j)^2 \left.\frac{d^2\phi}{d(R_i - R_j)^2}\right|_{R_i - R_j = a} \cdots$$

$$= U_{eq.} + \underline{\frac{1}{4}\sum_{i\neq j}(u_i - u_j)^2 \phi''(R_i - R_j)}$$



atom vibration $(u_i - u_j)$ harmonic oscilator.

$$U_{harmonic} = \frac{1}{4}\sum_{i\neq j}(u_i - u_j)^2 K_{ij} = \frac{K}{4}\sum_{j=2}^{N}\left[(u_{j+1} - u_j)^2 + (u_{j-1} - u_j)^2\right]$$

$(N+1 = 1.)$

$$K_{ij} = \begin{cases} K & i = j-1 \text{ or } i = j+1. \\ 0 & \text{otherwise} \end{cases}$$

$$F_j = -\frac{\partial U_{harmonic}}{\partial u_j}$$

$$= \frac{K}{2}\left[u_{j+1} + u_{j-1} - 2u_j\right]$$

$$\begin{pmatrix} u_{j+1}^2 - 2u_{j+1}u_j + u_j^2 \\ + u_{j-1}^2 - 2u_{j-1}u_j + u_j^2 \end{pmatrix}$$

$\frac{K}{2}(u_{j+1} - u_j)$

$-\frac{K}{2}(u_j - u_{j-1})$

u_{j+1}

· Use equation of motion ← spring model.

$$m\frac{d^2u_j}{dt} = F_j = \frac{K}{2}(u_{j+1} + u_{j-1} - 2u_j)$$

Note: $F = -kx$

$F = ma = m\frac{d^2x}{dt^2}$

$m\frac{d^2x}{dt^2} = -kx$

$x(t) = x_0 e^{-i\omega t}$

$\omega = \sqrt{k/m}$

· Use wave solution $u_j(x,t) = \underbrace{u_q(0)}_{\text{상수}}\underbrace{e^{-i\omega t}}_{\text{시간}}\underbrace{e^{iq(ja)}}_{\text{공간}(x)}$

$\overleftrightarrow{a}$

$$m\,\cancel{u_q(0)}\,\cancel{e^{-i\omega t}}\cdot\cancel{e^{iq(ja)}}\cdot(-i\omega)^2$$

$$= \frac{K}{2}\cancel{u_q(0)}\,\cancel{e^{-i\omega t}}\left\{e^{iq(\cancel{j}+1)a} + e^{iq(\cancel{j}-1)a} - 2\cancel{e^{iqja}}\right\}$$

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

$e^{ix} = \cos x + i\sin x$

$e^{-ix} = \cos x - i\sin x$

$\cos x = \frac{e^{ix} + e^{-ix}}{2}$

$$= \frac{K}{2}2(\cos qa - 1)$$

$$\cancel{-m\omega^2 = 2K\sin^2(\frac{qa}{2})}$$

$$\cancel{\omega = \sqrt{\frac{2K}{m}}\left|\sin\frac{qa}{2}\right|}$$

$$\omega^2 = \frac{2K}{m}(1 - \cos qa)$$

or

$$\omega^2 = \frac{4K}{m}\sin^2\left(\frac{qa}{2}\right) \quad \text{or} \quad \omega = \sqrt{\frac{4K}{m}}\left|\sin\frac{qa}{2}\right|.$$