①

Mid Term solution

Q1

3 atoms per basis $= n$

3D $= d$

$n \times d = 9$ branches

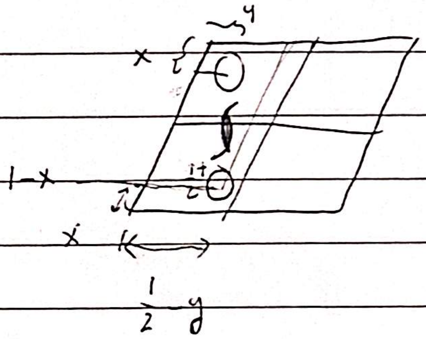
3 acoustic

$9-3 = 6$ optical

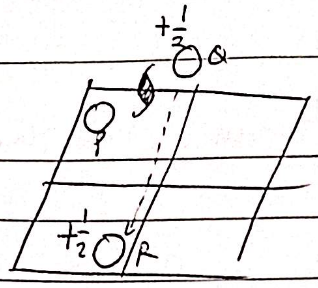
Q2

Action of 2_1 screw axis at $\left(\frac{1}{2}, \frac{1}{4}, z\right)$.

$$(x, y, z) \longrightarrow \left(1-x, \frac{1}{2}-y, z+\frac{1}{2}\right)$$

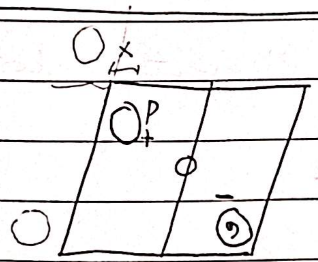


Action of 2_1 screw axis at $\left(0, \frac{1}{4}, 0\right)$



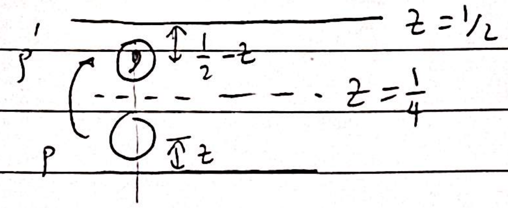
P goes to Q and then Q is equivalent to R.

Action of $\bar{1}$ at $\left(\frac{1}{2}, \frac{1}{2}, z\right)$

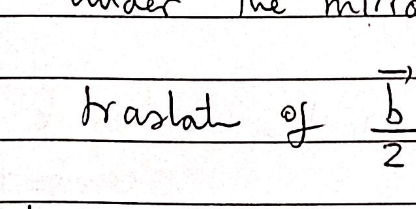


$$(x, y, z) \longrightarrow (\bar{x}, \bar{y}, \bar{z})$$

Action of b glide plane at height $z = \frac{1}{4}$



P goes to P' from height z to $\frac{1}{2} - z$ under the mirror plane at $z = \frac{1}{4}$. Follow this by a translation of $\frac{\vec{b}}{2}$, yielding Q, i.e $\left(x, \frac{1}{2} + y, \frac{1}{2} - z\right)$.



Hence all 4 equivalent positions are generated.

Q3

(a) Crystal system is orthorhombic because of the presence of a m plane and a 2_1 axis.

(b) Since it is orthorhombic, the three symmetry elements in the name specify elements along $\vec{a}$, $\vec{b}$ and $\vec{c}$ in the same order.

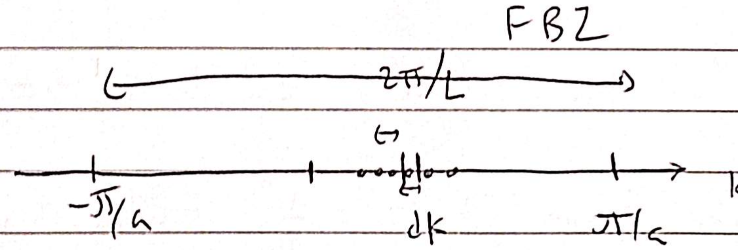
m (mirror plane) $\perp$ $\vec{a}$.

c (glide plane) $\perp$ $\vec{b}$;

2_1 (screw axis) along $\vec{c}$.

Q4

(a)



$$dN = \frac{dk}{(2\pi/L)} = \frac{1}{2} g(\omega)\, d\omega$$ (as k can be +ve or -ve)

$$g(\omega)\, d\omega = \frac{2L}{2\pi}\, dk$$

$$g(\omega) = \frac{L}{\pi}\left(\frac{1}{d\omega/dk}\right)$$

Now, $\omega = vk$ (sound, dispersionless)

$$\frac{d\omega}{dk} = v.$$

$$\therefore \boxed{g(\omega) = \frac{L}{\pi v}}.$$

(b)

$$\int_0^{\omega_D} g(\omega)\, d\omega = N \leftarrow \text{number of modes (2D)}$$

$$\frac{L}{\pi v}\omega_D = N$$

$$\boxed{\omega_D = \frac{N\pi v}{L}}, \quad k_B\theta_D = \hbar\omega_D$$

$$\theta_D = \frac{\hbar N\pi v}{L k_B}$$

$\frac{N}{L} = \frac{1}{a} \Rightarrow$ spacing in real space

$$\therefore \boxed{\theta_D = \frac{\hbar\pi v}{a k_B}}.$$

(c) $$U = \int_0^{\omega_D} d\omega \, g(\omega) \left(\hbar\omega\right) \frac{1}{e^{\hbar\omega/k_BT} - 1}$$

$T \to 0$ (low T) , $\dfrac{\hbar\omega}{k_BT} \to \infty$, $\omega_D \to \infty$

$$\cancel{U = \int_0^{\infty}}$$

Let $\dfrac{\hbar\omega}{k_BT} = x$

$$\omega = \frac{k_BT}{\hbar} x$$

$$d\omega = \frac{k_BT}{\hbar} dx$$

$$\omega_D = \frac{k_BT}{\hbar} x_D$$

$$U = \int_0^{x_D} \left(\frac{k_BT}{\hbar}\right) dx \, g(x) \, \cancel{\hbar} \left(\frac{k_BT}{\cancel{\hbar}}\right) x \left(\frac{1}{e^x - 1}\right)$$

$$= \frac{(k_BT)^2}{\hbar} \int_0^{x_D} dx \, g(x) \left(\frac{x}{e^x - 1}\right)$$

For small T, $x_D \to \infty$

$$U \simeq \frac{(k_BT)^2}{\hbar} \int_0^{\infty} dx \, g(x) \left(\frac{x}{e^x - 1}\right)$$

Now $g(\omega)\,d\omega = g(x)\,dx$.

$$g(\omega)\frac{d\omega}{dx} = g(x)$$

$$g(x) = \frac{g(\omega)}{dx/d\omega} = \frac{L}{\pi v}\cdot\frac{1}{\hbar/k_BT}$$

$$= \frac{Lk_BT}{\hbar\pi v}$$

∴

$$U \simeq \frac{(k_BT)^2}{\hbar}\int_0^\infty dx\left(\frac{x}{e^x-1}\right)\left(\frac{Lk_BT}{\hbar\pi v}\right)$$

$$U = \frac{(k_BT)^3 L}{\hbar^2\pi v}\int_0^\infty dx\left(\frac{x}{e^x-1}\right) \quad \text{——} \quad (1)$$

$$\cancel{C_v = \frac{\partial U}{\partial T}\Big|_V \propto T^2}$$

Now $C_v = \frac{\partial U}{\partial T}\Big|_{\text{const } V}$.

Now $\frac{\hbar\omega}{k_BT} = x \Rightarrow T = \frac{\hbar\omega}{k_B x}$

$$T = \frac{\hbar\omega}{k_B}(x)^{-1}$$

$$\frac{\partial U}{\partial T} = \frac{\partial U}{\partial x}\cdot\frac{\partial x}{\partial T} \qquad \frac{\partial T}{\partial x} = -\frac{\hbar\omega}{k_B}\frac{1}{x^2}$$

$$\therefore \frac{\partial U}{\partial T} = \cancel{\frac{-\hbar\omega}{k_B}\,\frac{(k_B T^2)}{\hbar^2\omega}}\;\frac{1}{\partial T/\partial x}\cdot\frac{\partial U}{\partial x}$$

$$= -\frac{k_B x^2}{\hbar\omega}\,\frac{\partial U}{\partial x}$$

$$= -\frac{\cancel{k_B}}{\cancel{\hbar\omega}}\cdot\frac{\hbar^2\omega^2}{k_B^2 T^2}\cdot\frac{\partial U}{\partial x}$$

Now $x = \dfrac{\hbar\omega}{k_B T}$

$$C_v = \frac{\partial U}{\partial T} = -\frac{\hbar\omega}{k_B T^2}\,\frac{(k_B T)^3 L}{\hbar^2 \pi v}\,\frac{\partial}{\partial x}\int_0^\infty dx\left(\frac{x}{e^x-1}\right)$$

$\Rightarrow C_v \sim T^1$. (at low temp, in 1 D).

Q5.

$a : b : c = 0.529 : 1 : 0.477$

Intercepts are $0.264 : 1 : 0.238$.

$$(h : k : l) = \left(\frac{a}{x} : \frac{b}{y} : \frac{c}{z} \right)$$

$$= \left(\frac{0.529}{0.264} : \frac{1}{1} : \frac{0.477}{0.238} \right)$$

$$= (2.004, 1, 2.004)$$

$$\simeq (2, 1, 2) = (212)$$ are the Miller indices.

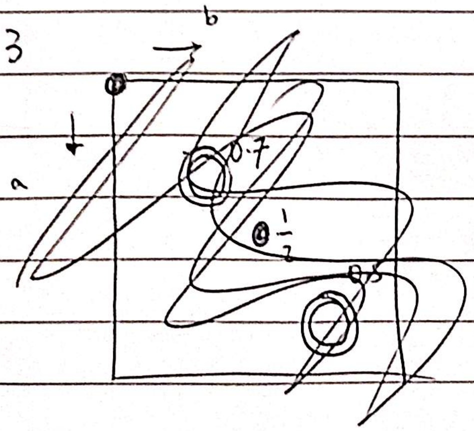
Q6.

Ti at 2a $\rightarrow$ $0,0,0$ and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

O at 4f $\rightarrow$ $x, x, 0$; $\bar{x}, \bar{x}, 0$; $x+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}$;

$x \simeq 0.3$

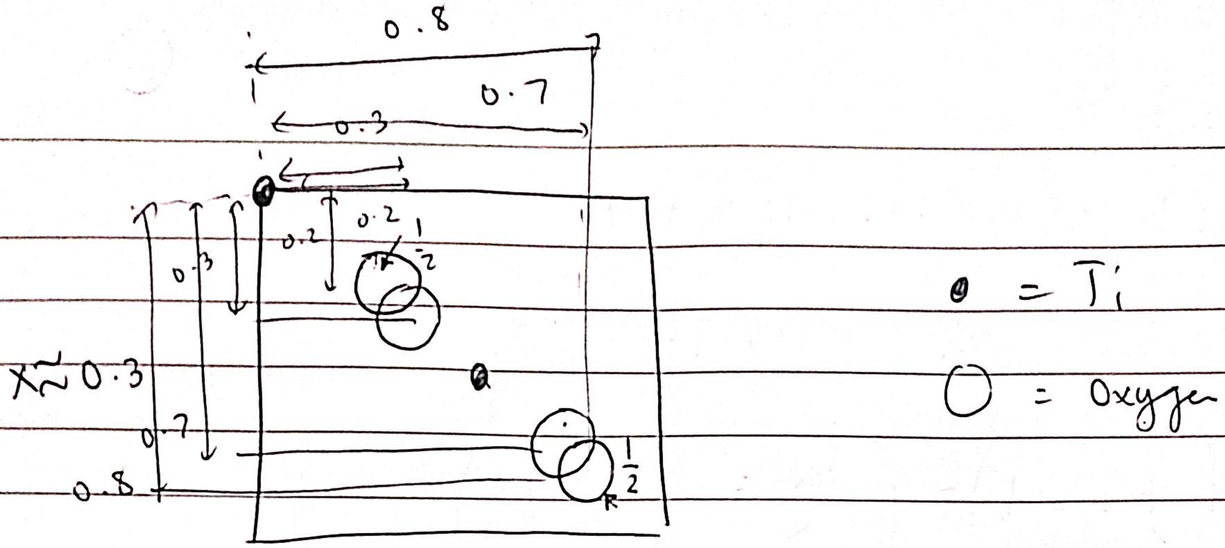
$\bar{x}+\frac{1}{2}, \bar{x}+\frac{1}{2}, \frac{1}{2}$.



● = Ti

○ = O

P.T.O.



Q7

$$S(hkl)_{\text{lattice}} = e^{i2\pi\left(\frac{h}{2}\right)} + e^{i\frac{2\pi}{2}\left(\cancel{x+y}\, h+k+l\right)}$$

$$= e^{i\pi h} + e^{i\pi(h+k+l)}$$

$$= e^{i\pi h}\left(1 + e^{i\pi(k+l)}\right)$$

$\neq 0$ when $k+l = 2n$ = even

which is the required reflection condition.