

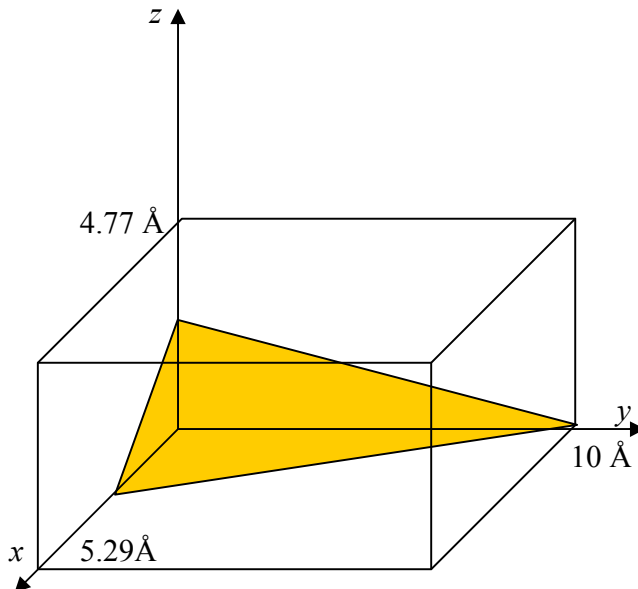
# PC3235 – Solid State Physics 2004/05

1(a)(i)

	h	k	l
A. Intercept (ratio)	$\frac{2.64}{5.29} = \frac{264}{529}$	$\frac{10}{10} = 1$	$\frac{2.38}{4.77} = \frac{238}{477}$
B = 1/A	$\frac{529}{264}$	1	$\frac{477}{238}$
C = B / smallest no.	2.003	1	2.004
Closest integer	2	1	2

Therefore, Plane [212]

(a)(ii)



(a)(iii) In units of Å, real lattice:  $\mathbf{u}_1 = 5.29 \mathbf{i}$ ,  $\mathbf{u}_2 = 10 \mathbf{j}$ ,  $\mathbf{u}_3 = 4.77 \mathbf{k}$

$$\mathbf{a}_1 \times \mathbf{a}_2 = 25.2333 \hat{j}$$

$$\mathbf{a}_2 \times \mathbf{a}_3 = 47.7 \hat{k}$$

$$\mathbf{a}_3 \times \mathbf{a}_1 = 52.9 \hat{i}$$

$$\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3 = 252.333$$

$$\text{Reciprocal lattice } \mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}; \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}; \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$

$$\therefore \mathbf{b}_1 = 2\pi \frac{47.7}{252.333} \hat{k} = \frac{200\pi}{529} \hat{k}; \mathbf{b}_2 = \frac{200\pi}{477} \hat{i}; \mathbf{b}_3 = \frac{2\pi}{10} \hat{j}$$

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 = v_1 \frac{200\pi}{529} \hat{k} + v_2 \frac{200\pi}{477} \hat{i} + v_3 \frac{2\pi}{10} \hat{j}$$

For separation between adjacent parallel (h k l), then

$$\mathbf{G} = h \frac{200\pi}{529} \hat{k} + k \frac{200\pi}{477} \hat{i} + l \frac{2\pi}{10} \hat{j} = 2 \left( \frac{200\pi}{529} \hat{k} \right) + \frac{200\pi}{477} \hat{i} + \left( \frac{2\pi}{10} \right) \hat{j}$$

$$= \frac{400\pi}{529} \hat{k} + \frac{200\pi}{477} \hat{i} + \frac{2\pi}{5} \hat{j}$$

$$|\mathbf{G}|^2 = \left( \frac{400\pi}{529} \right)^2 + \left( \frac{200\pi}{477} \right)^2 + \left( \frac{2\pi}{5} \right)^2$$

$$d = \frac{2\pi}{|\mathbf{G}|} = 2.10 \text{ \AA}$$

(b)(i) Using Bragg equation:  $2d \sin \theta = n\lambda$ , known parameters are  $\lambda$  and  $\theta$

- For a simple cubic lattice,  $d = \frac{2\pi}{|\mathbf{G}|} = \frac{a}{|h^2 + k^2 + l^2|^{\frac{1}{2}}}$
- We can compute d for every possible diffraction angle obtained from the diffraction experiment
- It is known that the scattering amplitude gives the possible reflection planes
- For reflection/ diffraction to occur, scattering amplitude must be more than 0
- Scattering amplitude  $S_G = \sum f(e^{i2\pi(xh+yk+zl)})$
- From above formula it can be deduced that

Cubic structure	<b>h, k, l</b>
Simple cubic	Any integer
Body Center Cubic(bcc)	All even
Face Center Cubic(fcc)	Unmixed integers—all odd or all even

And

Cubic structure	$h^2 + k^2 + l^2$
Simple cubic	1, 2, 3, 4...
Body Center Cubic(bcc)	2, 4, 6, 8...
Face Center Cubic(fcc)	3, 4, 8, 11...

- Take  $\frac{(\text{smallest integer of } |h^2 + k^2 + l^2|) \times \sin^2 \theta}{\text{smallest value of } \sin^2 \theta}$
- Compare above values with  $h^2 + k^2 + l^2$  sequence
- Largest number of matches with  $h^2 + k^2 + l^2$  sequence will be the cubic structure.

- Combining Bragg formula and inter-planar distance  $d$  for a simple cubic, it can be shown that  $a = \frac{n\lambda\sqrt{h^2 + k^2 + l^2}}{2\sin\theta}$  where  $a$  is the lattice parameter for a simple cubic structure.
- As error of  $a$  approaches 0 as the error of  $\theta$  approaches 0
- Therefore plotting graph of  $a$  against  $\frac{1}{\sin^2\theta}$ . Intercept of best fit line will be lattice parameter

(b)(ii) Given  $\lambda = 1.54\text{Å}$ ;  $\theta = 24^\circ$ ;  $(h \ k \ l) = (2 \ 1 \ 0)$

$$h^2 + k^2 + l^2 = 5$$

$$d = \frac{a}{\sqrt{5}}$$

$$2d \sin\theta = \lambda \Rightarrow d = \frac{\lambda}{2\sin\theta}$$

$$a = \frac{\sqrt{5}\lambda}{2\sin\theta} \approx 4.23\text{Å}$$

$$\therefore \text{volume of unit cell} = a^3 \approx 75.7\text{Å}^3$$

2(a)(i) At equilibrium distance net force = 0

$$F = 0 = 24\epsilon \left[ \frac{2\sigma^{12}}{R_0^{13}} - \frac{\sigma^6}{R_0^7} \right] \Rightarrow \frac{2\sigma^{12}}{R_0^{13}} = \frac{\sigma^6}{R_0^7}$$

$$\therefore R_0 \approx 3.82\text{Å}$$

(a)(ii) Let  $R = R_0 + u$

$$F = 24\epsilon \left[ \frac{2\sigma^{12}}{(R_0 + u)^{13}} - \frac{\sigma^6}{(R_0 + u)^7} \right] \approx 24\epsilon \left[ 2\sigma^{12}(R_0^{-13} - 13R_0^{-14}u) - \sigma^6(R_0^{-7} - 7R_0^{-8}u) \right]$$

$$\Rightarrow F \approx 24\epsilon \left[ 2\sigma^{12}(R_0^{-13} - 13R_0^{-14}u) - \sigma^6(R_0^{-7} - 7R_0^{-8}u) \right] = ku$$

$$\text{but } R_0^{-n} \ll u$$

$$k \approx 24\epsilon \left[ 2\sigma^{12}(-13R_0^{-14}u) - \sigma^6(-7R_0^{-8}u) \right] \approx 0.525$$

(b) 
$$U = N \left[ \frac{A}{R^n} - \frac{\alpha e^2}{4\pi\epsilon_0 R} \right]$$

At equilibrium, 
$$\frac{dU}{dR} = 0 = N \left[ -\frac{nA}{R_0^{n+1}} + \frac{\alpha e^2}{4\pi\epsilon_0 R_0^2} \right]$$

$$\frac{nA}{R_0^{n+1}} = \frac{\alpha e^2}{4\pi\epsilon_0 R_0^2}$$

$$\frac{A}{R_0^n} = \frac{\alpha e^2}{n4\pi\epsilon_0 R_0}$$

$$\therefore U = N \left[ \frac{\alpha e^2}{n4\pi\epsilon_0 R_0} - \frac{\alpha e^2}{4\pi\epsilon_0 R_0} \right] = \frac{N\alpha e^2}{4\pi\epsilon_0 R_0} \left[ \frac{1}{n} - 1 \right] = -\frac{N\alpha e^2}{4\pi\epsilon_0 R_0} \left[ 1 - \frac{1}{n} \right]$$

- 3(a)(i) A harmonic force has its directional acceleration always pointing towards the equilibrium position. In addition, the restoring force is proportional to the displacement from the equilibrium position.

Anharmonic forces do not always have the direction of acceleration pointing towards the equilibrium position.

- (a)(ii) Assume that all the atoms in the 1D monoatomic lattice be connected by a spring of spring constant  $c$  to its nearest neighbors only. Let the atoms be displaced slightly from its equilibrium position by  $u$ , where  $s$  denotes the  $s$ th atom of the chain.

$$\text{Let } u_s = u_0 e^{i(ska - \omega t)}, \quad \frac{d^2 u_s}{dt^2} = -\omega^2 u_0 e^{i(ska - \omega t)}$$

$$F = m \frac{d^2 u_s}{dt^2} = c(u_{s+1} + u_{s-1} - 2u_s)$$

$$\Rightarrow -m\omega^2 u_0 e^{i(ska - \omega t)} = cu_0 e^{i(ska - \omega t)} (e^{ika} + e^{-ika} - 2)$$

$$-m\omega^2 = c(2 \cos ka - 2)$$

$$\omega^2 = \frac{4c}{m} \sin^2 \frac{ka}{2}$$

- (a)(iii) Using ans in part (ii),  $\omega^2 = \frac{4c}{m} \sin^2 \frac{ka}{2}$

$$\omega^2 \text{ is maximum when } k = \frac{\pi}{a}$$

$$\therefore \omega = \sqrt{\frac{4c}{m}} \sin \frac{ka}{2}$$

For phonon,

$$E = \hbar\omega = \hbar \sqrt{\frac{4c}{m}} \sin \frac{ka}{2} \approx 2.79 \times 10^{-23} \text{ J}$$

$$p = \frac{h}{\lambda} = \hbar \times \left( \frac{2\pi}{\lambda} \right) = \hbar k \approx 6.83 \times 10^{-25} \text{ Nm}^{-1}$$

(a)(iv) Thermal conduction phenomenon is mainly due to two factors, the flow of phonons and electrons. In metals where the free electron density is high, the flow of electrons dominates while in non-metallic solids, mainly the flow of phonons determines the thermal conductivity. In a crystal lattice, the phonons collide with each other because of the anharmonic force factors. The phonon collision process is divided into Normal Processes and Umklapp Processes. In Normal Processes, a phonon with wavevector  $\mathbf{K}_1$  collides with another phonon with wavevector  $\mathbf{K}_2$  yields a third phonon with wavevector  $\mathbf{K}_3 = \mathbf{K}_1 + \mathbf{K}_2$ , the total phonon momentum is conserved. In Umklapp Processes,  $\mathbf{K}_1 + \mathbf{K}_2 = \mathbf{K}_3 + \mathbf{G}$ , where  $\mathbf{G}$  is a reciprocal lattice vector. This is because in a crystal lattice, the only meaningful phonon  $\mathbf{K}$ 's must lie in the first Brillouin zone so that any longer  $\mathbf{K}$  produced in a collision must be brought back into the first zone by addition of a  $\mathbf{G}$ . In both processes, energy is conserved. In a crystal lattice, phonon density is higher in the hotter end than that in the colder end, heat flows from the hotter end to the colder end as phonons flow. Therefore, the Normal Processes accounts for the thermal conductivity. If that is the only possible process, then the thermal resistivity would be nearly zero because collision between phonons does not change the total phonon momentum (except between a phonon and the crystal boundary) and the speed of phonon is of the order of the sound speed inside the crystal. The main factor leading to thermal resistivity is the Umklapp Processes because the total phonon momentum along the direction of heat flow is reduced by an Umklapp phonon collision process. The Umklapp Processes happen only for two phonons with larger wavevectors in the order of  $k_B\theta/2$  because otherwise the wavevector of the resultant phonon cannot be outside the first zone.

4(a)(i) The free electron theory suggests that in metals there is a high density of free electrons moving around. A conduction electron is not deflected by ion cores arranged on a periodic lattice because matter waves can propagate freely in a periodic structure. A conduction electron is scattered only infrequently by other conduction electrons because of the Pauli Exclusion Principle. In the ground state of a system of  $N$  free electrons, the occupied orbitals may be represented as points inside a sphere in  $\mathbf{k}$  space

$$J = \sigma E = -nev$$

$$\therefore \sigma = -\frac{nev}{E} \quad \dots(1)$$

$$F = m \frac{dv}{dt} = -eE \Rightarrow m \int_0^v dv = -eE \int_0^\tau dt$$

$$v = -\frac{eE\tau}{m} \quad \dots(2)$$

$$\text{Combining (1) and (2),} \quad \sigma = -\frac{ne}{E} \left( -\frac{eE\tau}{m} \right) = \frac{ne^2\tau}{m}$$

$$(a)(ii) \quad N = 2 \frac{\frac{4}{3}\pi k^3}{\left(\frac{2\pi}{a}\right)^3} = \frac{a^3}{3\pi^2} \left(\frac{2mE}{\hbar^2}\right)^{\frac{3}{2}}$$

Using  $a = 3.5 \times 10^{-10}$ ;  $E = 4.7 eV$

$N = 1.98017 \approx 2 \Rightarrow$  BCC structure  $\therefore$  2 atoms per lattice and monovalent

- (b)(i) A crystal may be an insulator when the highest band is filled with an even number of electrons.

For metals such as potassium, there is only 1 electron per lattice cell, therefore it is a metal

For elements such as Magnesium, there are 2 electrons per lattice cell. Therefore it may be an insulator. However, the electrons only partially fill up the electron bands due to overlap in energy. Therefore it is a metal but not a very good one.

For semiconductors such as silicon, the energy band is the same as that of an insulator. However, the band gap is significantly smaller as compared to that of an insulator.

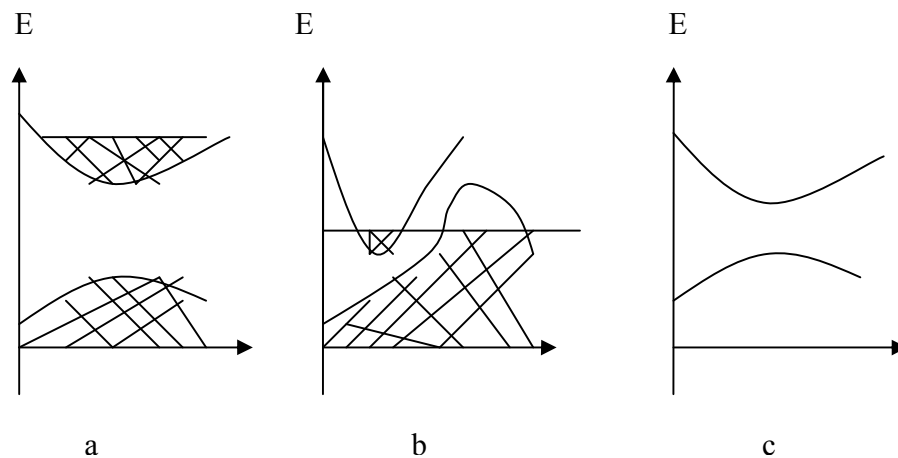


Fig 4: Energy band of (a) metal; (b)divalent metals; (c) insulators

- (ii) The dispersion relation plots for crystal considers the relative mass of the electron in the crystal instead of the actual mass of a free electron. This is because there are attractive forces between the nuclei and the electrons as well as frequent collisions between conductive electrons. This causes the electrons to be “heavier” than expected thus relative mass is more effective in representing the mass of the conduction electrons. Thus the dispersion relations of electrons in crystals will be slightly more complicated as well as different from that of a free electron because we are now using relative instead of actual mass of an electron which affects the wave vector plot.