

1) i) allowed \vec{k} val free e : $k = \text{periodic } \vec{k} = (k_x, k_y, k_z)$ where $k_i = \frac{2\pi}{L} \times n_i$
 free e energy $E(\vec{k}) = \frac{\hbar^2 k^2}{2m}$ ✓

$$\text{ii) } n^{\circ} \text{ points} = \frac{\text{vol sphere}}{\text{vol point}} = \frac{V k_F^3}{6\pi^2} = \frac{V}{2 \cdot 3\pi^2} \left[\left(\frac{2m\epsilon}{\hbar^2} \right)^{1/2} \right]^3$$

$$N(\epsilon) = 2 \cdot n^{\circ} \text{ points} = \frac{V}{3\pi^2} \left(\frac{2m\epsilon}{\hbar^2} \right)^{3/2}$$

iii) $g(\epsilon) = n^{\circ} e$ states per unit energy at ϵ

$$g(\epsilon) d\epsilon = N(\epsilon + d\epsilon) - N(\epsilon) = \Delta N(\epsilon)$$

$$\begin{aligned} g(\epsilon) &= \frac{dN(\epsilon)}{d\epsilon} \\ &= \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} d\epsilon \end{aligned}$$

iv) $N = \int_0^{\epsilon_F} g(\epsilon) d\epsilon \quad n = \frac{N}{V}$

$$\epsilon_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$$

$$\epsilon_F = \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V} \right)^{2/3}$$

$$\left(\epsilon_F \frac{2m}{\hbar^2} \right)^{3/2} = 3\pi^2 \frac{N}{V}$$

$$N = \left(\epsilon_F - \frac{\hbar^2}{2m} \right)^{3/2} \frac{V}{3\pi^2}$$

$$N = nV = \int_0^{\epsilon_F} g(\epsilon) d\epsilon$$

$$g(\epsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2}$$

$$N = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \frac{2\epsilon_F^{3/2}}{3}$$

$$= \frac{V}{2\pi^2} \frac{2}{3} \left(\epsilon_F \frac{2m}{\hbar^2} \right)^{3/2}$$

= confirmed

$$V_F = \frac{\hbar k_F}{m} \quad T_F = \frac{\epsilon_F}{k_B}$$

$$n \rightarrow k_F \rightarrow V_F \rightarrow \epsilon_F \rightarrow T_F$$

$$k_F = (3\pi^2 n)^{1/3} \quad \epsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

[Note: $\hbar = 1.055 \times 10^{-34} \text{ J s}$, $m = 9.1 \times 10^{-31} \text{ kg}$, $k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$ and $1 \text{ eV} = 1.60 \times 10^{-19} \text{ J}$.]

Element	$n (10^{22}/\text{cm}^3)$	$\epsilon_F (\text{eV})$	$T_F (10^4 \text{ K})$	$k_F (\text{\AA}^{-1})$	$v_F (10^6 \text{ m/sec})$
Cu	8.47				
Ca	4.61				
Al	18.1				

- Forget calc 2 refuse to go through this again

3) i) k val : $\vec{k} = (k_x, k_y, k_z)$ where $k_i = \frac{2\pi}{L} \times n_i$ ✓

$$v(\vec{k}) = \frac{\hbar^2 k^2}{2m}$$

$$E(n_i) = \frac{h^2}{2m}$$

$$\text{i)} n^{\circ}\text{ points sphere} = \frac{\text{vol sphere}}{\text{vol point}} = \frac{h_F^2}{6\pi^2} V$$

iii)

$g(\epsilon) d\epsilon = n^{\circ}$ electronic states with energies between ϵ and $\epsilon + d\epsilon$

$$N(\epsilon) = 2 \frac{\text{vol sphere}}{\text{vol per point}} = \frac{V}{3\pi^2} \left(\frac{2m\epsilon}{\hbar^2} \right)^{3/2}$$

$$g(\epsilon) d\epsilon = N(\epsilon + d\epsilon) - N(\epsilon) = \frac{dN(\epsilon)}{d\epsilon} d\epsilon = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} d\epsilon$$

$$\text{iv) a)} g_{2D}(\epsilon) = \frac{dN_{2D}(\epsilon)}{d\epsilon} = \frac{m A}{\pi \hbar^2} \quad A = L^2$$

Find Fermi E from N

$$N(\epsilon) = \frac{V}{3\pi^2} \left(\frac{2m\epsilon}{\hbar^2} \right)^{3/2} \rightarrow$$

$$= \frac{V}{3\pi^2} \left(\frac{2m\hbar^2 h_F^2}{2m\hbar^2} \right)^{3/2}$$

$$= \frac{V}{3\pi^2} h^3$$

$$\frac{dN(\epsilon)}{d\epsilon} = \frac{V}{3\pi^2} h^3 = \frac{m A}{\pi \hbar^2}$$

$$N = \int_0^{\epsilon_F} g_{2D}(\epsilon) d\epsilon$$

$$= \int_0^{\epsilon_F} \frac{Am}{\pi \hbar^2} d\epsilon$$

$$= \frac{Am}{\pi \hbar^2} \epsilon_F$$

$$\epsilon_F = \frac{N\pi\hbar^2}{Am}$$

$$= \frac{\pi\hbar^2}{m}$$

$$U = \int_0^{\epsilon_F} \epsilon g_{2D}(\epsilon) d\epsilon = \frac{Am}{2\pi\hbar^2} \epsilon_F^2$$

$$\langle \text{kinetic energy} \rangle = \frac{\frac{Am}{2\pi\hbar^2} \epsilon_F^2}{N} = \frac{Am}{2\pi\hbar^2} \times \frac{\pi\hbar^2}{Am} \frac{\epsilon_F^2}{N} = \frac{1}{2} \epsilon_F$$

4) i) the electrons become thermally excited. If the energy increase is sufficient some electrons might change energy level ✓ use key word

(i) (Bookwork.) At $T = 0$ all electron states up to the Fermi energy are occupied, and those above the Fermi energy are unoccupied. When the temperature is raised, some states become thermally excited and move to levels with energies of the order of $k_B T$ higher. Because of the Pauli exclusion principle, only states within $k_B T$ of the Fermi level are able to be excited into unoccupied levels – states much lower in energy cannot because the states within a range $\sim k_B T$ are already filled.



$$\text{ii) } n^0 \text{ elements Fermi level } \sim N\left(\frac{T}{T_F}\right)$$

$$\therefore \text{inverse e: } U(T) - U(0) \sim N\left(\frac{T}{T_F}\right) \times k_B T = N k_B \frac{T^2}{T_F}$$

$$\text{Heat capacity } C = \frac{\partial U}{\partial T} \sim 2 N k_B \frac{T}{T_F}$$

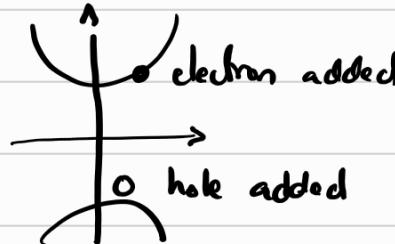
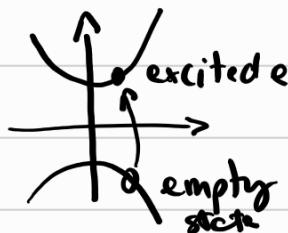
Classic:

$$U(T) = N \times \frac{3}{2} k_B T$$

$$C = \frac{3}{2} N k_B T$$

predict smaller by $\frac{T}{T_F}$

5)



$$\text{i) Monovalent atoms: } A = 1 \text{ eV}, B = -1 \text{ eV}, C = 5 \text{ eV}, D = 2 \text{ eV}, \alpha = 1$$

$$D = 2 \text{ eV}, \alpha = 1$$

$$6) n = AT^{3/2} e^{-(E_G - \mu)/k_B T}$$

$$p = BT^{3/2} e^{-\mu/k_B T}$$

Problem 6

Assuming that the electron and hole concentrations in a semiconductor are given (in the usual notation) by

$$n = AT^{3/2} e^{-(E_G - \mu)/k_B T} \quad p = BT^{3/2} e^{-\mu/k_B T}$$

where A and B are constants, show that in an intrinsic semiconductor, where n_i is the concentration of electrons in the conduction band, a plot of $\ln(n_i/T^{3/2})$ vs $1/T$ allows an estimate of the band gap.

What is the band gap if at $T = 500 \text{ K}$ $n_i = 4 \times 10^{14}/\text{cm}^3$ and at $T = 300 \text{ K}$ it is $2 \times 10^{10}/\text{cm}^3$.

In an intrinsic semiconductor the electron and hole concentrations are equal. Therefore

$$n = p = n_i \rightarrow n_i^2 = n \times p$$

Using the expressions in the question,

$$n_i^2 = AT^{3/2} e^{-(E_G - \mu)/k_B T} \times BT^{3/2} e^{-\mu/k_B T} = ABT^3 e^{-E_G/k_B T}$$

$$\text{so } n_i^2/T^3 = AB e^{-E_G/k_B T} \rightarrow n_i/T^{3/2} = \sqrt{AB} e^{-E_G/2k_B T}$$

$$\text{or } \ln(n_i/T^{3/2}) = \ln\sqrt{AB} - \frac{E_G}{2k_B T}$$

This equation is of the form $y = c + mx$, so a plot of $\ln(n_i/T^{3/2})$ vs $1/T$ is a straight line with gradient $-E_G/2k_B T$.

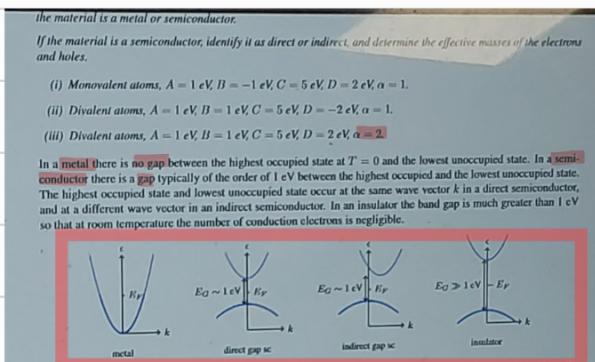
Assuming a straight line relationship, two points are enough to determine the gradient: $y_1 = c + mx_1, y_2 = c + mx_2$,

$$\text{so } (y_1 - y_2) = m(x_1 - x_2)$$

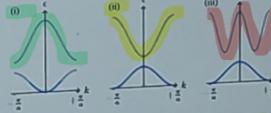
$$m = \frac{y_1 - y_2}{x_1 - x_2}$$

$$\text{Here } y_1 = \ln(4 \times 10^{14}/500^{1.5}) = 24.30, y_2 = \ln(2 \times 10^{10}/300^{1.5}) = 15.16, x_1 = 1/500 = 0.00200, x_2 = 1/300 = 0.00333, \text{ and putting into the expression for } m \text{ gives } m = -6850 \text{ K which can be equated to } -E_G/2k_B T.$$

Thus $E_G = 2 \times 6850 \times 1.38 \times 10^{-23} / (1.6 \times 10^{-19}) = 1.2 \text{ eV}$.



To classify the one-dimensional materials, remember that a full band can accommodate 2 electrons per primitive cell. A solid where the primitive cell contains a monovalent atom has one electron per primitive cell, enough to half fill a band. A divalent atom contributes two electrons, so a primitive cell containing a divalent atom has enough electrons to fill one band.



Case (i) is a metal, case (ii) a direct semiconductor, and (iii) an indirect semiconductor, the conduction band minimum and the valence band maximum occurring at different values of k .

For the effective masses, use $\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k^2}$ evaluating the expression at the wave vector k corresponding to the valence band maximum or conduction band minimum. For example, in (ii) for the valence band $\frac{\partial^2 E(k)}{\partial k^2} = -B a^2 \cos ka$ which is $-Ba^2$ at the band maximum at $k = 0$. This gives $1/m^* = -1.6 \times 10^{-19} \times (2 \times 10^{-10})^2 / (1.05 \times 10^{-34})^2 = -5.8 \times 10^{29} \text{ kg}^{-1}$, or $m^* = -1.7 \times 10^{-30} \text{ kg} = -1.9m$ where m is the free electron mass. Since $m_h^* = -m_e^*$, the hole mass is $m_h^* = 1.9m$.

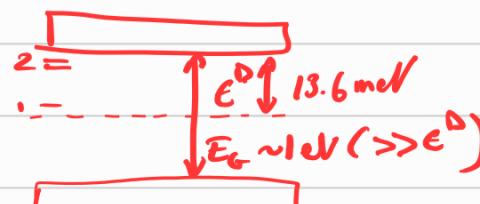
Other values: Case (ii) $m^* = 0.05m$, Case (iii) $m^* = 1.9m$, $m = 0.24m$.

$$7) E_G = 1.1 \text{ eV}$$

$$m_e^* = 0.1m$$

$$m_h^* = 0.8m$$

relative permittivity 10



$$\text{Dopant E levels: } E_n^\Delta = \frac{-m_e^* e^2}{2(4\pi\epsilon)^2 h^2} \times \frac{1}{n^2} = -\frac{13.6}{n^2} \text{ meV}$$

$$8) \text{ intrinsic } n = p$$

Using a sketch showing $\ln n$ vs $1/T$, where n is the carrier concentration, explain the temperature dependence of the carrier concentration in silicon doped with phosphorus.

semiconductor, in which the conduction properties arise from an equal number

Extrinsic n-type

An intrinsic semiconductor is a pure semiconductor with **no** electrons in the conduction band and **holes** in the valence band.

An **extrinsic** semiconductor is a semiconductor in which the conduction properties are dominated by the effects of **electrons** in the conduction band and **holes** in the valence band.

An **dopant atoms**, **donors** (*n*-type) or **acceptors** (*p*-type) which **increase** the **numbers** of conduction electrons or holes respectively.

Silicon is a group IV element, and phosphorus group V – you have a copy of the periodic table covering these elements in your notes; I would not expect you to know this in an exam.

Doping silicon with phosphorus will therefore produce an *n*-type semiconductor, one that has been doped with donor atoms which form impurity levels just below the conduction band minimum. At very low temperatures only a few electrons from the donor levels will be thermally excited into the conduction band — this is called carrier freeze out.

The carrier concentration varies like

$$n \sim N_C e^{-\epsilon^D / 2k_B T} \Rightarrow \ln n \approx \ln N_C - \frac{\epsilon^D}{2k_B T}$$

As the temperature is raised increasing numbers of electrons from the donor levels will be thermally excited into the conduction band. Eventually all donor impurities will be ionised and the concentration of conduction electrons will saturate at n_D , the donor concentration.

$$\ln n \approx \ln n_D$$

As the temperature is raised further an increasing number of electrons will be thermally excited from the valence band, and the carrier densities will begin to behave increasingly like that of an intrinsic semiconductor:

$$n \propto T^{3/2} e^{-E_G / 2k_B T} \Rightarrow \ln n \approx \ln A T^{3/2} - \frac{E_G}{2k_B T}$$

Your sketch should show the three linear regimes on the $\ln n$ vs $1/T$ plot and indicate the gradients/special values.

