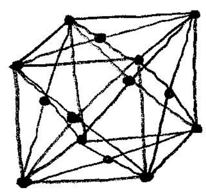
Question 1 (25)

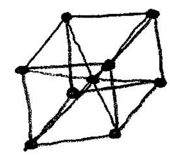
(a) (7) Using a schematic diagram show the difference between unit cells of a face-centred cubic (FCC) lattice and body-centred cubic (BCC) lattice. How many atoms each unit cell has?

FCC



$\underbrace{8\times 1/8}_{\text{corners}} + \underbrace{6\times 1/2}_{\text{faces}} = 4$ atoms

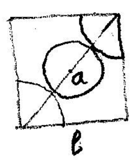
BCC



$\underbrace{8\times 1/8}_{\text{corners}} + \underbrace{1}_{\text{body}} = 2$ atoms

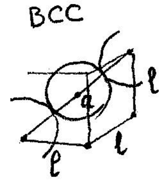
(b) (5) Assuming that atoms are hard spheres with diameter *a*, what is the sides of FCC and BCC unit cells, if atoms are closely-packed.

FCC



$\sqrt{2}\,l = 2a \rightarrow \boxed{l = \sqrt{2}\,a}$

BCC



$2a = \sqrt{3}\,l \rightarrow \boxed{l = \frac{2}{\sqrt{3}}a}$

(c) (7) What ratio of the unit cells are filled with atoms in FCC and BCC?

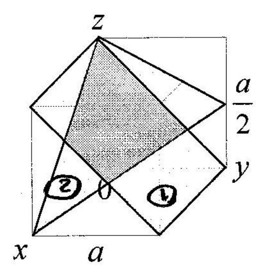
FCC:

$\frac{4\times 4/3\,\pi\left(\frac{a}{2}\right)^3}{(\sqrt{2}\,a)^3} = \boxed{\frac{\pi}{3\sqrt{2}}} = 1.74$

BCC:

$\frac{2\times 4/3\,\pi\,(a/2)^3}{\left(\frac{2}{\sqrt{3}}\right)^3 a^3} = \boxed{\frac{\sqrt{3}\,\pi}{8}} = 1.68$

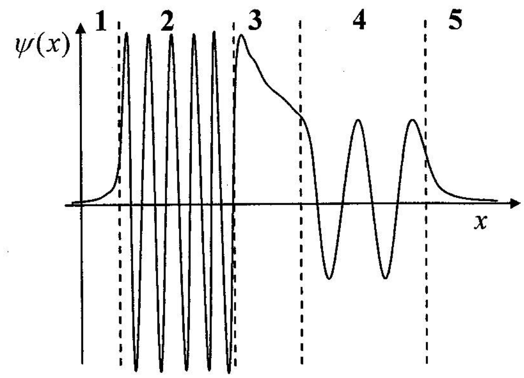
(d) (6) What are the Miller's indices for the two planes shown in the figure? What is the type of silicon unit cell?



	x	y	z		
① :	∞	1	1	$\longrightarrow$	(0 1 1)
② :	1	2	1	$\longrightarrow$	1 1/2 1 $\rightarrow$ (2 1 2)

Question 2 (15)

(a) (7) The figure on the right shows a wavefunction $\psi(x)$ for an electron with energy E. List the regions 1 to 5 in order of having the highest probability for the presence of the electron. Start with the highest probability. Explain your reason for choosing the order.



$|\psi|^2 \rightarrow$ probability :

② → ④ → ③ → ⑤ → ①

Regions ② and ④ have large amplitudes for electron waves.

〃 ① 〃 ⑤ have lowest amplitudes

(b) (3) In which region does the particle have the highest kinetic energy? Why?

②

$$E_{kinetic} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 (2\pi)^2}{2m\lambda^2}$$

region ② has smallest wave length.

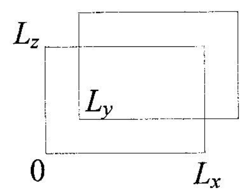
(c) (5) For which regions we have $E < U_i(x)$, where $U_i(x)$ is the potential energy in region i. Why?

Regions ①, ③ and ⑤ since the solution is not wave-like ($e^{\pm jkx}$). The solutions in these regions are exponential-like ($e^{\pm kx}$), and for these solutions we have $E < U_i$.

Question 3 (35)

(a) (5) For a 3-D infinite potential well with dimensions (L_x, L_y, L_z) and $U(x,y,z) = 0$ inside the well, write the Schrödinger wave equation for an electron inside the well.

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) = E\,\psi(x,y,z)$$



(b) (7) Using the separation of variable method show that $\psi(x,y,z) = AX(x)Y(y)Z(z)$ and $E = E_x + E_y + E_z$.

$$\psi(x,y,z) = A\,X(x)\,Y(y)\,Z(z)$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) X(x)Y(y)Z(z) = E\,X(x)Y(y)Z(z) \rightarrow$$

$$X''YZ + XY''Z + XYZ'' = \frac{2mE}{\hbar^2}XYZ \rightarrow$$

$$\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = \frac{2mE}{\hbar^2} \rightarrow \text{Constant.}$$

For this to hold for all x, y, z, we should have:

$$\frac{X''}{X} = k_x^2, \quad \frac{Y''}{Y} = k_y^2, \quad \frac{Z''}{Z} = k_z^2$$

$$k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2} \quad \text{or} \quad E = E_x + E_y + E_z, \quad E_x = \frac{\hbar^2 k_x^2}{2m}$$

(c) (6) Write the boundary conditions for z direction, and show that $Z(z) = \sin\left(\frac{n_z \pi z}{L_z}\right)$ and $E_z = \frac{n_z^2 \pi^2 \hbar^2}{2mL_z^2}$.

$$\frac{Z''}{Z} = k_z^2 \rightarrow \quad Z(z) = A e^{jk_z z} + B e^{-jk_z z}$$

$$Z(0) = 0 \rightarrow \quad A + B = 0$$

$$\rightarrow Z(z) = A\left(e^{jk_z z} - e^{-jk_z z}\right) = A_z \sin(k_z z)$$

$$Z(L_z) = 0 \rightarrow \quad k_z L_z = n_z \pi \rightarrow \quad k_z = \frac{n_z \pi}{L_z}$$

$$E_z = \frac{\hbar^2 \pi^2 n_z^2}{2m L_z^2}$$

(d) (5) Write the normalization equation and find A.

$$\int_0^{L_x}\int_0^{L_y}\int_0^{L_z} A^2\sin^2(k_z z)\sin^2(k_y y)\sin^2(k_z z)\,dz\,dy\,dx = 1$$

$$\int_0^{L_z}\sin^2(k_z z) = \int_0^{L_z}\frac{1-\cos(2\frac{n_z\pi}{L_z})}{2}\,dz = \frac{L_z}{2}$$

$$\rightarrow A^2\frac{L_x}{2}\frac{L_y}{2}\frac{L_z}{2} = 1$$

$$A = \sqrt{\frac{8}{L_x L_y L_z}}$$

(e) (6) For $L_x = L_y = a$ and $L_z = 1000a$ (the case for a nanowire), what is the energy $h\nu$ and wavelength (as a function of a) of a photon emitted when an electron makes the transition $\psi_{6,5,10} \rightarrow \psi_{5,6,3}$ (The index numbers are for quantum numbers n_x, n_y, and n_z).

$$E = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + \frac{n_z^2}{10^6}\right)$$

$$h\nu = E_{6,5,10} - E_{5,6,10} = \frac{\pi^2\hbar^2}{2ma^2}\left[\cancel{6^2}+\cancel{5^2}+\frac{100}{10^6}-\cancel{5^2}-\cancel{6^2}-\frac{9}{10^6}\right]$$

$$= \frac{91\pi^2\hbar^2}{2ma^2\times10^6}$$

$$\lambda\nu = c \rightarrow \lambda = \frac{hc}{h\nu}$$

(f) (6) How many states are available in the range $\frac{16}{2}\frac{\pi^2\hbar^2}{ma^2} < E < \frac{20}{2}\frac{\pi^2\hbar^2}{ma^2}$.

$$16 < n_x^2 + n_y^2 + \frac{n_z^2}{10^6} < 20$$

Changes in n_z change E by very little values, but change in n_x, n_y make big changes in E.

Number of states

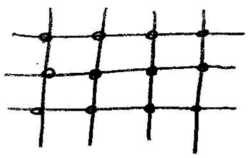
n_x, n_y		
1 1	$\rightarrow 16-2 < \frac{n_z^2}{10^6} < 20-2 \rightarrow 10^3\sqrt{16-2} < n_z < 10^3\sqrt{20-2}$	$\rightarrow 10^3(\sqrt{20-2}-\sqrt{16-2}) = 500$
1 2, 2 1	$\rightarrow n_x^2+n_y^2 = 1+4 = 5$	$\rightarrow 2\times10^3(\sqrt{20-5}-\sqrt{16-5}) = 1112$
1 3, 3 1	$\rightarrow n_x^2+n_y^2 = 1+9 = 10$	$\rightarrow 2\times10^3(\sqrt{20-10}-\sqrt{16-10}) = 1425$
3 3	$\rightarrow n_x^2+n_y^2 = 9+9 = 18 \rightarrow 10^3\sqrt{2} = 1414$	
2 2	$\rightarrow n_x^2+n_y^2 = 4+4 = 8$	$\rightarrow 10^3(\sqrt{12}-\sqrt{8}) = 635$
		$\rightarrow 10^3(\sqrt{7}-\sqrt{3}) = 1827$
2 3, 3 2	$\rightarrow n_x^2+n_y^2 = 4+9 = 13$	
1 4, 4 1	$\rightarrow n_x^2+n_y^2 = 1+16 = 17 \rightarrow 2\times10^3\times\sqrt{3} = 3464$	

$\boxed{\text{Total} = 10377}$

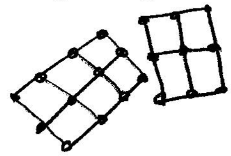
Question 4 (25)

(a) (9) Using lattice schematics, explain the difference between crystalline, polycrystalline and amorphous materials.

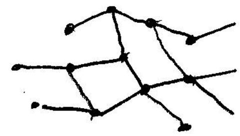
Crystalline
has perfect crystal structure.



Polycrystalline
Pieces of crystalline material connected with grain boundaries



Amorphous
No crystalline and ordered shape



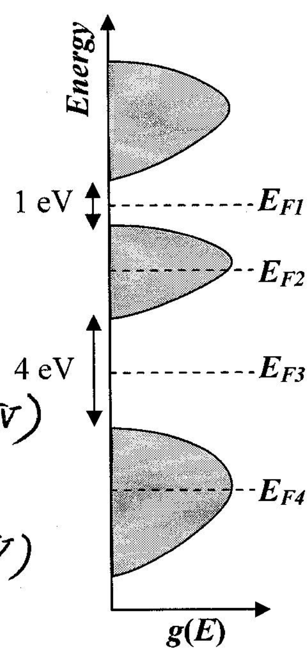
(b) (8) A semiconductor film (conductivity of 1 S/cm) wire has a length and width of 10 μm and thickness of 100 nm. Find the current that goes through this wire, if we apply 10 V to its sides.

$$R = \rho \frac{L}{S} = \frac{L}{\sigma S}$$

$$I = \frac{V}{R} = \frac{V \sigma S}{L} = \frac{(10\ V) \times (1\ S/cm) \times (\cancel{10 \times 10^{-4}} \times 100 \times 10^{-7})}{\cancel{10 \times 10^{-4}}}$$

$$= 10^{-4}\ A$$

(c) (8) Four different materials have identical band structures (shaded areas represent state bands), however, their intrinsic Fermi energy levels are different as shown in the figure. What are the best guesses for the type of these materials (metal, semiconductor, or dielectric)? Briefly explain why.



E_{F2}, E_{F4} in the middle of the band

2 and 4 → metal

E_{F1} between two bands (has band gap < 3 eV)

1 → semiconductor

E_{F3} between two bands (has bandgap > 3 eV)

3 → dielectric