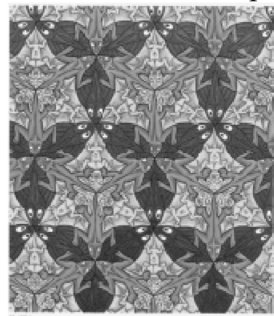
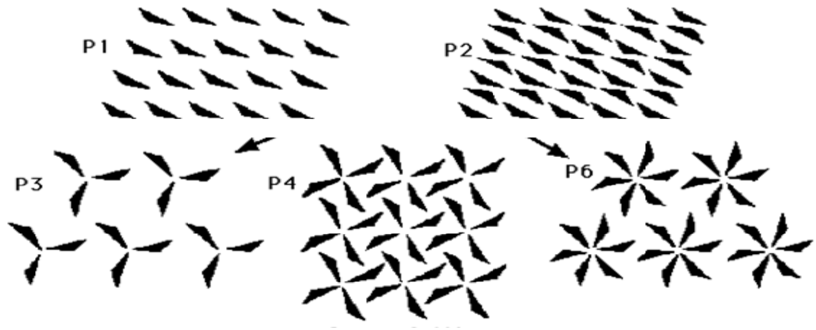
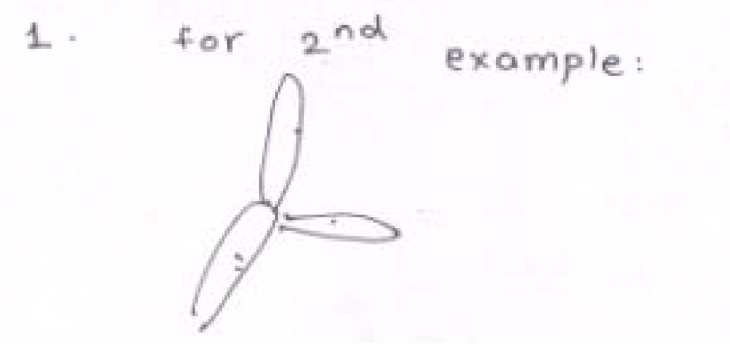
Fundamentals of Semiconductors
EPL213
Problem sheet 1

Aim: understanding unit cell, crystal structures, Brillouin zone, symmetry representation

1. Sketch the unit cell in these two examples. Can you identify how many lizards (now basis) for unit cell?



2. . Draw the *Wigner-Seitz* cell of a cubic lattice using the procedure given in your lecture notes. Label Symmetry points (How many you can see in this 2D (x-y) plane?)

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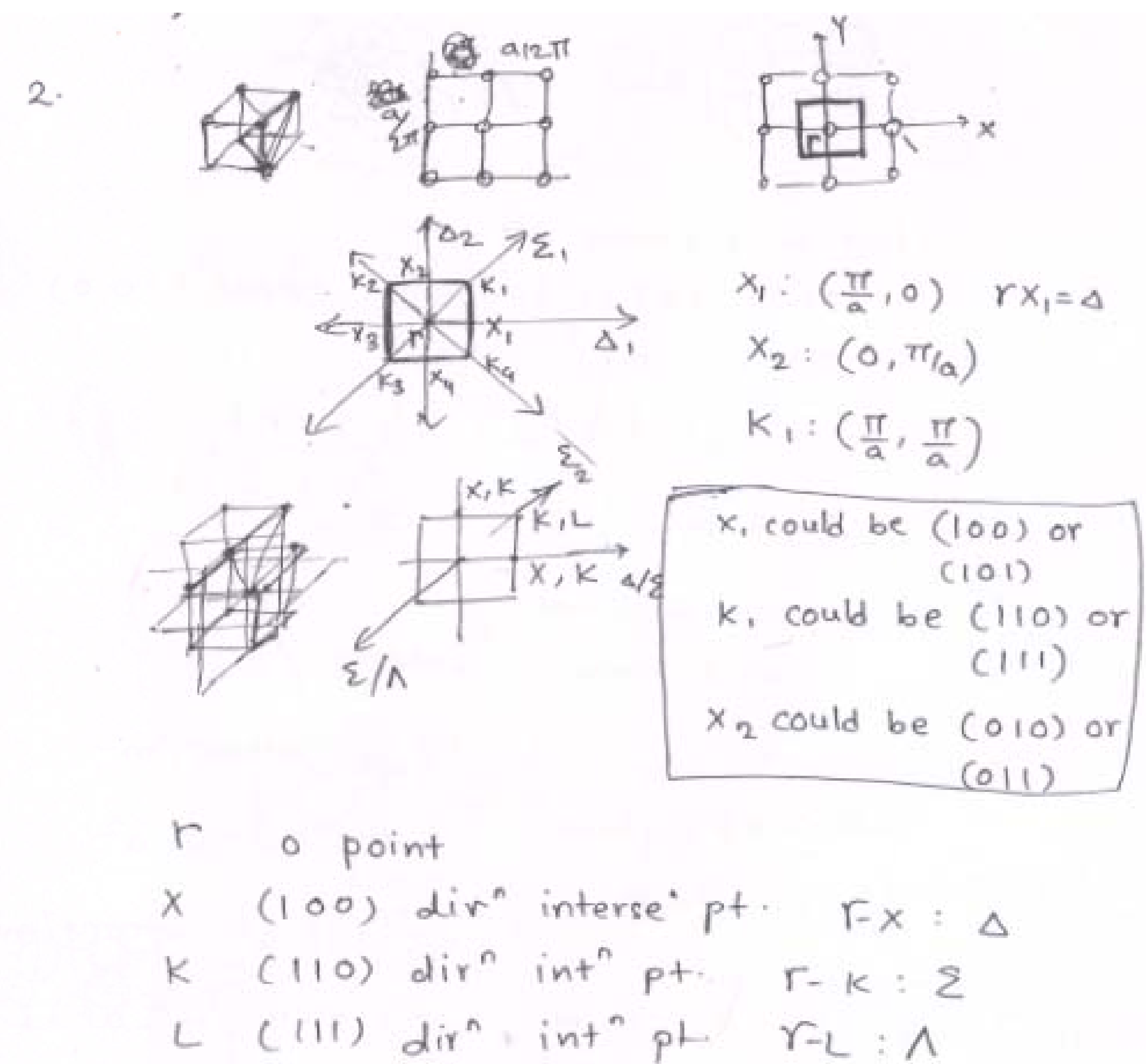
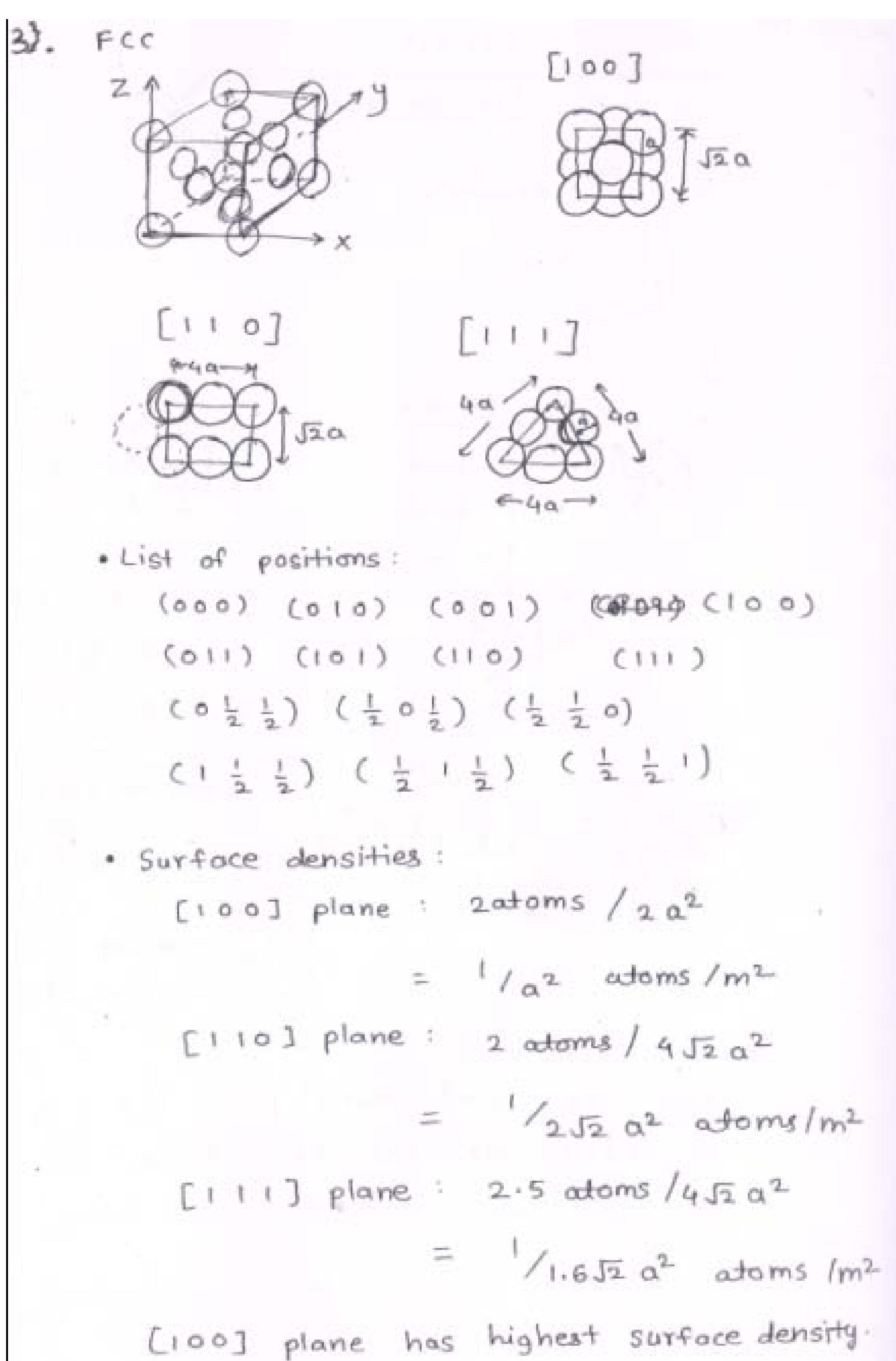


3. List the positions of the atoms in the basis of a face centred cubic lattice. Draw a unit cell (see your lecture notes, since this is a very important lattice type). Draw a plan view of the lattice seen along the [100], [110] and [111] directions, labelling the height of each atom. Which plane has the densest arrangement of atoms?



3). FCC

• List of positions:

(000) (010) (001) (100)

(011) (101) (110) (111)

$(0\,\frac{1}{2}\,\frac{1}{2})$ $(\frac{1}{2}\,0\,\frac{1}{2})$ $(\frac{1}{2}\,\frac{1}{2}\,0)$

$(1\,\frac{1}{2}\,\frac{1}{2})$ $(\frac{1}{2}\,1\,\frac{1}{2})$ $(\frac{1}{2}\,\frac{1}{2}\,1)$

• Surface densities:

[100] plane : 2 atoms $/ 2a^2$

$= 1/a^2$ atoms $/m^2$

[110] plane : 2 atoms $/ 4\sqrt{2}\,a^2$

$= 1/2\sqrt{2}\,a^2$ atoms$/m^2$

[111] plane : 2.5 atoms $/ 4\sqrt{2}\,a^2$

$= 1/1.6\sqrt{2}\,a^2$ atoms $/m^2$

[100] plane has highest surface density.

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4. You have been told that the hard spheres natural assembly is fcc packed lattice. Now, if the cubic cell width is a, can you find the packing fraction? (packing fraction is defined as number of spheres (or atoms) in the cell multiplied by volume of sphere(atom) divided by volume of unit cell)

4. Find P.f. of Fcc lattice.

$2\sqrt{2}a$ $\qquad V = (2\sqrt{2}a)^3 = 16\sqrt{2}a^3$

& total no. of atoms : 4

∴ volume occupied $= 4 \times \frac{4}{3}\pi a^3$

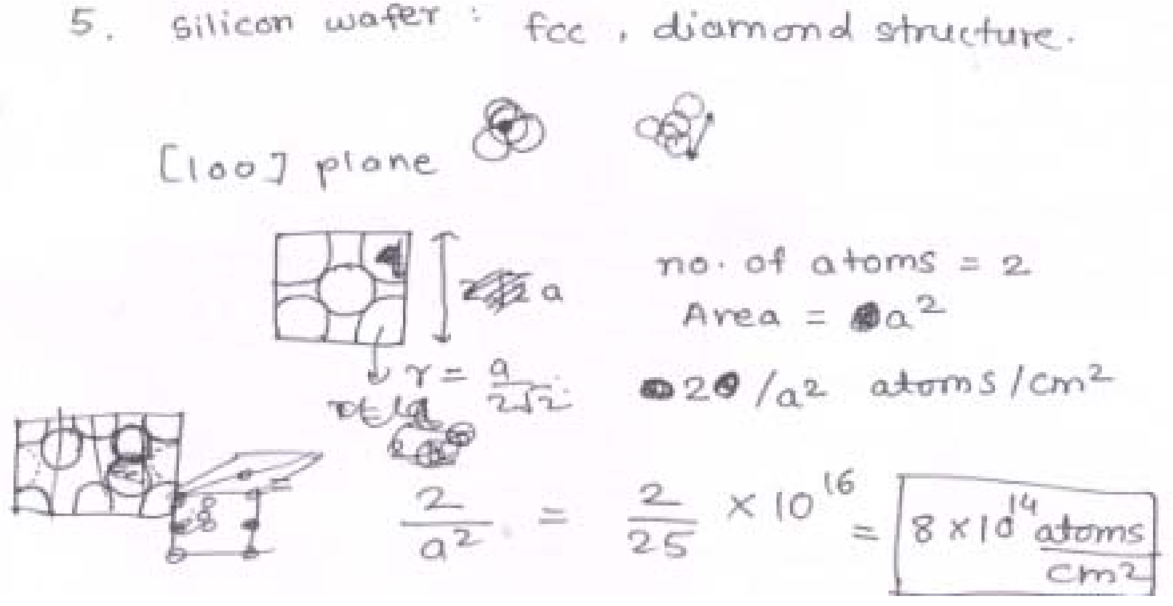
$V_{occ.} = \frac{16}{3} \times 3.14 a^3$

$$P.f. = \frac{1.0467}{\sqrt{2}} = \frac{1.0467}{1.417} \times 100\,\%$$

$$= \frac{104.67}{1.417}\,\%$$

$$\boxed{P.f. = 0.7423}$$

5. Find number of Silicon atoms/cm^2 in (100) surface of Silicon wafer. (a=5.43x10^{-8}cm)



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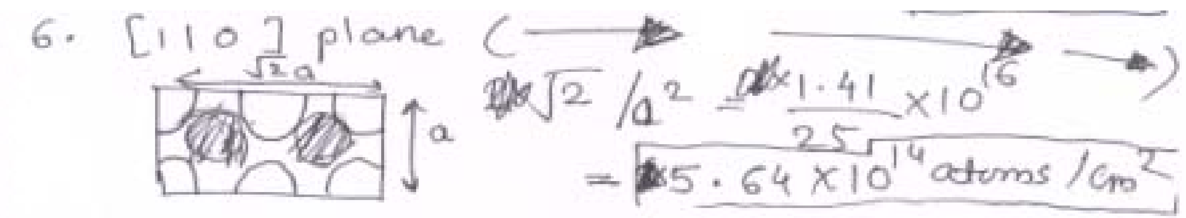
6. Similarly do it for (110) surface



7. Now you are in a position to extend the same philosophy to 3D model (Do you remember the Si crystal structure? Refer your lecture notes). Find Number Si atoms (per unit volume) in an unit cell and the density of Silicon. (*If necessary use, Avogadro Number= 6.02x10^{23} and Mol Weight of Si= 28.08g/mol*)

7. Si crystal is diamond structure.

Total no. of atoms in 1 lattice

$$= 4 \times \frac{1}{4} \text{ corner} + 6 \times \frac{1}{2} \text{ half} + 4 \text{ in voids}$$

$$= 8.$$

$$\therefore \text{Density of atoms } \rho_A = \frac{8}{a^3} \text{ atoms/cm}^3$$

$$\text{weight of 1 Si atom} = \frac{28.08}{6.02 \times 10^{23}} \text{ g}$$

$$\therefore \rho_{Si} = \frac{8}{a^3} \times \frac{28.08}{6.02 \times 10^{23}}$$

$$= \frac{8 \times 280.8}{125 \times 6.02}$$

$$\boxed{\rho_{Si} = 2.33 \text{ g/cm}^3}$$

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Fundamentals of Semiconductors

EPL213

Problem sheet 2

Aim: understanding the band structures, effective mass and the conduction valance energy levels, understanding of band gaps, density of states, intrinsic properties of semiconductors

1. Using Nearly-free electrons (consider one dimension) near the Brillouin zone edge of a cubic crystal (a=0.30 nm) are found to have allowed energies of 3.66eV and 4.66eV when given a momentum k_x = 10.00 nm^{-1} and –10.94 nm^{-1} respectively. By calculating $E_{1,2}$, find the strength in eV of the potential that scatters them and also find the possible energy separation.

1. Nearly free e^- model :

$a = 0.30$ nm

$E_1 = 3.66$ eV $k_1 = 10$ nm^{-1}

$E_2 = 4.66$ eV $k_2 = -10.94$ nm^{-1}

To find: $E_{1,2}$

$$E_{-10.94} = E_{10.00} + \sum \frac{V_n^2}{E_{-10.94} - E_{10.00}}$$

Find $V_n \rightarrow$ Potential.

Then,

$$E_+ = \frac{[E_1 + E_2]}{2} + \sqrt{\left[\frac{E_1 - E_2}{2}\right]^2 + V^2}$$

$$E_- = \left[\frac{E_1 + E_2}{2}\right] - \sqrt{\left[\frac{E_1 - E_2}{2}\right]^2 + V^2}$$

2. We have effective masses of various branches in conduction and valance bands of Si as following. Find the density of states masses for respective conduction and valance bands. $m_l^*=0.98m_0$, $m_t^*=0.19m_0$, $m_{lh}^*=0.16m_0$ and $m_{hh}^*=0.49m_0$

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2. **Given:** $m_l^* = 0.98\, m_0$, $m_t^* = 0.19\, m_0$

$m_{lh}^* = 0.16\, m_0$, $m_{hh}^* = 0.49\, m_0$.

Silicon

To find: m_{dos}^* for CB & VB.

Solution: Use formula:

for CB: $m_{dos}^* = (m_l^* m_t^{*2})^{1/3}\, 6^{2/3}$

for VB: $m_{dos}^* = \left[m_{lh}^{3/2} + m_{hh}^{3/2} \right]^{2/3}$

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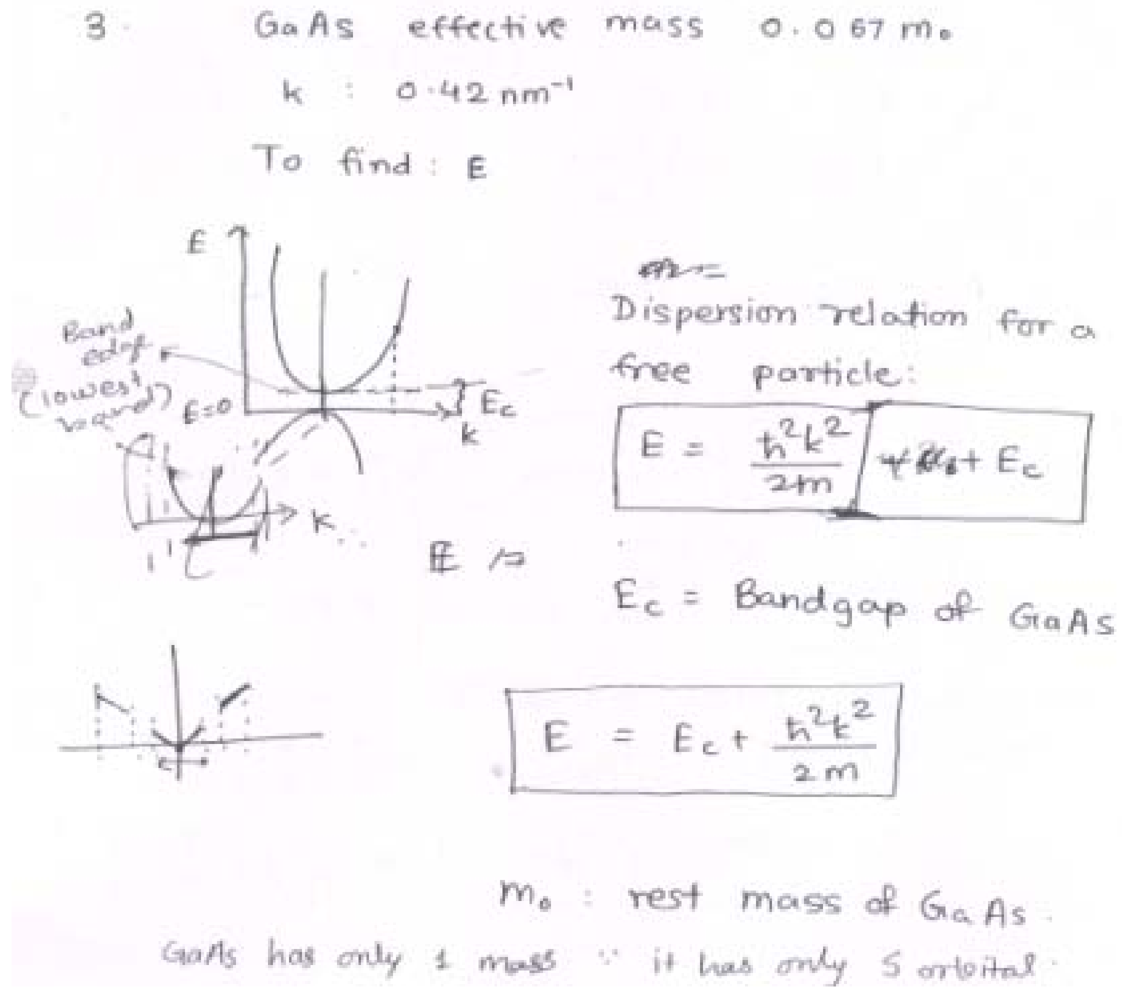
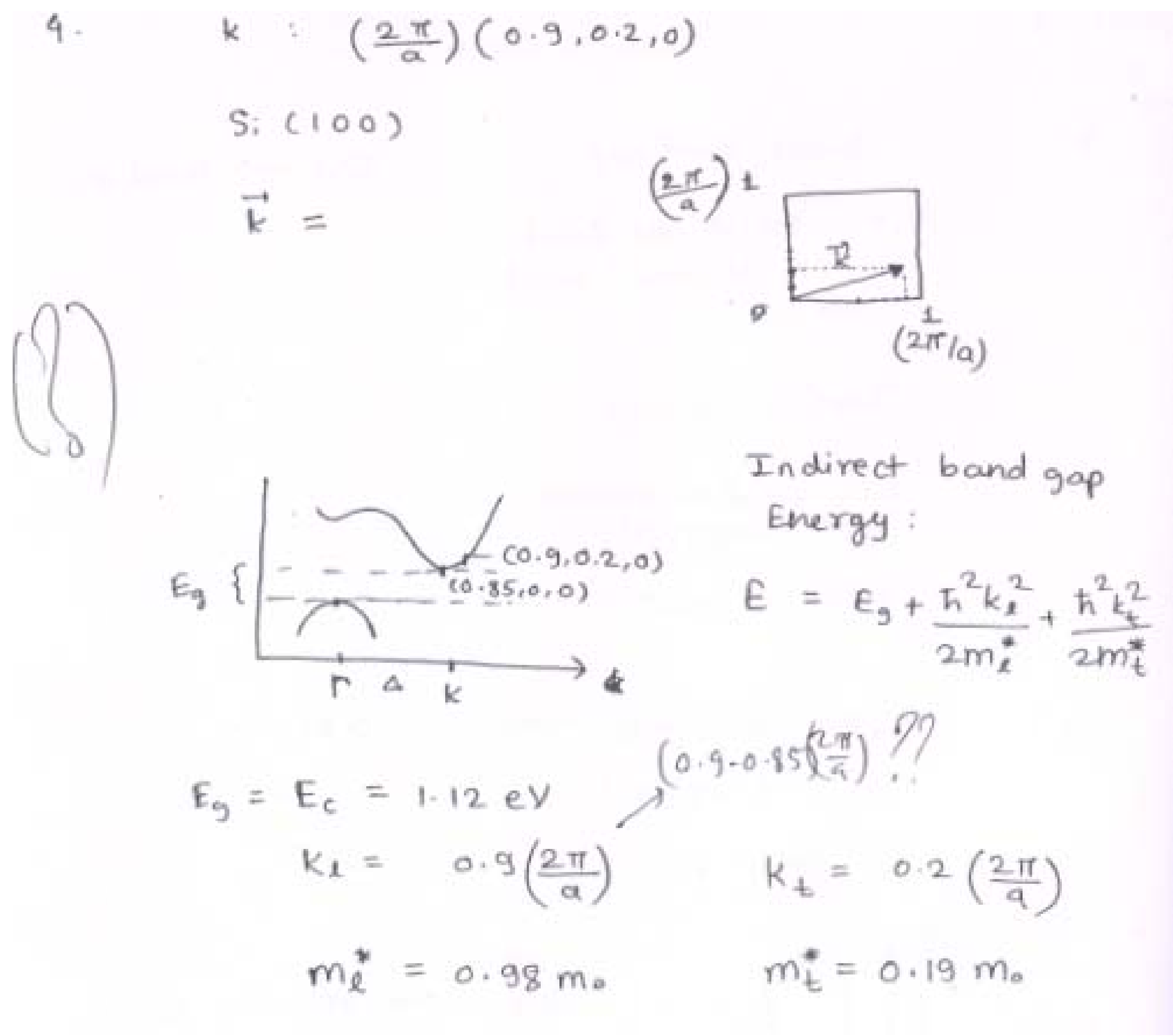
3. Calculate the conduction band energy level for the given k vector 0.42nm^{-1} (measured from band edge). The GaAs effective mass (you already know this) is $0.067m_0$. How about free space electron energy?



4. A conduction band electron in Si(100) occupy in k space $(2\pi/a)*(0.9,0.2,0)$. Estimate the energy level, measured from the conduction band edge.



5. Comment briefly on the following terms that are very much useful in understanding band structures.
- Direct and indirect band gap
- Effective masses at conduction and valance bands
- Heavy-hole, light-hole and split-off bands

$In_xGa_{1-x}As$
$InGa_xAs_{1-x}$
$In_xGa_{1-x}As_yP_{1-y}$
$In_xGa_yAs_{1-x}P_{1-y}$
$In_xGa_yAlAs_{1-x-y}$
$In_xGa_yAl_{1-x-y}As$

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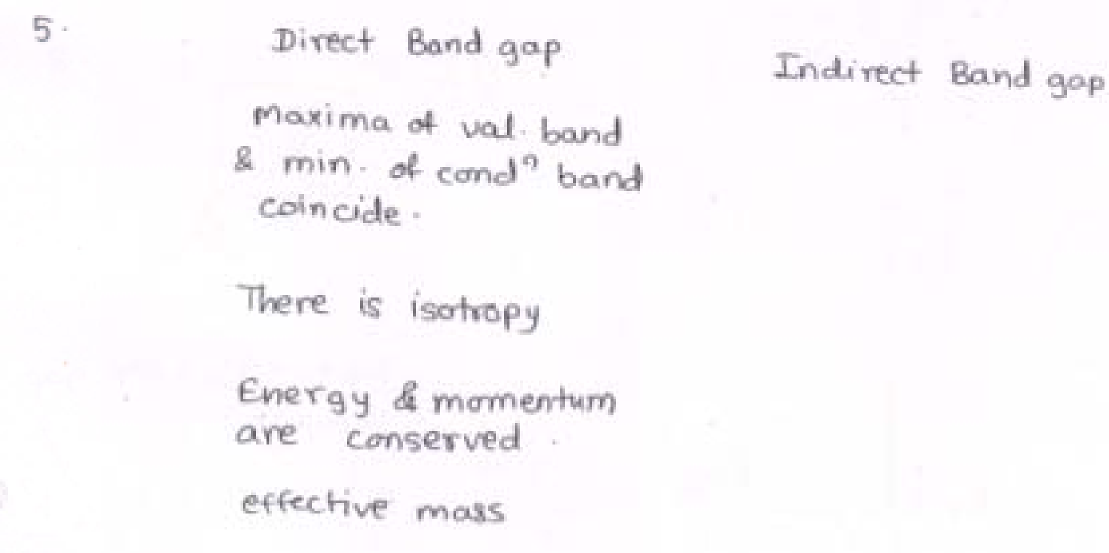

6. You have seen screen shots of the applet for alloy, AlGaAs condition and valance band estimation n your lecture. This is based on virtual crystal approximation using the following data at 300K

Conduction band energies measured from valance band edge

GaAs	AlAs
Γ point= 1.43eV X point= 1.91eV	Γ point= 2.75eV X point= 2.15eV

Calculate respective Γ and X points for intermediate compositions $Al_{0.3}Ga_{0.7}As$, $Al_{0.6}Ga_{0.4}As$. It is easy for you to say that GaAs is a direct band gap material and AlAs is an indirect one by just looking at the Γ and X points energies. How about the above compositions? (hint: (Here in this approximation, one simply uses the weight average of energies) . *Give a hint if the compositions given in the left side box are possible or not, tell me why?*

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GaAs	AlAs
Γ pt = 1.43 eV	Γ point = 2.75 eV
X pt = 1.91 eV	X pt = 2.15 eV

	Γ	X	Type
$Al_{0.3}Ga_{0.7}As$	1.826 eV ($1.43\times0.7+2.75\times0.3$)	1.982 eV	Direct
$Al_{0.6}Ga_{0.4}As$	2.222 eV	2.054 eV	Indirect

$In_xGa_{1-x}As$ ✓

$InGa_xAs_{1-x}$ ✗

$In_xGa_{1-x}As_yP_{1-y}$ ✓

$In_xGa_yAs_{1-x}P_{1-y}$ ✗

$In_xGa_yAlAs_{1-x-y}$ ✗

$In_xGa_yAl_{1-x-y}As$ ✓

Rule : In + Ga + Al = As + P

7. Estimate the (a) effective density of states for valance and conduction bands and (b) intrinsic carrier concentration for silicon at 300K

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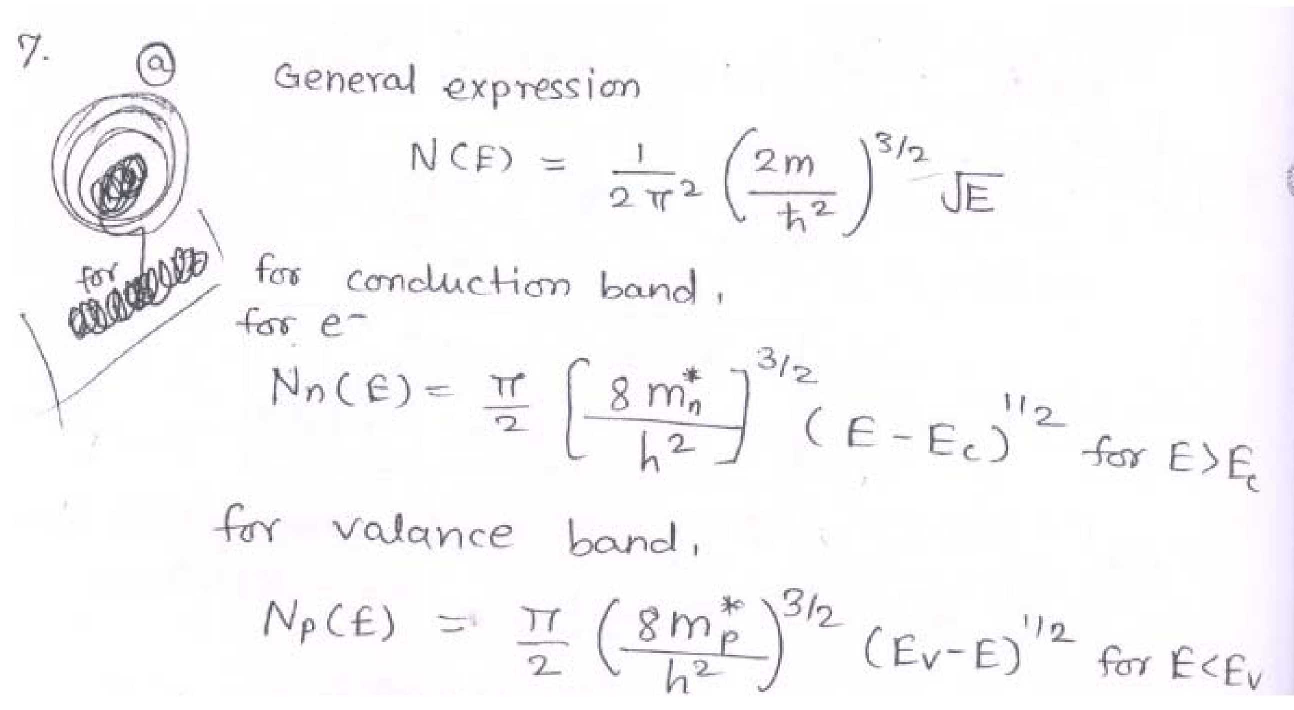

7. (a) General expression

$$N(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$$

for conduction band,
for e^-

$$N_n(E) = \frac{\pi}{2}\left[\frac{8m_n^*}{h^2}\right]^{3/2}(E-E_c)^{1/2} \quad \text{for } E>E_c$$

for valance band,

$$N_p(E) = \frac{\pi}{2}\left(\frac{8m_p^*}{h^2}\right)^{3/2}(E_v-E)^{1/2} \quad \text{for } E<E_v$$

8. An intrinsic GaAs light emitting device is operating at room temperature. Estimate any change in the emitted light wavelength with temperature.

(any help?: Refer your lecture notes for temperature dependence of band gap)

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8. $$E_g(T) = E_g(0) - \frac{\alpha T^2}{T+\beta} = \frac{hc}{\lambda}$$

$$\frac{hc}{\lambda_{300}} = 1.519 - \frac{\alpha(300)^2 \times 10^{-3}}{(300+204)}$$

$$\frac{hc}{\lambda_{300}} = 1.42 \text{ eV}$$

$$\lambda_{300} = 872.735 \text{ nm}$$

$$E_g(T+\Delta T) = E_g(0) - \frac{\alpha (T+\Delta T)^2}{T+\beta+\Delta T} = \frac{hc}{(\lambda_{300}+\Delta\lambda)}$$

$$-\frac{\alpha (T)^2}{T+\beta} + \frac{\alpha (T+\Delta T)^2}{T+\beta+\Delta T} = hc\left[\frac{\Delta\lambda}{\lambda_{300}^2}\right]$$

$$\frac{\Delta\lambda (hc)}{\lambda_{300}^2} = \alpha \left[\frac{(T^2 + 2T\Delta T + (\Delta T)^2)(T+\beta) - (T+\beta+\Delta T)\, T^2}{(T+\beta)^2}\right]$$

$$= \alpha \left[\frac{T^3 + 2T^2\Delta T + \beta T^2 + 2T\beta\Delta T - T^3 - \beta T^2 - T^2\Delta T}{(T+\beta)^2}\right]$$

$$\doteq \frac{\alpha\left[T^2\Delta T + 2T\beta\Delta T\right]}{(T+\beta)^2}$$

$$\Delta\lambda = \frac{\alpha\, \lambda_{300}^2\, \Delta T\, (T^2 + 2T\beta)}{hc\, (T+\beta)^2}$$

$$= 0.16 \text{ nm}$$

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add Q: Find E_{fi} of Si at room temp.

Ans:

$$E_{fi} = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln\left(\frac{N_v}{N_c}\right)$$

$$N_{v\,Si} = 1.04 \times 10^{19}\ cm^{-3}$$

$$N_{c\,Si} = 2.8 \times 10^{19}\ cm^{-1}$$

$$E_{fi} = \frac{E_g}{2} + \frac{k(300)}{2} \ln\left(\frac{1.04}{2.8}\right)$$

$$= \frac{1.12}{2} + \frac{8.617\,(300)}{2} \ln\left(\frac{1.04}{2.8}\right)$$

$$\boxed{E_{fi} = 0.5472\ eV}$$

9. Find the intrinsic Fermi level gradient with respect to temperature (*dE_{fi}/dT)* and . discuss your findings

   (Any help? k_B= 8.617e-5 eVK^{-1})

9.
$$E_{Fi} = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln\left(\frac{N_v}{N_c}\right)$$

$$= \frac{E_g}{2} + \frac{kT}{2} \ln\left(\frac{N_v}{N_c}\right)$$

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