ECE418 / ECE518 - Semiconductor Processing
Spring 2021
Homework 1 - Solutions
Due at the beginning of class Friday April 16th

Question 1 [6 marks]:
Gallium arsenide (GaAs) adopts the Zinc blende crystal structure (see Figure 1). The zinc blende structure is cubic, and similar to the diamond crystal structure (adopted by silicon), but the two interpenetrating face-centered-cubic structures consist of different atoms. The lattice constant in GaAs is $a = 5.65\text{Å}$. The mass of Ga atoms are 69.72 amu and the mass of As atoms are 74.92 amu. You will need to know that 1 amu $= 1.66 \times 10^{-27}\text{kg}$.

![Figure 1: Crystal structure of gallium arsenide.](image)

a) What is the nearest neighbor distance between gallium and arsenic atoms (in Å)? [2 marks]

In the zinc blende structure, the two interpenetrating fcc lattices are offset by $\frac{1}{4}$ of the unit cell length in all directions (as with diamond). Hence the distance between two different atoms is the length of a the vector $\mathbf{r} = (a/4, a/4, a/4)$. See the figure below:

![Diagram](image)

From Pythagoras, in the xy-plane the diagonal distance is:

$$d = \sqrt{\left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2}$$
The length of the vector \( r \), is then:

\[
r = \sqrt{\left(\frac{a}{4}\right)^2 + d^2}
\]

\[
r = \sqrt{\left(\frac{a}{4}\right)^2 + \left(\frac{a^2}{8}\right)^2}
\]

\[
r = \sqrt{\frac{a^2}{16} + \frac{a^2}{8}} = \sqrt{\frac{2a^2}{16} + \frac{a^2}{16}} = \sqrt{\frac{3a^2}{16}}
\]

\[
r = \frac{\sqrt{3}a}{4}
\]

We are told the lattice constant in GaAs is \( a = 5.65 \text{Å} \), so the length is therefore: 2.45Å.

b) What is the atomic density of gallium arsenide (in atoms/cm\(^3\))? [2 marks]

This is similar to the problem you observed in class, but there are now two different atoms in the lattice. Take a look at the figure below.

There are:
- 8 corner Ga atoms.
- 6 face Ga atoms.
- 4 internal As atoms.

From class we know:
- Corner atoms contribute 1/8 atom per cell.
- Face atoms contribute 1/2 atom per cell.
- Internal atoms contribute 1 atoms per cell.

Therefore there are:
- \( \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4 \) Ga atoms per cell
\[ 1 \times 4 = 4 \text{ As atoms per cell.} \]

So a total of 8 atoms per cell.

The volume of the cubic unit cell is simply just \( a^3 \). We are told the length of the unit cell in GaAs is \( 5.65 \text{Å} = 5.65 \times 10^{-10} \text{m} = 5.65 \times 10^{-8} \text{cm} \). So the volume of the unit cell is:

\[ (5.65 \times 10^{-8})^3 \text{cm}^3 = 1.81 \times 10^{-22} \text{cm}^3 \]

Therefore the number density is:

\[ \frac{8}{1.81 \times 10^{-22}} = 4.43 \times 10^{22} \text{ cm}^{-3} \]

c) What is the mass density of gallium arsenide (in g/cm\(^3\))? [2 mark]

From the solution to 1(b) we know there are 4 Ga atoms and 4 As atoms per unit cell. The mass of Ga atoms are 69.72 amu and the mass of As atoms are 74.92 amu. So the total mass in amu is:

\[ 4 \times 69.72 + 4 \times 74.92 = 578.58 \text{amu} \]

We are told 1 amu = \( 1.66 \times 10^{-27} \text{kg} \), therefore the mass in kg of the unit cell is:

\[ 578.58 \times 1.66 \times 10^{-27} \text{kg} = 9.60 \times 10^{-25} \text{kg} \]

Which is \( 9.60 \times 10^{-22} \text{ g} \).

From 1(b) we know that the volume of the GaAs unit cell is \( 1.81 \times 10^{-22} \text{ cm}^3 \). Therefore the mass density is:

\[ \frac{9.60 \times 10^{-22}}{1.81 \times 10^{-22}} = 5.30 \text{ g/cm}^3 \]

Question 2 [9 marks]:

a) Explain why we require high purity silicon for microelectronics. [2 marks]

Charge carriers (electrons and holes) move very quickly in crystalline silicon (their mobility is high). However any trap states that exist in the band gap of silicon are very likely to cause charges to become trapped. These trap states stop current from flowing, and makes devices non-operational or not-operating as expected. Traps in silicon are caused by impurities and it turns out a very high quality of silicon (99.9999999%) is required for sufficient operation.

b) Explain why we require single-crystal (rather than polycrystalline or amorphous) silicon for microelectronics. [2 marks]

While the mobility in polycrystalline silicon is a lower than in single-crystalline silicon it is not prohibitively low. The main issue with polycrystalline silicon is that the introduction of grain-boundaries cause significant device-to-device variation. This makes devices unpredictable and unreliable.

While amorphous silicon is homogenous, the charge carrier mobility is about 1000 times lower in amorphous silicon compared to single-crystalline silicon. It is far too for processor applications.
c) As part of an industrial process, the top-half a phosphorus-doped silicon ingot is used for some further processing. Using the normal freezing relationship, determine the average phosphorus concentration (in atoms / cm$^3$) throughout the top half of an ingot pulled from a melt containing an impurity concentration of $1 \times 10^{16}$ cm$^{-3}$. Remember, $X$ in the normal freezing relation is the fraction of the melt solidified. So if $X = 0.25$ for example, 25% of the melt has been solidified and 75% remains as liquid. The segregation coefficient for phosphorus in silicon is 0.35. [5 marks]

Here we need to determine the average concentration in a volume of the ingot, rather than at a particular position. In this case we are given the concentration in the melt: $C_0 = 1 \times 10^{16}$ cm$^{-3}$, and we need to determine the average concentration over a region of the solid: $\bar{C}_s$. Note: I am using a bar to denote average.

Since the impurity concentration in the ingot will vary as a function of position: $C_s = C_s(X)$, we need to integrate the concentration over the region of interest (the top half of the ingot) and divide by this length to get the average. We are interested in the top half of the ingot, so the length is just 0.5, and we are integrating from $X=0$ to $X=0.5$ (recall $X$ is melt fraction solidified):

$$\bar{C}_s = \frac{1}{0.5} \int_0^{0.5} C_s(X) dX$$

Putting in the normal freezing relation:

$$\bar{C}_s = \frac{1}{0.5} \int_0^{0.5} k_0 C_0 (1 - X)^{k_0-1} dX$$

To integrate this we will use a change of variables:

$$Y = 1 - X$$

$$\frac{dY}{dX} = -1$$

Therefore:

$$dX = -dY$$

We also need to change the limits from $X$ to $Y$:

Recall, $Y = 1 - X$, so the upper limit is: $Y = 1 - 0.5 = 0.5$ and the bottom limit is $Y = 1 - 0 = 1$.

Therefore the integral in terms of $Y$ is then:

$$\bar{C}_s = \frac{1}{0.5} \int_1^{0.5} k_0 C_0 Y^{k_0-1} (-dY)$$

Bring the constants out the front:

$$\bar{C}_s = \frac{-k_0 C_0}{0.5} \int_1^{0.5} Y^{k_0-1} dY$$

Now we can integrate:

$$\bar{C}_s = \frac{-k_0 C_0}{0.5} \left[ \frac{Y^{k_0}}{k_0} \right]_1^{0.5}$$
\[
\bar{C}_s = \frac{-C_0}{0.5} (0.5^{k_0} - 1^{k_0})
\]
\[
\bar{C}_s = \frac{-C_0}{0.5} (0.5^{k_0} - 1)
\]
\[
\bar{C}_s = \frac{C_0}{0.5} (1 - 0.5^{k_0})
\]

We can now put in the values:
\[
\bar{C}_s = \frac{1 \times 10^{16}}{0.5} (1 - 0.5^{0.35})
\]

Giving us an average concentration of: \(\bar{C}_s = 4.3 \times 10^{15} \text{ cm}^{-3}\).

2 out of 4 marks will be awarded if you just evaluated the concentration at \(X = 0.5\), rather than the average throughout the top.

**Question 3 [10 marks]:**

a) For clean Si(111) surfaces it has been determined that the sticking coefficient for O\(_2\) is \(S_c = 0.15\) for coverages of < 0.7 monolayer, and \(S_c = 0.015\) for coverages > 0.7 monolayer. How long will it take for 1 monolayer of O\(_2\) to be adsorbed on the Si(111) surface at an oxygen pressure of \(1.0 \times 10^{-7}\) torr and at 25ºC? Use the assumption that an O\(_2\) monolayer will be formed of a square lattice of O\(_2\) molecules on the surface. Assume the diameter of O\(_2\) molecule is 2.96Å. Give your answer in hours. [7 marks]

We have to first work out how long it takes to form a layer with coverage of 0.7 ML:

\[
t_1 = 0.7 \frac{n_{2D}}{J_A S_{c1}}
\]

We know the sticking coefficient for this coverage \(S_{c1} = 0.15\). After this time, the remaining growth of 0.3 ML will occur with a sticking coefficient of \(S_{c2} = 0.015\):

\[
t_2 = 0.3 \frac{n_{2D}}{J_A S_{c2}}
\]

The density of a 2-dimensional layer \(n_{2D}\) and the flux \(J_A\) will remain constant, so we can just say the total time to form the monolayer is:

\[
t = t_1 + t_2 = \frac{n_{2D}}{J_A} \left( \frac{0.7}{S_{c1}} + \frac{0.3}{S_{c2}} \right)
\]

\[
t = \frac{n_{2D}}{J_A} \left( \frac{0.7}{0.15} + \frac{0.3}{0.015} \right)
\]

\[
t = \frac{n_{2D}}{J_A} \times 24.67
\]

Now we just have to work out the 2-dimensional density of the monolayer and the flux of atoms.
Start with density. Assume the monolayer forms a square lattice, hence we can say the area occupied by each O$_2$ molecule on the surface is:

$$A = d^2$$

Where $d$ is the diameter of an O$_2$ molecule, $d = 2.96\text{Å}$. Work in cm:

$$d = 2.96 \times 10^{-10} \text{ m}$$

$$d = 2.96 \times 10^{-8} \text{ cm}$$

$$A = (2.96 \times 10^{-8})^2 = 8.76 \times 10^{-16} \text{ cm}^2$$

Hence the areal density of these molecules is just:

$$n_{2D} = \frac{1}{A} = \frac{1}{8.76 \times 10^{-16}} = 1.14 \times 10^{15} \text{ cm}^{-2}$$

Now we need to determine the impingement rate (flux) on the surface ($J_A$). This is given by:

$$J_A = \frac{1}{4} n \bar{v}$$

So we need to determine what the 3-dimensional number density of gas molecules ($n$) and the mean particle velocity ($\bar{v}$). Let’s start with the particle density, use the Ideal Gas Law:

$$P = n k_B T$$

$$n = \frac{P}{k_B T}$$

We are given the pressure in Torr: $P = 1.0 \times 10^{-7}$ Torr. Hence in Pascals:

$$P = \frac{101325}{760} \times 10^{-7} = 1.33 \times 10^{-5} \text{ Pa}$$

The temperature is given in °C, $T = 25°\text{C}$. In Kelvin:

$$T = 25 + 273 = 298 \text{ K}$$

We can then enter the values to determine the number density of gas molecules:

$$n = \frac{1.33 \times 10^{-5}}{1.38 \times 10^{-23} \times 298} = 3.24 \times 10^{15} \text{ m}^{-3}$$

We are working in cm, so:

$$n = 3.24 \times 10^9 \text{ cm}^{-3}$$

Now we just need to just work out the mean particle velocity:
\[ \bar{c} = \sqrt{\frac{8k_BT}{\pi m}} \]

We know the temperature is \( T = 298 \text{ K} \). The mass of the \( \text{O}_2 \) molecule is just:

\[ m = 2 \times 16 = 32 \text{ amu} \]
\[ m = 32 \times 1.66 \times 10^{-27} = 5.31 \times 10^{-26} \text{ kg} \]

We can now just put the numbers in to get the mean particle velocity:

\[ \bar{c} = \sqrt{\frac{8 \times 1.38 \times 10^{-23} \times 298}{\pi \times 5.31 \times 10^{-26}}} \]
\[ \bar{c} = \sqrt{1.97 \times 10^{-5}} = 444 \text{ m/s} \]

Again, we work in cm:

\[ \bar{c} = 44,407 \text{ cm/s} \]

Now we can work out the impingement rate:

\[ J_A = \frac{1}{4} n \bar{c} \]
\[ J_A = \frac{1}{4} \times 3.24 \times 10^9 \times 44,407 \]
\[ J_A = 3.60 \times 10^{13} \text{ cm}^{-2} \text{s}^{-1} \]

With this we can finally work out the total time to form a monolayer:

\[ t = \frac{n_2D}{J_A} \times 24.67 \]
\[ t = \frac{1.14 \times 10^{15}}{3.60 \times 10^{13}} \times 24.67 \]
\[ t = 782 \text{ s} \]
\[ t = 0.22 \text{ hr} \]

b) Provide a reason why a cryogenic pump is designed to adsorb helium and hydrogen atoms rather than condense them.[1 mark]

The melting point of both helium and hydrogen are above (or close to) the cryogen used in a cryogenic pump (He).
c) Very briefly explain why Turbomolecular pumps cannot be run until they are already under a vacuum. [2 marks]

The rotors in the turbomolecular pump are fragile and designed to spin extremely quickly (~10k rpm). They can only do so when the system is already under vacuum. If the turbo pump is exposed to atmosphere while spinning the rotors can be damaged.