MSE160 Problem Set 9

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1 Question 1.

Question 1. a)

To calculate atomic density, we take the theoretical density, ρ, given by:

$$\rho = \frac{nA}{V_C N_A}$$

and apply the formula for atomic density, n_{At}:

$$n_{At} = \frac{\rho_d N_A}{A_{Na}}$$

In a diamond cubic structure, there are 8 atoms per unit cell and the atomic mass of germanium is 72.64 g/mol. Since the structure is cubic, the volume is $a^3 = 1.811 \times 10^{-22}$ cm^3.

$$\rho = \frac{8 \times 72.64}{1.811 \times 10^{-22} \times 6.022 \times 10^{23}} = 5.33 \frac{\text{g}}{\text{cm}^3}$$

The atomic density can now be calculated as follows:

$$n_{At} = \frac{\rho_d N_A}{A_{Ge}} = \frac{5.33 \cdot 6.022 \times 10^{23}}{72.64} = 4.42 \times 10^{22} \text{cm}^{-3}$$

The ratio between the intrinsic carrier density and the atomic density is:

$$R = \frac{n_i}{n_{At}} = \frac{2.4 \times 10^{13}}{4.42 \times 10^{22}} = 5.43 \times 10^{-10}$$

Question 1. b)

For intrinsic germanium at 300 K, the concentration of electrons promoted to the conduction band is equal to the concentration of holes in the valence band since one hole is created per promoted electron. In addition, both are equal to the intrinsic carrier concentration. Thus:

$$n = p = n_i = 2.4 \times 10^{13} \text{ cm}^{-3}$$

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To calculate conductivity, σ, we can use the formula:

$$\sigma = nq(\mu_n + \mu_p)$$

where q is the fundamental charge, 1.602×10^{-19} C.

$$\sigma = (2.4 \times 10^{13})(1.602 \times 10^{-19})(3900 + 1900) = 0.0223$$

The unit can be complicated to derive, but we know that a Coulomb is an Ampere-second and an Ohm is a Volt per Ampere:

$$(\text{cm}^{-3})(\text{C})(\frac{\text{cm}^2}{\text{V} \cdot \text{s}}) = \frac{(\text{A} \cdot \text{s} \cdot \text{cm}^2)}{(\text{V} \cdot \text{s} \cdot \text{cm}^3)} = \frac{1}{\Omega \cdot \text{cm}}$$

Thus, the conductivity of germanium at 300 K is 0.0223 $(\Omega \text{·cm})^{-1}$.

Question 1. c)

We first have to calculate n_{At}:

$$n_{At} = \frac{\rho N_A}{M_{At}}$$

where ρ is the atomic density, N_A is Avogadro's Number, and M_{At} is the atomic mass. The atomic density can be calculated like in q1a). In an FCC structure, we know there are 4 atoms per unit cell, the volume is $a^3 = 6.643 \times 10^{-23}$ cm^3 and the atomic weight is 26.98 g/mol.

$$\rho = \frac{nA}{V_C N_A} = \frac{4 \cdot 26.98}{6.643 \times 10^{-23} \cdot 6.022 \times 10^{23}} = 2.70 \frac{\text{g}}{\text{cm}^3}$$

Now, we can evaluate n_{At}:

$$n_{At} = \frac{2.70 \cdot 6.022 \times 10^{23}}{26.98} = 6.02 \times 10^{22} \text{cm}^{-3}$$

To calculate the number of electrons that are freed per atom, we find a ratio between n_{At} and the concentration of electrons, n:

$$3 = \frac{n}{n_{At}} \longrightarrow n = 3n_{At} = 1.806 \times 10^{23} \text{ cm}^{-3}$$

Now that we know n, we can calculate for conductivity:

$$\sigma = nq\mu_e = (1.806 \times 10^{23})(1.602 \times 10^{-19})(13) = 376202 \frac{1}{\Omega \cdot \text{cm}}$$

Question 1. d)

The reason the conductivity of aluminum is so much higher than germanium is because aluminum is a metal, whereas germanium is a pure semiconductor material (a metalloid). Generally, metals have the highest conductivity out of all materials, which is why aluminum's conductivity is almost a factor of 10^6 greater than germanium.

2 Question 2.
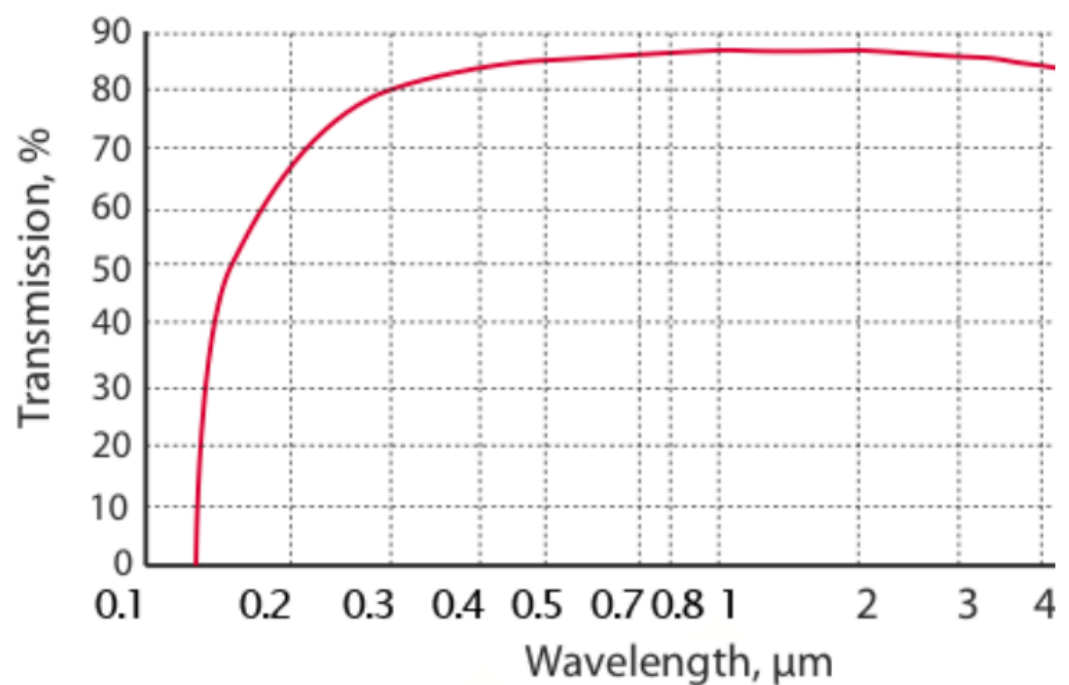
Question 2. a)

This material is optically transparent because as the wavelength of the light approaches the range of visible light (from 0.4 - 0.7 μm), the transmission % of the material is between 80 to 90%, which means the majority of the light can be transmitted through the material.

Question 2. b)

As the material is optically transparent, we can safely assume that the material is most likely an insulator, which have a band gap of $\geq$ 4 eV. However, this is not a sufficient estimate as we can determine a lower limit of energy of the band gap at the point where the material begins to absorb energy. For instance, if 50% of the photons are being transmitted through the material, 50% of the photons will be absorbed. Thus, the optical absorption function will be identical but reflected about the x-axis, as shown below.

<p align="center">Optical Absorption Function</p>
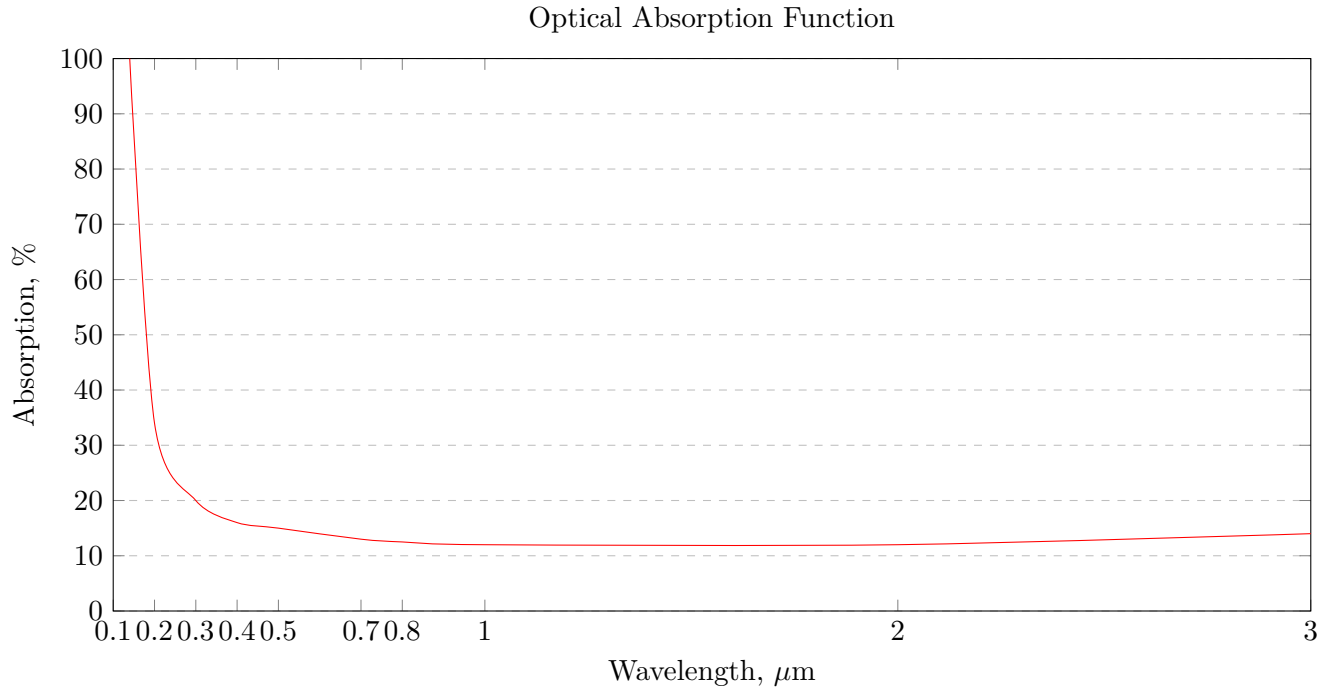
The wavelength of photon where the material begins to absorb energy is around the range of 0.15 to 0.3 micrometers, where the curve's slope begins to change from being flat.

The bandgap energy, E_g, can then be calculated as a range using equation for photon energy:

$$E = \frac{hc}{\lambda}$$

$$E_g = \frac{6.626 \times 10^{-34} \cdot 3.00 \times 10^8}{0.15 \text{ to } 0.3 \times 10^{-6}}$$

$$E_g = 1.325 \times 10^{-18} \text{ J to } 6.626 \times 10^{-19} \text{ J}$$

$$E_g = 8.27 \text{ eV to } 4.13 \text{ eV}$$

The estimate for the bandgap energy also respects the fact that the energy will be ≥ 4 eV, confirming the fact that the material is an insulator.

3   Question 3.

The molar mass of gallium and arsenic, respectively, are 69.72 g/mol and 74.92 g/mol. In the zincblende structure, it is a diamond cubic structure, in which the gallium and arsenic are alternating, meaning in the 8 atom unit cell of the diamond cubic structure, 4 are gallium and 4 are arsenic. We can use the same density formula to calculate the gallium arsenide's density:

$$\rho = \frac{nA}{V_C N_A}$$

The volume of this unit cell is also calculated by $a^3 = 1.804 \times 10^{-22}$ cm^3.

$$\rho = \frac{(4 \cdot 69.72) + (4 \cdot 74.92)}{1.804 \times 10^{-22} \cdot 6.022 \times 10^{23}} = 5.33 \frac{\text{g}}{\text{cm}^3}$$
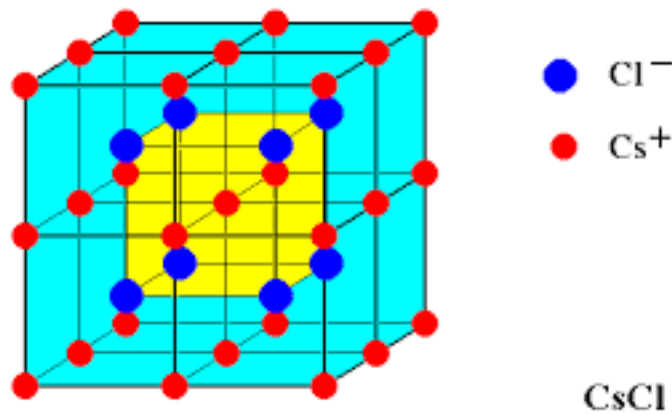
The density of gallium arsenide is 5.33 g/cm^3.

4   Question 4.

The Madelung Constant, M, is defined as:

$$M = \sum_j \frac{\pm}{r_{ij}}$$

If we take a look at the lattice structure of cesium chloride:

We can note that the first Madelung constant can be determined by starting with the center cesium cation and working our way to the chlorine anions. It approaches 8 chlorine anions, with a distance of $\frac{\sqrt{3}a}{2}$ (suppose that the distance from 1 cesium cation to another is a). Also, since the Cs^+ and Cl^- are of opposite signs, the Madelung constant begins with a +. Thus the first Madelung constant is $\frac{8}{\frac{\sqrt{3}a}{2}} = \frac{16}{\sqrt{3}a}$.

The second Madelung constant can be determined by next working our way to the cesium anions directly adjacent to the cesium cation in the centre. It approaches 6 adjacent cesium cations, with a distance of a. Since the two Cs^+ have the same charge, the Madelung constant will begin with a -. Thus the second Madelung constant will be $-\frac{6}{a}$.

Finally, the third Madelung constant can be determined by working our way from the centre cesium cation to the cesium cations diagonally adjacent. If we let the centre cesium cation have coordinates (0, 0, 0), the diagonally adjacent cesium cations would have coordinates (1, 0, ±1), (-1, 0, ±1), (0, 1, ±1), (0, -1, ±1), (1, ±1, 0), and (-1, ±1, 0), for a total of 12 adjacent diagonals. The distance from the centre cation to these cations is $\sqrt{2}a$, and since the charges of the two Cs^+ cations are the same, the Madelung constant will begin with a -. Thus the third Madelung constant will be $-\frac{12}{\sqrt{2}a}$.

$$M_{CsCl} = \frac{16}{\sqrt{3}a} - \frac{6}{a} - \frac{12}{\sqrt{2}a}...$$

$$E = \frac{-e^2}{4\pi\varepsilon_0} \frac{1}{a} \left[\frac{16}{\sqrt{3}} - 6 - \frac{12}{\sqrt{2}} \right] = \frac{5.25e^2}{4\pi\varepsilon_0 a}$$