# MSE160 [Winter 2023] - Problem Set # 3

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## Problem 1 -

What are the full electron configurations of the following atoms (3 points)

- a. Cu<sup>2</sup>
- b. Ni
- c. O<sup>2</sup>
- d. Ar
- e. Au
- f. Na<sup>1+</sup>

 $Cu^{2+}$ :  $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^9$ 

Ni:  $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^8$ 

 $0^{2-}$ :  $1s^2, 2s^2, 2p^6$ 

Ar:  $1s^2, 2s^2, 2p^6, 3s^2, 3p^6$ 

Au:  $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}, 5p^6, 6s^1, 4f^{14}, 5d^{10}$ 

 $Na^{1+}$ :  $1s^2, 2s^2, 2p^6$ 

# Problem 2 -

A 100-lumen laser is directed at a 2L of water at 20°C. Let us say that it takes 4200 J to heat 1L of water 1 degree. If it takes 6 days for the water to heat up to 30°C, assuming perfect delivery and absorption of energy and no energy loss over this time, what is the wavelength of the laser that was used?

Assume that 1 lumen = 4.09\*1015 photons/s. (4 points)

Since it takes 4200 J of energy to heat 1L of water by 1 degree. Then it takes twice the amount of heat 2L of water by 1 degree. Therefore, to heat 2L of by 1 degree we need 8400 J of energy.

For the water to heat up by 10° (difference between 30°C and 20°C) we need:

$$10 \times 8400 = 84000 J$$

Using the given conversion:

 $100 \ lumen = 4.09 \times 10^{15} \times 100 \ photons/s = 4.09 \times 10^{17} \ photons/s$ 

Converting the duration of 6 days into seconds:

$$6 \ days = 6 \times 24 \times 60 \times 60 \ s = 518400 \ s$$

Hence, we can determine the number of photons that were released in this duration:

# of photons = 
$$4.09 \times 10^{17} \times 518400 = 2.12 \times 10^{23}$$

Using the number of photons, we can compute the energy per photon:

$$E = \frac{84000}{2.12 \times 10^{23}} = 3.962 \times 10^{-19} J per photon$$

The equation  $E = \frac{hc}{\lambda}$  can be rearranged with respect to  $\lambda = \frac{hc}{E}$ .

Substituting the values of h, c and E into the equation:

$$\lambda = \frac{hc}{E} = \frac{(6.62607015 \times 10^{-34})(3 \times 10^8)}{3.962 \times 10^{-19}} = 5.0172 \times 10^{-7} \, m$$

We can rewrite this in terms of nm:

$$\lambda = 5.02 \times 10^{-7} \, m = 502 \times 10^{-9} \, m = 502 \, nm$$

$$\therefore \lambda = 502 \, nm$$

#### Problem 3 -

The conductivity of an unknown intrinsic semiconductor was measured to increase by a factor of 10 between the two temperatures 25°C and 100°C. Recall that the relationship between conductivity and

temperature should follow an Arrhenius-type relationship of the form  $\sigma = \sigma_o e^{\frac{-E_g}{2k_bT}}$ , assuming that electron and hole mobilities do not change over this temperature range. Determine the band gap of this unknown semiconductor. (6 points)

We need to write the temperatures on the kelvin scale:

$$T_1 = 100 + 273 = 373 \text{ K}$$
  
 $T_2 = 25 + 273 = 298 \text{ K}$ 

We can compute the band gap  $E_g$  by manipulating the Arrhenius-type equation and the given information:

$$10 = \frac{\sigma_0 e^{\frac{-E_g}{2k_b T_1}}}{\sigma_0 e^{\frac{-E_g}{2k_b T_2}}} = e^{\left(\frac{-E_g}{2k_b T_1} - \frac{-E_g}{2k_b T_2}\right)} = e^{\frac{-E_g}{2k_b}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)}$$

Taking the natural logarithm of both sides, we get:

$$\ln(10) = \frac{-E_g}{2k_h} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

We can rearrange this for the band gap  $E_g$ :

$$E_{g} = -\frac{\ln(10) \times 2 \times k_{b}}{(\frac{1}{T_{1}} - \frac{1}{T_{2}})}$$

Substituting the values of the Boltzmann constant and the temperature we get the band gap as:

$$E_{g} = -\frac{\ln(10) \times 2 \times 1.380649 \times 10^{-23}}{(\frac{1}{373} - \frac{1}{298})} = 9.423 \times 10^{-20} \text{ J}$$

Now for convenience we can convert this band gap from joules into electron-volts:

$$E_g = 9.423 \times 10^{-20} \times 6.242 \times 10^{18} = 0.5881 \text{ eV}$$

$$\therefore E_{\rm g} = 0.588 \, \rm eV$$

#### Problem 4 -

What is the conductivity of pure germanium at 26°C if n-I at that temperature is  $4 \times 10^{13}~cm^{-3}$  while the electron and hole mobilities are 3600 and 1700  $cm^2$ /Vs, respectively? (2 points)

Because pure germanium is an intrinsic semiconductor, we can use the formula:

$$\sigma = n_i e (\mu_n + \mu_p)$$

Substituting the values of the constants and the variables we get:

$$\sigma = (4 \times 10^{13})(1.602176634 \times 10^{-19})(3600 + 1700) = 0.0339 (mhos/cm)$$

$$\sigma = 0.034 \, (mhos/cm)$$

## Problem 5 -

Assume that Gd atoms in Gd metal act as isolated Gd atoms in terms of their magnetic moment. Calculate the saturation magnetization of Gd metal. Note: Gd has a density of 7.9 g/cm<sup>3</sup> and a molar mass of 157.25 g/mol. (5 points)

To determine the number of atoms of Gd per cubic meter, we will use stoichiometry equations:

$$\rho = \frac{m}{V} = \frac{n \times M_r}{V} = \frac{\frac{N}{N_A} \times M_r}{V} = \frac{N \times M_r}{N_A \times V}$$

where n is the number of moles, N is the number of atoms,  $N_A$  is the Avogadro's constant and V is the volume.

Rearranging this equation for  $\frac{N}{V}$ , we can get the number of atoms of Gd metal per cubic meter:

$$\frac{N}{V} = \frac{\rho \times N_A}{M_r} = \frac{(7.9 \times 10^6) \times (6.0221 \times 10^{23})}{(157.25)} = 3.025 \times 10^{28} atoms \ per \ cm^3$$

We know that 1 atom of gadolinium has a magnetic moment of 7.98 Bohr Magnetons Using this information, we can compute the saturation magnetization of Gd metal:

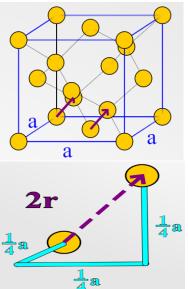
$$M_B = 7.98 \times M_B \times \frac{N}{V} = 7.98 \times 9.27 \times 10^{-24} \times 3.025 \times 10^{28} = 2.24 \times 10^6 \frac{A}{m}$$

$$M_B = 2.24 \times 10^6 \frac{A}{m}$$

# Problem 6 -

Calculate the theoretical density of diamond. The molar mass of carbon is 12 g/mol and the atomic radius is 70pm. (7 points)

We need to first determine the lattice parameter, a, for the diamond cubic crystal structure:



In the diamond crystal cubic structure there are carbons at the FCC positions and at tetrahedral positions. In this specific crystal structure atoms touch in the purple direction (as shown on the figure on the left). When atoms touch each other, the distance between their centers is given by 2r. We can consider on of the atoms at the tetrahedral positions whose coordinates are  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ . We can assume that the corner carbon atom is directly touching the carbon atom at the tetrahedral position.

Using Pythagoras theorem and the carbon atoms with the coordinates (0, 0, 0) and  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ :

$$2r = \sqrt{(\frac{1}{4}a)^2 + (\frac{1}{4}a)^2 + (\frac{1}{4}a)^2}$$

Simplifying this equation, we get:

$$2r = \sqrt{3} \left(\frac{1}{4}a\right)$$

Rearranging this equation for the lattice parameter:

$$a = \frac{8}{\sqrt{3}}r$$

Now we can substitute the atomic radius of carbon to determine the lattice parameter of the diamond crystal cubic structure:

$$a = \frac{8}{\sqrt{3}}r = \frac{8}{\sqrt{3}} \times (70 \times 10^{-12}) = 3.2331 \times 10^{-10} m$$

We can determine the volume of the unit cell by

$$V_{cell} = a^3 = (3.2331 \times 10^{-10})^3 = 3.38 \times 10^{-29}$$

Using the formula of theoretical density, we know that:

$$\rho = \frac{n \times A_w}{V_{cell} \times N_A}$$

where n is the number of atoms in the unit diamond cubic crystal structure, A is the molar mass of carbon, V is the volume of the unit cell and  $N_A$  is the Avogadro's number.

In a diamond cubic crystal structure there are 8 carbon atoms, and therefore n = 8.

Substituting all the constants and known variables into the theoretical density equation we get:

$$\rho = \frac{8 \times (12)}{(3.38 \times 10^{-29}) \times (6.0221 \times 10^{23})} = 4716355.9 \, \frac{g}{m^3} = 4.72 \, \frac{g}{cm^3}$$

$$\therefore \rho = 4.72 \ g \ cm^{-3}$$

## Problem 7 -

If we want to make an LED that is formed from Ga<sub>2</sub>Al<sub>0-3</sub>As that emits at a wavelength of 450 nm, what is x? (3 pts)

We can determine the band gap of this semiconductor using the following formula:

$$E = \frac{hc}{\lambda} = \frac{(6.62607015 \times 10^{-34})(3 \times 10^8)}{450 \times 10^{-9}} = 4.417 \times 10^{-19} J = 2.76 \text{ eV}$$

We know that the band gap for GaAs is 1.4 eV and the band gap for AlAs is 3.14 eV.

To determine the value of x, we can use the equation.

$$1.4(x) + 3.14(1-x) = 2.756 \, eV \, (found \, above)$$

Solving the equation for the value of x, we get:

$$\therefore x = 0.22$$