<u>Note:</u> These questions will be discussed during the tutorial sessions on September **10th** and **14th**. The In-Tutorial Exercise will be on September **17th** and **21st**.

<u>Question 1:</u>

i) For each of the following compounds, state whether the bonding is essentially metallic, covalent, ionic, van der Waals, or hydrogen:

(a) Ni, (b) ZrO_2, (c) graphite, (d) solid Kr, (e) Si, (f) BN, (g) SiC, (h) Fe_2O_3, (i) MgO, (j) W, (k) H_2O within the molecules, (l) H_2O between the molecules.

If ionic and covalent bonds are involved in the bonding of any of the compounds listed, calculate the percentage ionic character in the compound.

ii) Describe the atomic bonding between magnesium and chlorine.

<u>Solution</u>

i)

(a) Ni:	Nickel bonding is primarily metallic.
(b) ZrO_2:	From Pauling's equation, the Zr–O bond is 73.4% ionic and 26.6% covalent, where x_A and x_B are the electronegativities of zirconium and oxygen, respectively.
(c) Graphite:	The bonding is covalent within the layers and secondary between the layers.
(d) Solid Kr:	The bonding represents van der Waals due to fluctuating dipoles.
(e) Si:	Silicon bonding is covalent.
(f) BN:	The B–N bond, from Pauling's equation (2-10), is 26.1% ionic and 73.9% covalent.
(g) SiC:	From Eq. (2-10), the Si–C bond is 11% ionic and 89% covalent.
(h) Fe_2O_3:	From Eq. (2-10), the Fe-O bond is 55.5% ionic and 44.5% covalent.
(i) MgO:	From Eq. (2-10), the Mg-O bond is 70.2% ionic and 29.8% covalent.
(j) W:	Tungsten bonding primarily consists of metallic bonding with some covalent character.
(k) H_2O within the molecules:	The H–O bond is 38.7% ionic and 61.3% covalent.
(l) H_2O between the molecules:	Hydrogen bonding exists between H_2O molecules.

ii) Applying Pauling's equation to $MgCl_2$ component:

for $MgCl_2$, X_{Mg}= 1.2 and X_{Cl}=3.0, therefore:

$$\%IC = \left[1 - e^{-(0.25)(3-1.2)^2}\right] \times 100 = 55.5\%$$

Metals and non-metals often form ionic bonds because of the difference in their electronegativity values. Electronegativity is basically a measure of how strongly an element will attract electrons toward it. Chlorine (a non-metal) has an electronegativity value of 3.0 and magnesium (a metal) has an electronegativity value of 1.3. This makes a difference of 3.0-1.3= 1.7. In general, any electronegativity difference of 1.6 or more is considered an ionic bond and $MgCl_2$ falls in this category.

Ionic bonds are when atoms gain or lose electrons to become charged species (ions) that share an electrostatic called an ionic bond. Magnesium forms a positive ion (cation) with a 2+ charges and chlorine forms a negative ion (anion) with a 1- charge. So two chlorine atoms form an ionic bond with one magnesium to form $MgCl_2$.

Question 2:

The interaction energy between Na^+ and Cl^- ions in the NaCl crystal can be written as:

$$E(r) = -\frac{4.03 \times 10^{-28}}{r} + \frac{6.97 \times 10^{-96}}{r^8}$$

Where the energy is given in joules per ion pair, and the interionic separation *r* is in meters. Calculate the binding energy and the equilibrium separation between the Na^+ and Cl^- ions. Also estimate the elastic modulus Y of NaCl given that:

$$Y = \frac{1}{6r_0}\left[\frac{d^2E}{dr^2}\right]_{r=r_0}$$

Solution:

$$@\ equilibrium: \left.\frac{dE(r)}{dr}\right]_{@r_0} = 0 \Rightarrow 4.03 \times 10^{-28} r_0^{-2} - 8 \times 6.97 \times 10^{-96} r_0^{-9} = 0 \xrightarrow{yields} r_0 = 2.81 \times 10^{-10}$$

$$E(r_0) = -\frac{4.03 \times 10^{-28}}{2.81 \times 10^{-10}} + \frac{6.97 \times 10^{-96}}{(2.81 \times 10^{-10})^8} = 1.255 \times 10^{-18} \frac{J}{ion\ pair}$$

$$Y = \frac{1}{6r_0}\left[\frac{d^2E}{dr^2}\right]_{r=r_0} = \frac{1}{6r_0}\left[-2(4.03 \times 10^{-28}) r_0^{-3} + (-8)(-9)(6.97 \times 10^{-96}) r_0^{-10}\right]$$

$$Y = \frac{1}{6 \times 2.81 \times 10^{-10}}\left[-2(4.03 \times 10^{-28})(2.81 \times 10^{-10})^{-3} + (-8)(-9)(6.97 \times 10^{-96})(2.81 \times 10^{-10})^{-10}\right]$$

$$Y = 7.543 \times 10^{10}\ Pa = 75.43\ GPa$$

Question 3:

a) A gold wire is 0.70 mm in diameter and 8.0 cm. in length. How many atoms does it contain?

b) Calculate and compare the number of atoms per cubic centimeter in lead and lithium.

c) An intermetallic compound has the general chemical formula Mg_xAl_y, where x and y are simple integers. What is the simplest chemical formula of a magnesium aluminide intermetallic compound that consists of 15.68 wt % Mg and 84.32 wt % Al?

Solution:

a) The density of gold is 19.3 g/cm^3

$m_{Au}=\rho V$ & ρ=19.3 g/cm^3 , d=0.7mm= 0.07 cm

V of wire= A×L ; which A is cross section area of wire and L is length

$V=\frac{\pi d^2}{4}\times L=\frac{\pi(0.07)^2}{4}\times(8.0cm)=0.0308cm^3$

$m_{Au}=\rho V=(19.3\ g/cm^3)(0.0308cm^3)=0.5944\ g$

Atomic mass of Au (1 mole of Au) is equal to 196.97 g

No. of Atoms Au= $(0.5944g_{Au})(\frac{6.02\times10^{23} atoms\ /mol}{196.97\ g/mol})=1.82\times10^{21}$ atoms of Au

b) The density of lead is 11.36 g/cm^3

No. of lead atoms = $(\rho V)(\frac{Avogadro's\ number}{atomic\ mass})$

Atomic mass of lead is 207.19 g/mol

For V= 1 cm^3

No. of lead atoms = $\frac{(11.36)(1)(6.02\times10^{23})}{207.19}=3.3\times10^{22}$ atoms

For Lithium; density of lithium is 0.534 g/cm^3, atomic mass of Lithium is 6.941 g/mol

No. of lithium atoms = $(\rho V)(\frac{Avogadro's\ number}{atomic\ mass})=(0.534g/cm^3)(1cm^3)(\frac{6.02\times10^{23}}{6.941})=4.6\times10^{22}$ atoms

This means that the same mass of Li has around 40% larger number of atoms than Pb because Li is much lighter atom.

c) Firstly, we have to determine the gram-mole fractions of Mg and Al. So, using a basis of 100 g of intermetallic compound,

No. of gram-mole of Mg = $\frac{15.68\ g}{24.31\ g/mol}=0.645$ mol

Atomic mass of Mg is 24.31 g/mol

No. of gram-mole of Al = $\frac{84.32\ g}{26.98\ g/mol}=3.125$ mol

Atomic mass of Al is 26.98 g/mol

Total gram-mole of component = 3.770 mol

x as gram-mole fraction of Mg = $(\frac{0.645\ mol}{3.77\ mol})=0.17$

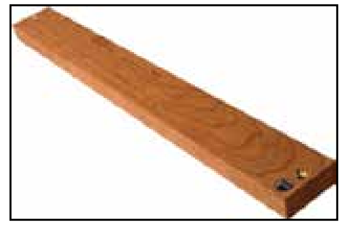
y as gram-mole fraction of Al = $(\frac{3.125\ mol}{3.77\ mol})=0.83$

Thus we have $Mg_{0.17}Al_{0.83}$ or multiplying by 6, $\mathbf{MgAl_5}$

<u>Question 4:</u>

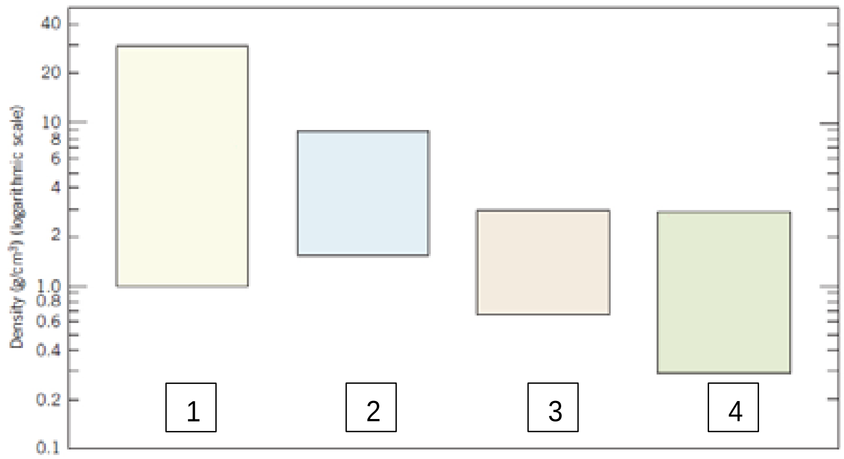
From the pictures below, materials can be classified into four general categories.



a) What are these categories?

b) Based on these categories, label the blocks in the figure below to match with their suitable densities.



c) What is the difference between composites and other types of materials? Give an example for composite materials.

<u>Solution:</u>

a) From left to right images

- metals (metallic elements)
- ceramics (compounds between metallic and nonmetallic elements)
- polymers (compounds composed of carbon, hydrogen, and other nonmetallic elements)
- composites

b)

1) Metals
2) Ceramics
3) Polymers
4) Composites

c) Composites are composed of at least two different material types. Glass fibre reinforced plastic is the common type of composites. Woods are also considered natural composites.