Question 1

On the basis of ionic charge and ionic radii, predict crystal structures for the following materials:

a) CsI
b) NiO
c) KI
d) NiS

Solution:

a) For CsI, using data from Table 12.3:

$$\frac{r_{Cs^+}}{r_{I^-}} = \frac{0.170\ nm}{0.220\ nm} = 0.773$$

Therefore, according to Table 12.2, the coordination number for each cation (Cs^+) is eight, and, using Table 12.4, the predicted crystal structure is cesium chloride.

b) For NiO, using data from Table 12.3

$$\frac{r_{Ni^{2+}}}{r_{O^{2-}}} = \frac{0.069\ nm}{0.140\ nm} = 0.493$$

The coordination number is six (Table 12.2), and the predicted crystal structure is sodium chloride (Table 12.4).

c) For KI, using data from Table 12.3

$$\frac{r_{K^+}}{r_{I^-}} = \frac{0.138\ nm}{0.220\ nm} = 0.627$$

The coordination number is six (Table 12.2), and the predicted crystal structure is sodium chloride (Table 12.4).

d) For NiS, using data from Table 12.3

$$\frac{r_{Ni^{2+}}}{r_{S^{2-}}} = \frac{0.069\ nm}{0.184\ nm} = 0.375$$

The coordination number is four (Table 12.2), and the predicted crystal structure is zinc blende (Table 12.4).

Question 2:

The unit cell for Al_2O_3 has hexagonal symmetry with lattice parameters a = 0.4759 nm and c = 1.2989 nm. If the density of this material is 3.99 g/cm^3, calculate its atomic packing factor. Ionic radius for Al^{+3} is 0.053 nm and for O^{-2} is 0.140 nm.

Solution:

To calculate the AFP, firstly we have to determine the value of n' in Equation (12.1). This necessitates that we calculate the value of V_C, the unit cell volume. In Example Problem 3.3 it was shown that the area of the hexagonal base (AREA) is related to **a** as

AREA= $\frac{3a^2\sqrt{3}}{2} = \frac{3}{2}\times(4.759\times10^{-8}\text{ cm})^2\times(1.732) = 5.88\times10^{-15}\text{ cm}^2$

So the unit cell volume now is just

V_C= (AREA).(c) = $(5.88\times10^{-15}\text{ cm})(1.2989\times10^{-7}\text{ cm}) = 7.64\times10^{-22}\text{ cm}^3$

Now for n' yields

$$n' = \frac{\rho N_A V_c}{\sum A_c + \sum A_A} = \frac{(3.99\ g/cm^3)(6.023\times10^{23})(7.64\times10^{-22}cm^3)}{2\left(26.98\frac{g}{mol}\right) + 3(16.00\ \frac{g}{mol})}$$

$$n' = 18\ formula\ units/unit\ cell$$

Thus, there are 18 Al2O3 units per unit cell, or 36 Al^{3+} ions and 54 O^{2-} ions. The radius of these ions types are 0.053 and 0.140 nm, respectively. Thus, the total sphere volume, Vs is

$V_S = n_{Al^{3+}}\frac{4}{3}\pi a^3 + n_{O^{2-}}\frac{4}{3}\pi a^3 = (36)\left(\frac{4}{3}\pi\right)(5.3\times10^{-9}\text{ cm})^3 + (54)\left(\frac{4}{3}\pi\right)(1.4\times10^{-8}\text{ cm})^3$

$V_S = 6.43\times10^{-22}\text{ cm}^3$

Finally, APF is

$$APF = \frac{V_S}{V_C} = \frac{6.43\times10^{-22}}{7.64\times10^{-22}} = 0.842$$

Question 3:

A ceramic material, in the form of a circular bar with radius 5mm, is tested in 3-point bending. The length between the support points is 50 mm. If the load required to cause fracture is 2380 N, determine the flexure strength of this ceramic.

a) If this material has a fracture toughness of 4.5 MPa.m$^{1/2}$ what is the size of the longest internal crack? Assume the geometric parameter Y is equal to 1.

b) Knowing that the modulus of elasticity for the nonporous material is 400 GPa, what is the elastic modulus of the porous ceramic if it has 10 vol% porosity?

Solution:

$$a)\ \sigma_{fs} = \frac{F_f L}{\pi R^3} = \frac{2380\ N \times 0.05\ m}{\pi \times (0.005m)^3} = 303.03 \times 10^6 \frac{N}{m^2} = 303.03\ MPa$$

$$K_{1C} = Y\sigma_f\sqrt{\pi a} \rightarrow a = \frac{1}{\pi}\left(\frac{K_{1C}}{Y\sigma_f}\right)^2 = \frac{1}{\pi}\left(\frac{4.5\ MPa.m^{1/2}}{1 \times 303.03\ MPa}\right)^2 = 70.19 \times 10^{-6} m = 70.19 \mu m$$

$$b)\ E = E_0(1 - 1.9P + 0.9P^2) = 400\ GPa \times (1 - 1.9 \times 0.1 + 0.9 \times 0.1^2) = 327.6\ GP$$

<u>Question 4:</u>

The tensile strength and number-average molecular weight for two polyethylene materials are as follows:

Tensile Strength (MPa)	Number-Average Molecular Weight (g/mol)
85	12,700
150	28,500

Estimate the number-average molecular weight that is required to give a tensile strength of 195 MPa.

<u>Solution:</u>

This problem gives us the tensile strengths and associated number-average molecular weights for two polyethylene materials and then asks that we estimate the $\overline{M}_n$ that is required for a tensile strength of 195 MPa. Equation 15.3 cites the dependence of the tensile strength on $\overline{M}_n$. Thus, using the data provided in the problem statement, we may set up two simultaneous equations from which it is possible to solve for the two constants TS∞ and A. These equations are as follows:

$$85 \text{ MPa} = TS_\infty - \frac{A}{12{,}700 \text{ g/mol}}$$

$$150 \text{ MPa} = TS_\infty - \frac{A}{28{,}500 \text{ g/mol}}$$

Thus, the values of the two constants are: TS∞ = 202 MPa and A = 1.489 ´ 106 MPa-g/mol. Solving for $\overline{M}_n$ in Equation 15.3 and substituting TS = 195 MPa as well as the above values for TS∞ and A leads to

$$\overline{M}_n = \frac{A}{TS_\infty - TS}$$

$$= \frac{1.489 \times 10^6 \text{ MPa-g/mol}}{202 \text{ MPa} - 195 \text{ MPa}} = 213{,}000 \text{ g/mol}$$

Question 5:

Briefly explain how each of the following influences the tensile or yield strength of a semicrystalline polymer and why:

(a) Molecular weight
(b) Degree of crystallinity
(c) Deformation by drawing
(d) Annealing of an undeformed material

Solution

(a) The tensile strength of a semicrystalline polymer increases with increasing molecular weight. This effect is explained by increased chain entanglements at higher molecular weights.

(b) Increasing the degree of crystallinity of a semicrystalline polymer leads to an enhancement of the tensile strength. Again, this is due to enhanced interchain bonding and forces; in response to applied stresses, interchain motions are thus inhibited.

(c) Deformation by drawing increases the tensile strength of a semicrystalline polymer. This effect is due to the highly oriented chain structure that is produced by drawing, which gives rise to higher interchain secondary bonding forces.

(d) Annealing an undeformed semicrystalline polymer produces an increase in its tensile strength.