HW #9 MSEG 302 Spring 2018 answer key

**1. Calculate the density and atomic packing factor for cesium chloride assuming the radius of the Cs+ cation is 0.170 nm, and the Cl- anion is 0.181 nm, assuming that the ions touch along the cube diagonals.**

Per Figure 12.3, CsCl is simple cubic, with a chlorine atom at the corner of the unit cell and a cesium atom in the center (BCC-like) position. Since the atoms touch along the body diagonal, this means 2 rCl + 2 rCs = Sqrt[3] a, where rCl and rCs are the radius of the chlorine and cesium atoms respectively, and a is the length of the unit cell. Given the values of rCs and rCl from the problem statement, and solving for a gives a = 0.405 nm. So the density = (MCs + MCl) / a3, where MCs and MCl are the mass of a single Cs and Cl atom. MCs = 132.9 g/mol / Nav, and MCl = 35.45 g/mol / Nav, where Nav = 6.02 x 1023 / mol (Avogadro’s number). Solving and changing units (1 cm = 107 nm) gives density = 4.20 g/cm3. Wikipedia says actual density of CsCl = 3.99 g/cm3. Atomic packing factor = Volume of atoms / volume of unit cell. Volume of an atomic sphere Vatom = 4  r3 / 3. So APF = VCs + VCl / a3 = 0.682. This is similar to that of BCC, as it should be since the structure is quite similar to BCC overall.

**2. A mixture of 92 kg of CaO with 8 kg of ZrO2 is melted into a liquid at high temperature.**

**a) On slow cooling, at what temperature will solid first appear?**

**b) What is the composition of this solid?**

**c) At what temperature will the sample become completely solid?**

**c’) As the sample continues to cool, at what temperature will a second solid phase begin to precipitate?**

**d) What is the composition of this solid phase?**

**e) What is the expected composition and relative amounts of the phases expected to be present at room temperature?**

Total mass is 92+8 = 100 kg, so this sample is 8wt% CaO, 92wt% ZrO2. From phase diagram (Figure 12.24), a) first solid will appear at about 2550 C on cooling from the melt, with b) composition of 3 wt% CaO – 97 wt% ZrO2. Sample becomes completely solid (cubic ZrO2) at c) 2350 C. After continued cooling, second phase begins to precipitate c’) at 1000 C; second phase is d) CaZr4O9, with a composition just above 10 wt% CaO. At room temperature, assuming no other phase transitions occur, sample will be e) a mixture of monoclinic ZrO2 (essentially pure), with CaZr4O9 (10.2% wt CaO. From the lever rule, there will be 80% CaZr4O9 and 20% ZrO2 in the mixture.

**3. For a certain ceramic material, mechanical tests of samples with 10 vol% porosity show stiffnesses and strengths that are 82% and 50% of their values for the corresponding fully dense materials, respectively. Estimate the stiffness and strength expected for samples with 20 vol% porosity.**

From text and class notes, for modulus (stiffness) E/E0 = 1-1.9P+0.9P2, and for flexural strength s/s0 = exp(-n P), with P the porosity in units of volume fraction. Using P=0.1 and solving for n gives 0.5 = exp(-n (0.1)), so n = 6.93. For P=0.2, E/E0 = 0.66 = 66%, and s/s0 = exp(-6.93 0.2) = 0.25 = 25%.

**4. A 15 cm long rectangular bar of fused silica with a cross section of 1 cm x 2 cm is measured in a three-point flexural test. In the first experiment the bar is lying flat, with the load coming from above. If the supported length of the bar is 10 cm, what is force required to cause fracture? If the rod is now rotated by 90 degrees around its long axis and re-tested, what will be the load required to cause fracture?**

Equation 12.7a in text and from class gives fs = 3 FfL / 2bd2, where Ff is the load at failure, L the supported length, d the dimension parallel to the force (height of bar), and b the direction perpendicular to the force (width of bar; see Figure 12.30). Flexural strength of fused silica is estimated to be 110 MPa (Table 12.5). So in the first case, b=2 cm, d=1 cm, giving

110 MPa = 3 Ff (10 cm)/2(1 cm)(2 cm)2. Solving for Ff gives 2933 N. Rotating the bar by 90 degrees means d becomes b, and b become d. Substituting in values accordingly gives Ff = 1467 N.

**5. The tensile strength of a poly(methyl methacrylate) (PMMA) polymer with a number-average molecular weight of 30,000 g/mol is found to be 50 MPa, while the tensile strength of a second sample having a number average molecular weight of 50,000 g/mol is 150 MPa.**

**a) Estimate the tensile strength at a number average molecular weight of 40,000 g/mol.**

**b) Estimate the tensile strength at a number average molecular weight of 1,000 g/mol.**

**c) Estimate the tensile strength at a number average molecular weight of 1,000,000 g/mol.**

From text and class notes, expect tensile strength to vary as TS = TSinf – A/Mn (equation 15.3), with A some constant. So 50 = TSinf – A/30000, and 150 = TSinf – A/50000. Solving gives TSinf = 300 MPa, A=7,500,000 MPa g /mol. So a) 300- A/40000 = 112.5 MPa. b) 300-7500000/1000 = -7200 MPa. But this is physically unrealistic… equation actually predicts that TS -> 0 at 25000 g/mol. So estimate TS ~ 0. c) 300-7500000/1000000 = 292.5 MPa

**6. A sample of polystyrene is examined by measuring the stress relaxation as a function of time at various temperatures after the application of a fixed amount of strain of 0.1 (10%). What is the expected stress on the sample after 10 seconds of deformation at a) 80 C, b) 120 C, and c) 190 C? What would be the expected stress on the sample at 190 C, assuming it had been lightly crosslinked?**

Equation 15.1 gives Er(t) = (t)/e0, where Er(t) is the relaxation modulus at a time t, e0 the applied strain, and (t) the stress. Solving for  (t) gives Er(t) e0. Values of Er(t) for 10 seconds are given in figure 15.7 and 15.8 for polystyrene. So at a) 80 C,  (t) = 3 x 103 MPa (0.1) = 3 x 102 MPa = 300 MPa. At b) 120 C, 0.7 (0.1) = 0.07 MPa = 70 kPa. At c) 190 C, 2 x 10-3 MPa (0.1) = 2 x 10-4 MPa = 200 Pa. If lightly crosslinked, sample would retain the rubbery modulus (see Figure 15.8)… so about stress about 70 kPa (like at 120 C).