# 3.091 OCW Scholar Self-Assessment Exam Crystalline Materials

Write your answers on these pages.

State your assumptions and show calculations that support your conclusions.

RESOURCES PERMITTED: PERIODIC TABLE OF THE ELEMENTS, TABLE OF CONSTANTS, AN AID SHEET (ONE PAGE 8½" × 11"), AND A CALCULATOR.

NO BOOKS OR OTHER NOTES ALLOWED.

Exam 2, Problem #1



(a) For each unit cell above, draw the crystallographic feature indicated and label it clearly.

(b) Named after Salvadore Dali, dalium (Da) is BCC. Its molar volume is 6.66 cm<sup>3</sup>/mol. Calculate the density of atoms in (001) of Da. Express your answer in atoms/cm<sup>2</sup>.

(c) Here is the (011) plane in a unit cell of magnesium oxide (MgO) which is FCC. Indicate the positions of all atoms lying in the plane. Represent atoms as 2-dimensional slices of space-filling spheres. The values of ionic radii are Mg<sup>2+</sup> = 0.65 Å and O<sup>2-</sup> = 1.34 Å. Your sketch need not be drawn to scale; however, you must convey relative values of the ionic dimensions.



#### Exam 2, Problem #2

(a) You discover that someone has been using your x-ray generator and has changed the target/anode. To determine the chemical identity of the new target, you go ahead and operate the x-ray generator and find the wavelength,  $\lambda$ , of the  $K_{\alpha}$  peak to be 0.250 Å. What element is the target made of?

(b) Hilary Sheldon conducts an experiment with her x-ray diffractometer. A specimen of tantalum (Ta) is exposed to a beam of monochromatic x-rays of wavelength set by the  $K_{\alpha}$  line of titanium (Ti). Calculate the value of the smallest Bragg angle,  $\theta_{hkl}$ , at which Hilary can expect to observe reflections from the Ta specimen.

DATA:  $\lambda_{K_{\alpha}}$  of Ti = 2.75 Å; lattice constant of Ta, a = 3.31 Å

(c) Sketch the emission spectrum (intensity *versus* wavelength) of an x-ray target that has been bombarded with *photons* instead of with electrons. Assume that the incident photons have more than enough energy to dislodge *K*-shell electrons in the target. On your spectrum label the features associated with  $K_{\alpha}$  radiation,  $K_{\beta}$  radiation, and  $L_{\alpha}$  radiation.

## Exam 3, Problem #1

Silver bromide (AgBr) has rock salt crystal structure, i.e., FCC Bravais lattice with the ion pair,  $Ag^+$  and  $Br^-$  as basis. The dominant defect in AgBr is the Frenkel disorder.

- (a) Does the Frenkel disorder in AgBr create vacancies of Ag<sup>+</sup>, vacancies of Br<sup>-</sup>, or both? Explain. The ionic radii are 0.67 Å for Ag<sup>+</sup> and 1.96 Å for Br<sup>-</sup>.
- (b) Calculate the temperature at which the fraction of Frenkel defects in a crystal of AgBr exceeds 1 part per billion = 1 ppb =  $10^{-9}$ . The enthalpy of Frenkel defect formation,  $\Delta H_F$ , has a value of 1.16 eV / defect, and the entropic prefactor, *A*, has a value of 3.091.

#### Exam 3, Problem #2

(b) On each of three separate drawings of one face of an FCC unit cell, indicate one of each of the following: (1) substitutional impurity; (2) vacancy; (3) interstitial impurity.

## Final Exam, Problem #3

(b) Calculate the atomic packing density along [011] direction of aluminum (Al). Express your answer in units of atoms cm<sup>-1</sup>.

# Final Exam, Problem #4

Give the rotational symmetry of each of the following patterns. Express your answer as *n*-fold.







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