MATRL 100A: Structure and Properties I, Problem Set 3

This problem set is due in lecture on Wednesday, Oct 21st in hard copy. Write neatly, show your work clearly, and include units in all answers. While you are free to discuss this problem set with your classmates, the product that you turn in must be your own work. Do not copy or paraphrase each other’s work.

Chapter 3

1. Iodine has an orthorhombic unit cell for which the \(a\), \(b\), and \(c\) lattice parameters are 0.479, 0.725, and 0.978 nm, respectively.
   
   (a) If the atomic packing factor and atomic radius are 0.547 and 0.177 nm, respectively, determine the number of atoms in each unit cell. \([2]\]
   
   (b) The atomic weight of iodine is 126.91 g/mol; compute its theoretical density. \([2]\]

2. The accompanying Figure (1) shows a unit cell for a hypothetical metal.

   ![Figure 1: Crystal structure for hypothetical metal](image)

   (a) To which crystal system does this unit cell belong? \([1]\)
   
   (b) What would this crystal structure be called? \([1]\)
   
   (c) Calculate the density of the material, given that its atomic weight is 141 g/mol. \([2]\)

3. List the point coordinates for all atoms, or partial atoms, that are contained in an FCC unit cell (Figure 3.1 in text). \([3]\)

4. Draw an orthorhombic unit cell, and within that cell a \([12\bar{1}]\) and \([101]\) direction. \([7]\)

5. For tetragonal crystals, cite the indices of directions that are equivalent to each of the following directions: [001], [110], and [010]. It will be beneficial to sketch a tetragonal unit cell for your reference. \([3]\)

6. Draw an orthorhombic unit cell, and within that cell a (210), (111), and (001) planes. Please draw separate unit cells for each plane. \([6]\)
7. Determine the Miller indices for the planes shown in the following unit cell (Figure 7):

![Unit cell for Problem 7](image)

Figure 2: Unit cell for Problem 7

8. Figure 3 shows the atomic packing schemes for several different crystallographic directions for a hypothetical metal. For each direction, the circles represent only the atoms contained within a unit cell; the circles are reduced from their actual size.

![Deconstructed view of the unit cell](image)

Figure 3: Deconstructed view of the unit cell in Problem 8

(a) To what crystal system does the unit cell belong? [2]
(b) What would this crystal structure be called? [2]
(c) Make a sketch of the 3D unit cell. [3]

9. (a) Derive linear density expressions (atoms/nm) for FCC [100] and [111] directions in terms of the atomic radius \( R \). [2]
(b) Compute and compare linear density values for these same two directions for silver. The radius of a silver atom is 0.144 nm. [2]

10. (a) Derive planar density expressions (atoms/nm\(^3\)) for BCC (100) and (110) planes in terms of the atomic radius \( R \). Make sketches indicating the (100) and (110) planes. [2]
(b) Compute and compare planar density values for these same two directions for vanadium. The radius of a vanadium atom is 0.132 nm. [2]
11. Molybdenum is BCC with an atomic radius of 0.1363 nm. Compute the interplanar spacing for the (111) set of planes. Be sure to sketch a BCC unit cell and indicate the (111) plane. [3]

12. The metal iridium has an FCC crystal structure. If the angle of diffraction for the (220) set of planes occurs at \(2\theta = 69.2^\circ\) (first-order reflection) when monochromatic x-radiation having a wavelength of 0.1542 nm is used, compute

   (a) the interplanar spacing for this set of planes and \([2]\)
   (b) the atomic radius for an iridium atom. \([3]\)

*Hint:* \(d_{220} = 2d_{110}\)