NORTHERN ILLINOIS UNIVERSITY

PHYSICS DEPARTMENT

Physics 580 – Solid State Physics Fall 2024

Problem Set #3

Problem Set Due: Thurs, Sept. 19, 2024
Read Kittel: Chapter 2, powerpoint: *X-ray Diffraction*

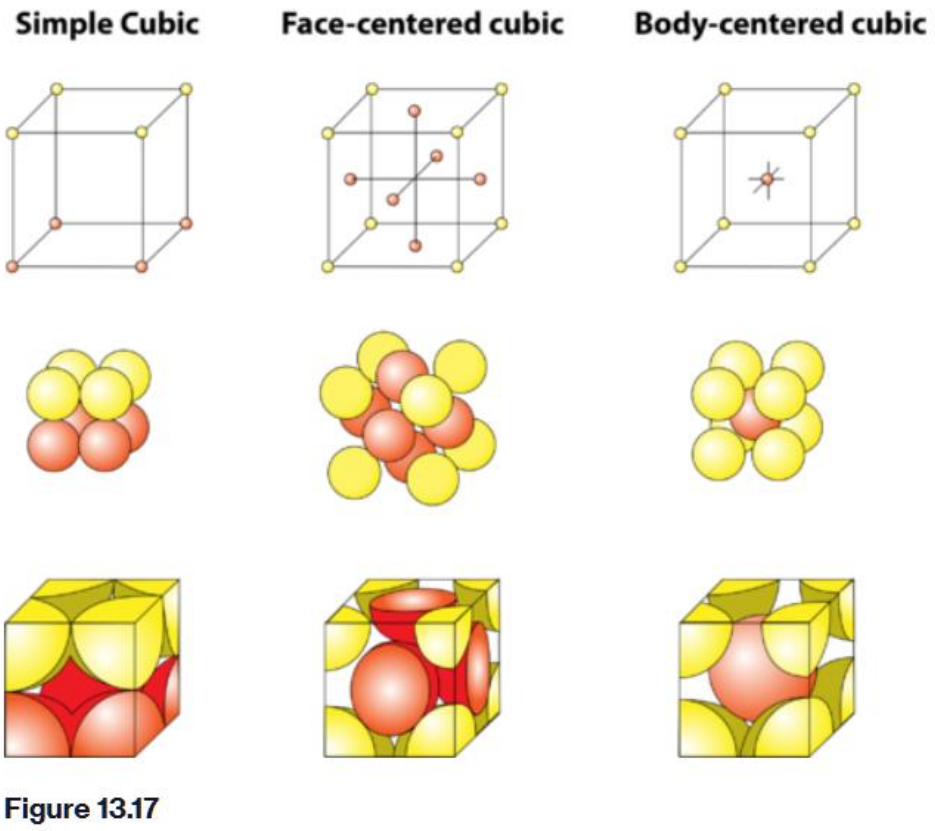


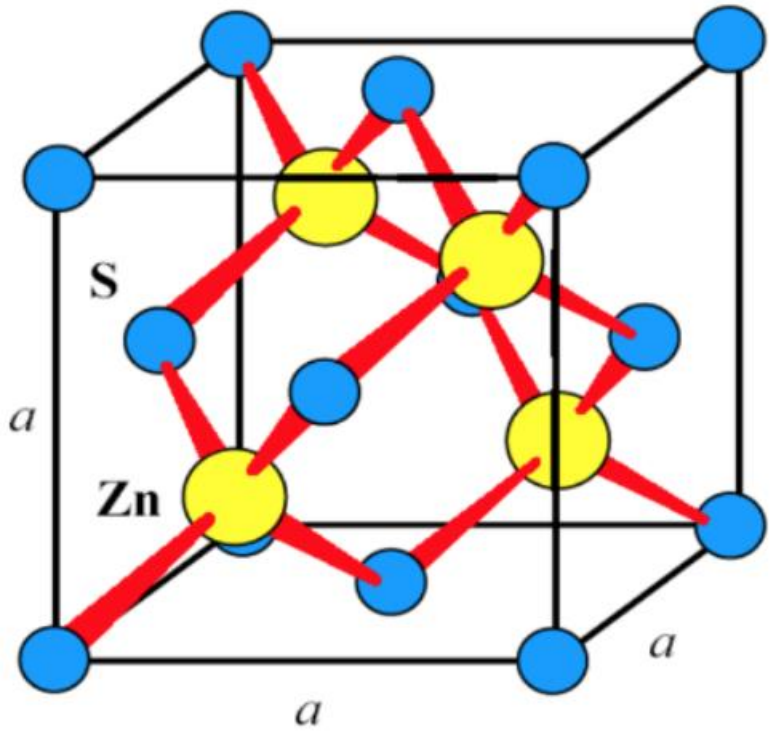
Figure 13.17

1. from webpage: https://www.coursehero.com/study-guides/cheminter/unit-cells/

   (a) What is the coordination number (number of nearest neighbors) for each of the structures above?

   (b) Calculate the atomic radius, R, in terms of the lattice parameter a_0 for the simple cubic and fcc structures above (you did this for a bcc structure in the last problem set).

(c) Gold crystallizes in a cubic close-packed structure (face-centered cubic unit cell) and has a density of 19.3 g/cm^3. Calculate the atomic radius of an Au atom in angstroms (Å). Use only these values: Avogadro's number and the molecular weight (or molar mass) of Au from the periodic table of the elements. Assume the atoms pack the unit cell as shown above for the fcc structure. How does your value compare with the actual atomic radius of gold in an fcc structure? That is, how much % larger or smaller is your value? (Go to the **WebElements** website)



2. ZnS crystallizes into what is referred to as a zincblende structure. The zincblende structure is an fcc lattice with a diatomic base with one atom at (0, 0, 0) and the other atom at (¼, ¼, ¼). The atoms are tetrahedrally coordinated, each atom having four neighboring atoms.

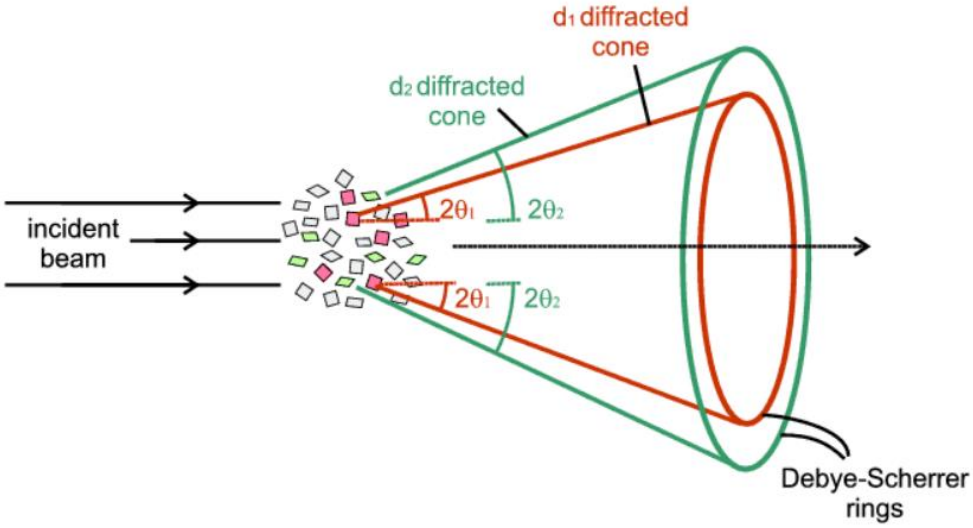
   (a) How many of each atom are contained within a unit cell of ZnS?

   (b) Many types of compounds crystallizes into the zincblende structure: BP (boron phosphide), ZnTe (zinc telluride), GaAs (gallium arsenide), MgSe (mercury selenide), to name a few. What is the difference between the diamond structure and the zincblende structure? (that is, why is the diamond crystal structure not called the zincblende structure?)

3. The edge length of the NaCl unit cell is 5.64 Å. Determine the density of NaCl in g/cm^3 using the molecular weight of Na and Cl from the periodic table of the elements and Avogadro's number. Make certain it agrees with the value given in **Wikipedia** (what is this value, and does your answer agree with it?).

4. Read through the powerpoint *X-ray Diffraction* located on Blackboard.

   (a) Write down Bragg's law with the Miller indices in mind as is done in the *X-ray Diffraction* powerpoint.



   from webpage: http://pd.chem.ucl.ac.uk/pdnn/diff2/kinemat2.htm

   (b) Why does a polycrystalline material (see figure above) give rise to Debye-Scherrer rings for diffracted x-ray beams.

   (c) The special someone in your life recently gave you diamond, however you have come to suspect that it is not a real diamond and might actually be cubic zirconia. To confirm its structure, you have performed powder XRD on the diamond using a system equipped with a Cu K_a X-ray source ($\lambda = 0.1542$ nm). The peak assignments from the diffraction pattern are as follows:

2θ (deg)	(hkl) assignment
43.99	(111)
75.41	(022)
91.64	(113)
119.74	(004)
104.95	(133)

Calculate the lattice constant of sample. Given that the lattice constant for diamond is 3.56 Å and 5.17Å for cubic zirconia, is your sample a real diamond or a fake?