

CHEM 3420: Physical Chemistry II — Spring 2009

Homework 9

Due in Class: Wednesday, April 22, 2009

1. Determine the fraction of the total cell volume occupied by atoms for the following structures:
 - (a) body-centered cubic (assume atoms touch along a body diagonal)
 - (b) primitive cubic (assume the atoms touch along the cell edge)

In each case assume that there is only one atom placed at each lattice point.

2. On a piece of ordinary graph paper draw an array of lattice points that define a square lattice.
 - (a) Connect the lattice points to define
 - i. a primitive cell
 - ii. a double cell
 - iii. a triple cell
 - (b) For the primitive cell that you have drawn:
 - i. Draw lines in the directions defined by $[12]$ and $[21]$.
 - ii. Draw the “planes” (lines, actually, in two dimensions but which are defined by indices h and k analogous to what one does in 3-D) with indices (13) and (31) .
3. Iron ($\rho = 7.86 \text{ g/cm}^3$) crystallizes in a BCC unit cell at room temperature. Calculate the radius of an iron atom in this crystal. At temperatures above 910°C iron prefers to be FCC. If we neglect the temperature dependence of the radius of the iron atom on the grounds that it is negligible, we can calculate the density of FCC iron. Use this to determine whether iron expands or contracts when it undergoes transformation from the BCC to the FCC structure.
4. Nickel has an FCC structure with a lattice parameter $a = 3.52 \text{ \AA}$. A powder sample is irradiated with Cu K_α radiation ($\lambda_{\text{Cu K}_\alpha} = 1.5418 \text{ \AA}$). At what angles (2θ) would you find the diffracted beams from the (111) , (220) , and (400) planes.