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CHEM 3420: Physical Chemistry II — Spring 2009

Homework 9 — Model Solutions

1. (a) There are 2 atoms per unit cell in BCC, so the fraction of space that is occupied by atoms is:

$$fraction = \frac{2 * \frac{4}{3}\pi r^3}{a^3}$$

where r is the atomic radius and a is the lattice constant. For BCC, the radius and lattice constant are related:

$$4r = \sqrt{3}a$$

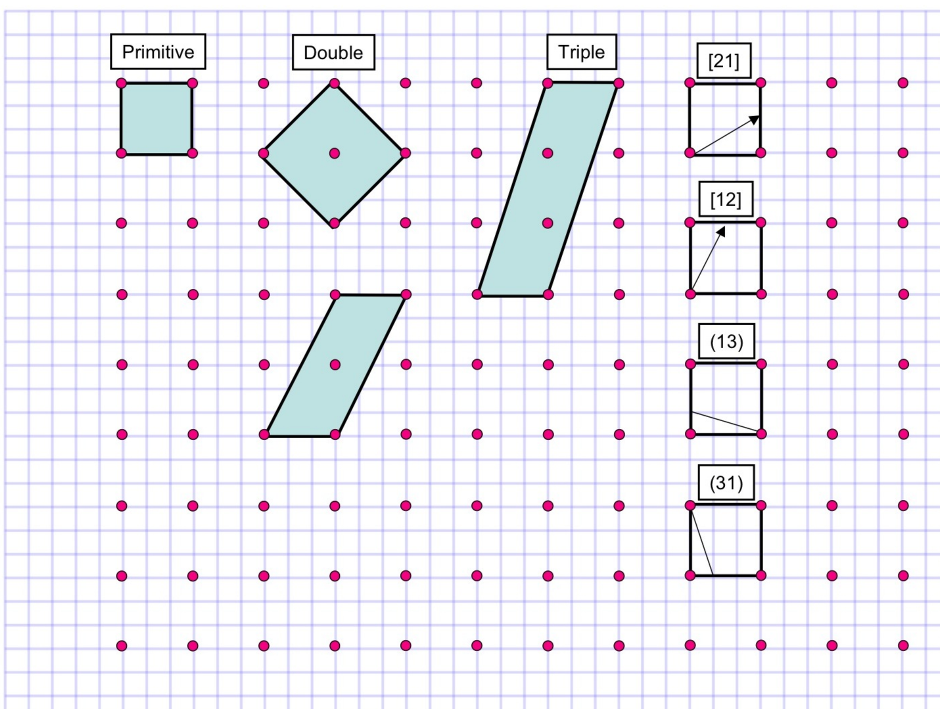
So:

$$fraction = \frac{2 * \frac{4}{3}\pi}{\left(\frac{4}{\sqrt{3}}\right)^3} = 0.680$$

(b) For primitive cubic, there is one atom per unit cell and $2r = a$.

$$fraction = \frac{\frac{4}{3}\pi r^3}{a^3} = \frac{\frac{4}{3}\pi r^3}{2^3 r^3} = 0.524$$

2. The figure below has the unit cells, directions, and planes asked for in problem 1.



3. The important pieces of information needed to solve this problem are the density (given), the volume of the unit cell (a^3), and the number of atoms per unit cell in BCC iron (2 per cell).

$$\frac{2}{a^3} = \frac{N_a}{V_{molar}}$$

where a is the lattice constant of BCC iron, N_a is Avagadro's number, and V_{molar} is the molar volume which can be found by using the density and molecular weight of iron:

$$V_{molar} = \frac{MW_{Fe}}{\rho} = \frac{55.85\ g/mol}{7.86\ g/cm^3} = 7.11\ cm^3/mol$$

So, making sure we use consistent units:

$$\frac{2}{a^3} = \frac{6.02 \times 10^{23}\ atoms/mol}{7.11\ cm^3/g}$$

$$a = 2.87 \times 10^{-8}\ cm$$

Remebering that the atoms in BCC are in contact along the body diagonal, or the ¡111¿ directions:

$$4r = \sqrt{3}a$$

$$\boxed{r_{Fe} = 1.24 \times 10^{-8}\ \text{cm} = 1.24\ \text{Å}}$$

Now to find the density of FCC iron we can work backwards using the value of the radius calculated previously. It is important to remember in the FCC structure, the atoms are in contact along the ¡110¿ directions, yielding the following relationship between a and r:

$$4r = \sqrt{2}a$$

$$a = 2\sqrt{2}r$$

So the density can be written as:

$$\rho_{FCC} = \frac{4MW_{Fe}}{N_a a^3} = \frac{4MW_{Fe}}{N_a(2\sqrt{2}r)^3} = \frac{4 * 55.85}{6.02 \times 10^{23}(2\sqrt{2} * 1.24 \times 10^{-8}\ cm)^3}$$

$$\boxed{\rho_{FCC} = 8.60\ \text{g/cm}^3}$$

FCC iron is more closely packed than BCC suggesting that iron contracts upon changing from BCC to FCC. This is consistent with how efficiently the atoms are packed in each structure. FCC is close packed, meaning 74% of the volume is filled with atoms (or it is 74% dense) while BCC is packed less efficiently with only 68% of the volume being filled. The ratio of the two densities calculated here are the same as the ratio of packing efficiency.

4. This problem is geared to get you comfortable with using Bragg's Law. We need to find the spacing between planes (d_{hkl}) in order to use Bragg's Law. For a cubic crystal we can write:

$$d_{hkl}^2 = \frac{a^2}{h^2 + k^2 + l^2}$$

Rearranging Bragg's Law and using $\lambda_{Cu_{K_\alpha}} = 1.5418$ Å:

$$\sin\theta = \frac{\lambda}{2d}$$

$$2\theta = 2\sin^{-1}\left(\frac{\lambda\sqrt{h^2 + k^2 + l^2}}{2a}\right)$$

Plane	2θ
(111)	44.6
(220)	76.4
(400)	122.3