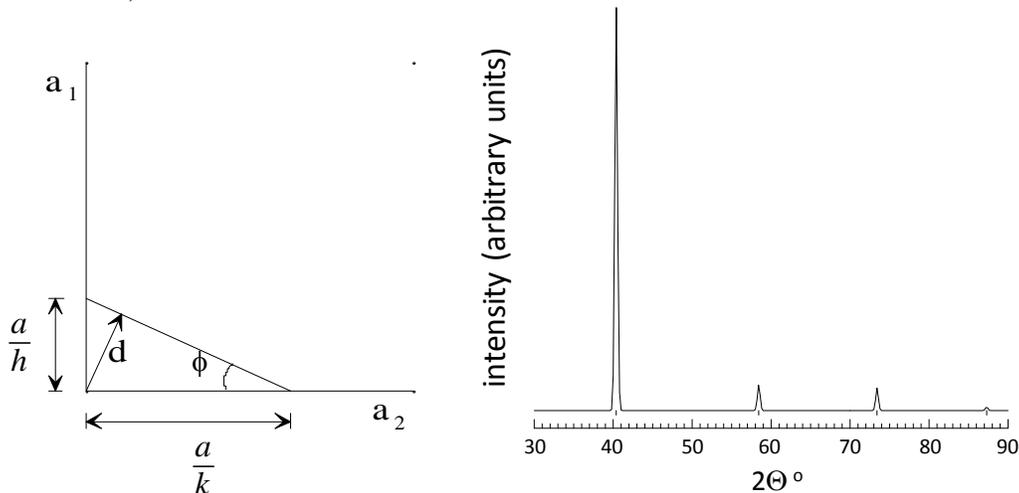


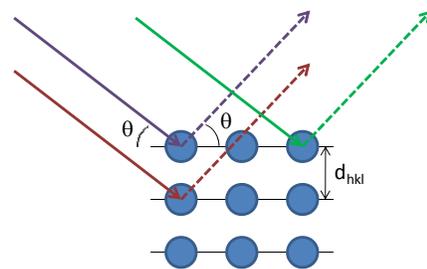
MS 115a, Problem Set #4

assigned 10/24/12
due 10/31/12

1. What are the planes of highest density in the CCP, HCP and BCC structures? What are the directions of highest density within those planes?
2. Using the left-side diagram below, show that for a 2-dimensional square lattice, the distance, d_{hk} , between planes of index (h, k) is given by $d_{hk} = a/(h^2 + k^2)^{1/2}$.
3. The right-side figure below shows the first four peaks of the x-ray diffraction pattern for tungsten, which has a loose-packed BCC crystal structure. The data were collected using monochromatic x-radiation having a wavelength of 1.542 Å.
 - (a) Index (*i.e.* give $h, k,$ and l indices for) each of these peaks
 - (d) Determine the interplanar spacing, d_{hkl} , for each of the peaks
 - (c) Determine the lattice constant of BCC tungsten.
 - (d) From (c), determine the atomic radius of W. Compare that to the actual value (use your reference of choice, but make sure you reference the **atomic** radius rather than the ionic radius).



4. In lecture we derived Bragg's law by considering the path-length difference between x-rays scattered from atoms on different diffraction planes. Specifically, we considered the path-length difference between the purple and brown waves in the drawing to the right. What is the path-length difference between the purple and the green waves? What is it between the red and the green waves?



5. An X-ray powder diffraction experiment is performed on sodium chloride, which has lattice constant 5.644 Å, using X-radiation with wavelength 1.541 Å. Specify the structure type and lattice type of sodium chloride. Calculate the 2θ peak positions of the first 5 diffraction peaks. Give the miller indices of the planes that correspond to these peaks.

6. Calculate the equilibrium concentration (#/#) and equilibrium number (#/volume) of vacancies in iron at 800°C. The activation energy for vacancy formation is 1.08 eV/atom, the density at 800°C is 7.75 g/cm³, and the atomic weight is 55.85 g/mol.
7. What is the composition, in atom percent, of an alloy that consists of 25 wt% Zn and 75 wt% Cu?
8. Carbon is added to iron to form steel. The BCC form of iron (known as ferrite, or the α form) is stable from room temperature to 912°C. At higher temperatures, it transforms to a CCP form (known as austenite, or the γ form), and this form can also exist at 900°C. Which form of iron (at 900°C) do you anticipate is capable of dissolving more carbon? Why? Hints: in CCP iron carbon sits at $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, whereas in BCC iron it sits at $0, \frac{1}{2}, \frac{1}{4}$. Compute the radius of the atom that will just fit into these sites.
9. The diffusion coefficient of C in the two forms of iron are characterized as
- | phase | D_0 (m ² /s) | ΔH (eV/atom) |
|---------------|---------------------------|----------------------|
| α -BCC | 6.2×10^{-7} | 0.83 |
| γ -FCC | 2.3×10^{-5} | 1.53 |
- Compute the diffusion coefficient for both phases at 900°C and rationalize the difference in the values in terms of the crystal structures (see problem 8).
10. (a) Suppose Li₂O is added as an impurity to CaO. If the Li⁺ substitutes for Ca²⁺, what kind of vacancies would you expect to form? How many of these vacancies are created for every Li⁺ added. (b) Suppose CaCl₂ is added as an impurity to CaO. If the Cl⁻ substitutes for O²⁻, what kind of vacancies would you expect to form? How many of the vacancies are created for every Cl⁻ added?
11. Hydrogen can be purified from a mixed gas composition by placing the mixed gas next to a foil of Pd, which will allow only the hydrogen to diffuse through it. Compute the hydrogen mass flux (mass/time*area) that passes through a 6 mm thick sheet of Pd at 500°C if the hydrogen concentrations on the two sides of the membrane are 2.7 and 0.4 kg/m³. The hydrogen diffusion coefficient through Pd is 1.0×10^{-8} m²/s at this temperature.
12. Show that $C(x) = \frac{B}{\sqrt{Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$, where B is a constant, is a solution to Fick's second law.
13. The self-diffusion coefficient for cerium in cerium dioxide is given at two temperatures
- | T (K) | D (m ² /s) |
|---------|-------------------------|
| 1273 | 9.8×10^{-17} |
| 1473 | 2.1×10^{-15} |
- (a) Determine the values of the pre-exponential term, D_0 , and the activation enthalpy, ΔH (also given the symbol Q) for self-diffusion.
- (b) Determine the magnitude of the self-diffusion coefficient at 1100°C.