

MS 115a, Problem Set #3

assigned 10/17/07

due 10/24/07

1. When considering the location of impurity atoms in metals we note that the radius of the impurity atom must be smaller than that afforded by the interstitial site. When considering the location of cations in ionic compounds in which anions are in a close-packed array, we note that the cation must be larger than that afforded by the interstitial site. Explain why we treat these two situations differently.

2. The compounds ZrO_2 (zirconia) and CeO_2 (ceria) can take on the ideal fluorite structure. Calculate the expected coordination numbers for Zr and Ce (based on the radius ratios) and compare it with that for the cation in the ideal fluorite structure. Which of these two compounds is more stable in the ideal fluorite structure?

$$R(\text{O}^{2-}) = 1.38 \text{ \AA} \quad R(\text{Zr}^{4+}) = 0.84 \text{ \AA} \quad R(\text{Ce}^{4+}) = 1.14 \text{ \AA}$$

3. In fact, ZrO_2 exists in three forms. At very high temperatures (2400-2700°C) it is cubic with the fluorite structure and lattice constant 5.09 Å.

At slightly lower temperatures (1240-2400°C) the structure becomes slightly distorted, and takes on a tetragonal lattice. The a and c lattice constants are 5.15 and 5.27 Å, respectively.

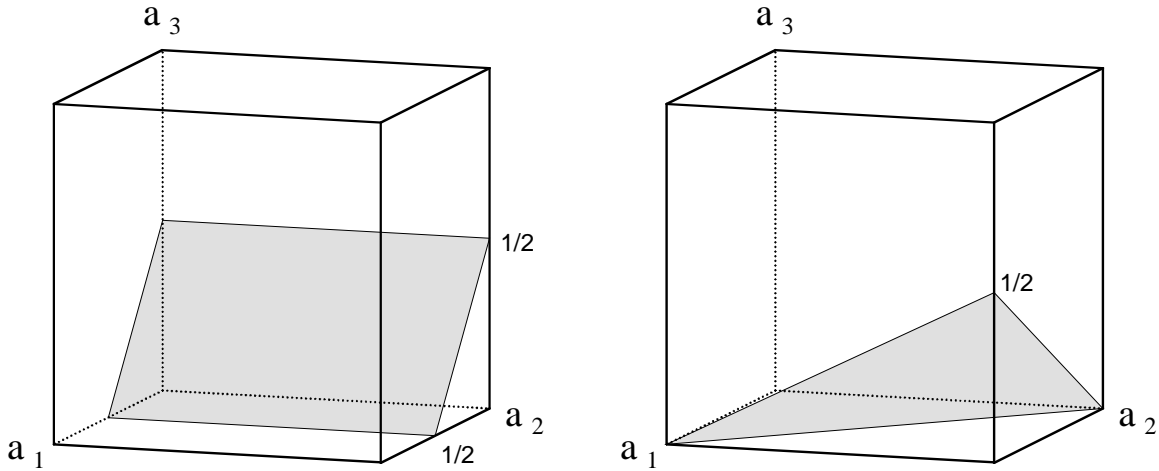
At even lower temperatures (room temperature-1240°C) the structure becomes distorted further, and takes on a monoclinic lattice.

With the exception of these slight distortions, the structure in the tetragonal and monoclinic forms are essentially the same as in the cubic form.

What is the fractional change in volume, $\Delta V/V_{\text{cubic}}$, upon transforming from the cubic to the tetragonal structure? Is this the type of volume change you would expect for a material that is being cooled?

4. Draw a two-dimensional square lattice with lattice constant a_0 . Show on this drawing the vector extending from 2,6 to -1,4. Give the indices for the direction of (a) this specific vector and (b) those of each member in the family of equivalent directions.
5. Draw a two-dimensional hexagonal lattice with lattice constant a_0 . Show on this drawing the vector extending from 1,1 to 2,3. Give the indices for the direction of (a) this specific vector and (b) those of each member in the family of equivalent directions.
6. Sketch the $(1\bar{1}01)$ and $(11\bar{2}0)$ planes in a hexagonal unit cell.

7. Determine the Miller indices for the planes shown in the unit cell shown below. Does the answer depend on the crystal system of the unit cell?



the plane in the right-side image leans forward.

8. 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 $d_{hk} = a/(h^2 + k^2)^{1/2}$
9. The right-side figure below shows the first four peaks of the x-ray diffraction pattern for copper, which has a CCP crystal structure. The data were collected using monochromatic x-radiation having a wavelength of 1.542 \AA .

(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 CCP copper.

(d) From (c), determine the atomic radius of Cu. Compare that to the actual value (use your reference of choice, but make sure you reference the **atomic** radius rather than the ionic radius).

