

MS 115a, Problem Set #3

assigned 10/17/12

due 10/24/12

1. The ceramic compound SrTiO_3 adopts the ideal perovskite structure and has a lattice constant of 3.905 \AA . Compute its density.
2. The compounds NaTaO_3 and SrRuO_3 also adopt the perovskite structure. Based on the ionic radii, predict whether these will be ideal cubic structures or will be distorted. Use the following ionic radii appropriate for the coordination environments:

$$R(\text{O}^{2-}) = 1.38 \text{ \AA}; R(\text{Na}^{1+}) = 1.39 \text{ \AA}; R(\text{Ta}^{5+}) = 0.72 \text{ \AA}; R(\text{Sr}^{2+}) = 1.44 \text{ \AA}; R(\text{Ru}^{4+}) = 0.62 \text{ \AA}$$

3. The compounds ZrO_2 (zirconia) and CaF_2 (the mineral fluorite) can take on the ideal fluorite structure. Calculate the expected coordination numbers for Zr and Ca (based on the cation:anion radius ratios) and compare the results with the actual coordination number for a cation in the ideal fluorite structure. Which of these two compounds is more stable in the ideal fluorite structure?

$$R(\text{O}^{2-}) = 1.38 \text{ \AA} \quad R(\text{Zr}^{4+}) = 0.84 \text{ \AA} \quad R(\text{F}^{1-}) = 1.31 \text{ \AA} \quad R(\text{Ca}^{2+}) = 1.12 \text{ \AA}$$

4. In fact, ZrO_2 exists in three forms. At very high temperatures ($2400\text{-}2700^\circ\text{C}$) it is cubic with the fluorite structure and lattice constant 5.09 \AA .

At slightly lower temperatures ($1240\text{-}2400^\circ\text{C}$) the structure becomes slightly distorted, and takes on a tetragonal lattice. The a and c lattice constants are 5.15 and 5.27 \AA , respectively.

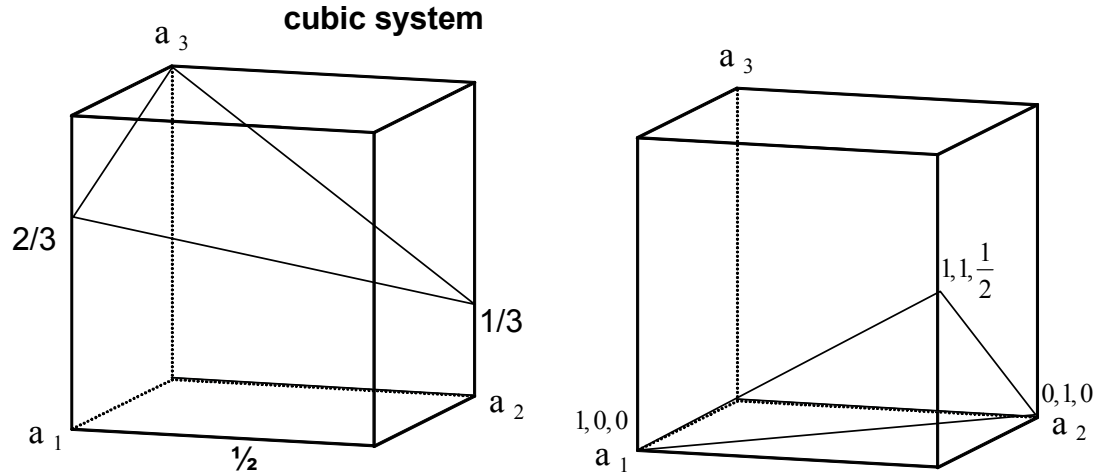
At even lower temperatures (room temperature- 1240°C) the structure becomes distorted further, and takes on a monoclinic lattice.

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?

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

8. 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?



Selected z-coordinates (fractional) are indicated in the left-side cell. The plane in the right-side image leans forward and (fractional) coordinates indicate where the plane intercepts the depicted unit cell.

9. A sample of polyvinyl chloride has the following distribution of molecular weights, as recorded in terms of number fraction and weight fraction.

Molecular weight range (g/mol)	x_i (number fraction)	w_i (weight fraction)
5,000-10,000	0.05	0.02
10,000-15,000	0.16	0.10
15,000-20,000	0.22	0.18
20,000-25,000	0.27	0.29
25,000-30,000	0.20	0.26
30,000-35,000	0.08	0.13
35,000-40,000	0.02	0.02

Based on these data, compute:

- (a) the number-average molecular weight; (b) the number-average degree of polymerization; and (c) the weight-average molecular weight.
- (d) plot the molecular weight distribution in terms of number fraction and indicate on this plot the position of the number-average and weight-average molecular weights.
10. The density of crystals of polyethylene is 998 kg m^{-3} , and the orthorhombic unit cell has dimensions $a = 0.741$, $b = 0.494$, and $c = 0.255 \text{ nm}$. (a) How many CH_2 units are there in a unit cell? (b) How many 'mer' ($\text{CH}_2\text{-CH}_2$) units are there?
11. The density of amorphous polyethylene is 810 kg m^{-3} . Estimate the crystallinity of low-density polyethylene (920 kg m^{-3}), of medium density polyethylene (933 kg m^{-3}), and of high-density polyethylene (950 kg m^{-3}). State your assumptions.