Week 02

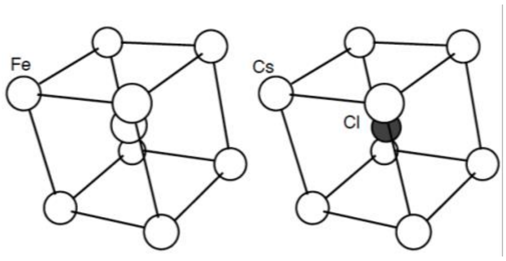
Crystallography
Lattice&Motif, interstitial sites,
Metal and Ionic crystals

Exercise 1 : Answer these questions by true or false

	True	False
1. All crystalline materials are single crystals.		
2. The structure of Ionic crystals depends on the relative size of the ions only for 1 anion - 1 cation systems.		
3. A motif represents the chemical nature of a material.		
4. Crystals have the same properties along all crystal directions.		
5.In the cubic structure, the volume of the primitive cell is equal to the volume of the conventional cell divided by the number of motifs in the conventional cell.		

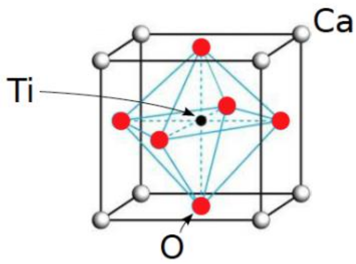
Exercise 2 : Motifs and Bravais lattices

2a. Find the crystal structure (primitive cubic, bcc, fcc) and the motifs of the following materials:



2b. Consider the material to the right. What is its crystal structure?

2c. By counting the number of each kind of atom in the cell. Can you find the chemical formula of this material ? Circle the motif.



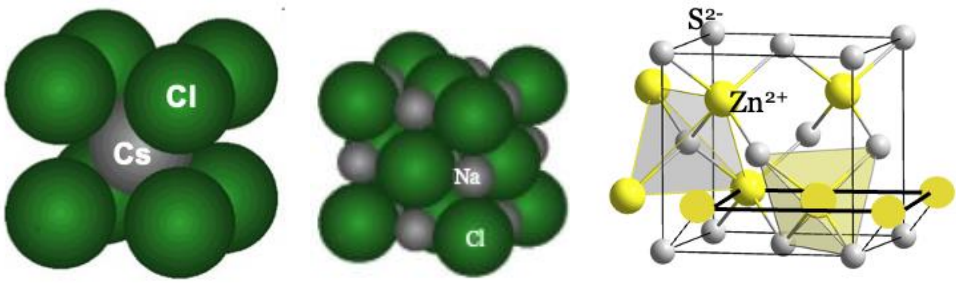
Exercise 3: Interstitial sites in Iron

3a. Using the schematics of the interstitial sites of the FCC and BCC structures shown in class, compare the size of the FCC interstitial site at the center of the cube, and the size of the BCC interstitial site at the center of a face of the cube.

Hint: we assume that the radius of the Fe atom is the same in the BCC and FCC structure, only the cube edge will change.

3b. Can you deduct why Carbon is more soluble in the Austenite (FCC) structure of Iron as visible in the phase diagram of Fe and C shown in class, despite the fact that the FCC structure has a higher density than the BCC (Ferrite) structure ?

Exercise 4: Ionic Crystal



NaCl

4a. Using geometrical considerations, derive the critical ratio of the radius cation/anion for the crystal structure shown above: CsCl, NaCl and ZnS. The critical radius occurs when the cations just fit into the space left by the anions so that the anions and cations just touch each other.

Show that the critical ratios correspond to $\sqrt{3}$-1, $\sqrt{2}$-1, $\sqrt{6}$/2-1

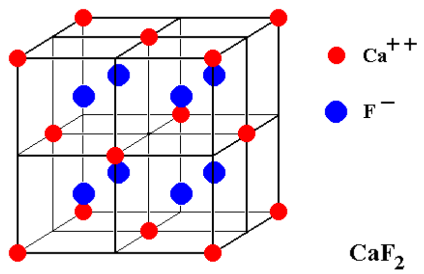
4b. Verify that the rule $\rho = \sqrt{\frac{12}{12-CN}} - 1$ is fullfilled for the case of NaCl

4c. Show that the packing factor $p(\rho)$ for an ionic crystal with the CsCl structure as shown in class is given by $p(\rho) = \frac{\sqrt{3}\pi}{2}\left(\frac{1+\rho^3}{(1+\rho)^3}\right)$,

where ρ is the ratio of the cation to anion radius, $\rho = \frac{r_{Cs}}{r_{Cl}}$.

Hint: here we consider the stable structure, rather than the stability limit, the presence of Cs separates the Cl atoms, so they touch on the diagonal, but not anymore along the cube edge.

4d. We look at the ionic crystal CaF_2 as shown below



i) Consider the structure first as a fcc structure of Ca^{2+}. In which interstitial sites are the F^- located?

ii) What is the coordination of a Ca cation and what is the coordination of the F anion?

iii) Considering radius ratio, what is the geometry of the interstital sites you expect considering an ionic radius of the Ca anion is 1.17 Å and that of the F anion is 1.26 Å. Discuss the result