Week 01

Introduction – The hard sphere model

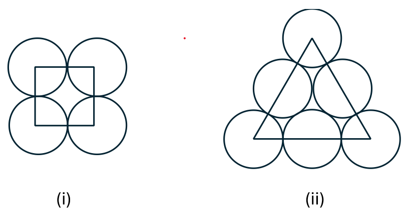
Exercise 1 :

Answer these questions by true or false:

	True	False
1. Materials in nature are always in a crystalline state.		
2. Metals tend to crystallize into dense structures.		
3. The packing parameter depends on the nature of the crystal structure, and not on the nature of the material.		

Exercise 2 : 2D packing parameters

We consider the following 2D figures where circles of radius R are placed at the corners of a square of edge length a in configuration (i), and the vertices (or corners) of an equilateral triangle of edge length b in configuration (ii).



2a. Find a relationship between a and b.

2b. In configurations (i):

(1) what is the total surface area $S_{cirlces}$ of the square covered by the circles, as a function of a ?

(2) Deduce the 2D packing density.

2c. In configurations (ii):

(1) what is the total surface area $S_{cirlces}$ of the triangle covered by the circles, as a function of a ?

(2) Deduce the 2D packing density.

Exercise 3 : From the FCC to the Diamond structure

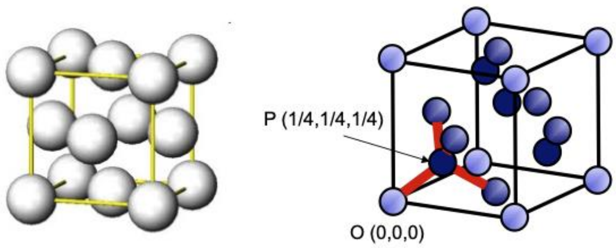
The face-centered cubic (FCC) structure, in the case of 1 atom per motif, has atoms that sits at the corner of a cube and at the center of its faces (see figure below). We consider the hard sphere model where atoms are represented by spheres of radius R. The edge of the cube has a length a.

3a. Knowing that the spheres are in contact along the diagonals of the cube's faces, show that the relationship between a and R is given by: $a\sqrt{2} = 4R$

3b. Deduce the volume of one sphere as a function of a.

3c. How much volume of spheres can we count inside the cube ?

3d. Deduce the packing factor of the FCC structure. Does it depend on a?



FCC structure Diamond structure

The diamond structure shown above consists of tetrahedra of carbon atoms arranged in space to form the crystal. This arrangement turns out to be represented by a motif of two carbon atoms translated in the face-centered cubic structure. In the motif, one atom has its center at one corner of the cube that could be an origin O (0,0,0), and the other one is shifted along the diagonal at position (¼, ¼, ¼). The two spheres representing the two atoms are in contact with each other (to the contrary of what is shown on the schematic for clarity).

3e.

(1) Show that the length of the diagonal of a cube of edge length a is $a\sqrt{3}$.

(2) What is the number of closest neighbors ?

(3) Deduce the relation between R and a in this case.

3f. How much volume of spheres can we count inside the cube for the Diamond structure?

3g. Deduce the packing fraction of the Diamond structure.

3h. Why is it so much smaller than the packing fraction of the FCC structure ?