

9. Homework “Unit cell, Wigner-Seitz unit cell”

1. What is the difference between a crystallographic unit cell and a Wigner-Seitz unit cell? Is the Wigner-Seitz unit cell depends on the choice of basis vectors? Please draw the Wigner-Seitz unit cell of the lattice, which have the following lattice constants:

- a) $a=1, b=2, \alpha =70^\circ$
- b) $a=1, b=1, \alpha =60^\circ$
- c) $a=1, b=2, \alpha =115^\circ$

2. The 2D crystal structure has a 3-fold axis. Define type of Bravais lattice for this crystal. The atomic layers in a unit cell by mean of the vectors $A=[x,y]$ described:

- a) $[x,y]=[0.2,0.1]$
- b) $[x,y]=[1/3,2/3]$
- c) $[x,y]=[1/3,1/7]$
- d) $[x,y]=[0.3,0.7]$

Find all the positions of symmetry equivalent atoms in the crystallographic unit cell.

3. The structure of a 2D crystal can be describes by a centred rectangular crystal system. This structure has a mirror plane m , which is parallel to the crystallographic b -axis ($[-x,y]$ transformation). The atomic positions are given by the following vectors $A=[x,y]$:

- a) $[x,y]=[0.2,0.1];$
- b) $[x,y]=[0,0];$
- c) $[x,y]=[0.25,0.25];$
- d) $[x,y]=[0.3,0.7];$

Find the positions of all symmetry-equivalent atoms in the crystallographic unit cell (the unit cell is not primitive).

4. The NaCl crystal structure has an FCC crystal lattice. The symmetry independent atoms Na and Cl have positions $[0,0,0]$ (for Na-atom Nr. 1) and

[1/2,1/2,1/2] (Cl-atom Nr. 14). Find the positions of all other atoms in the non-primitive unit cell. Find the coordinates of the atoms, which are shown in Fig. 1.

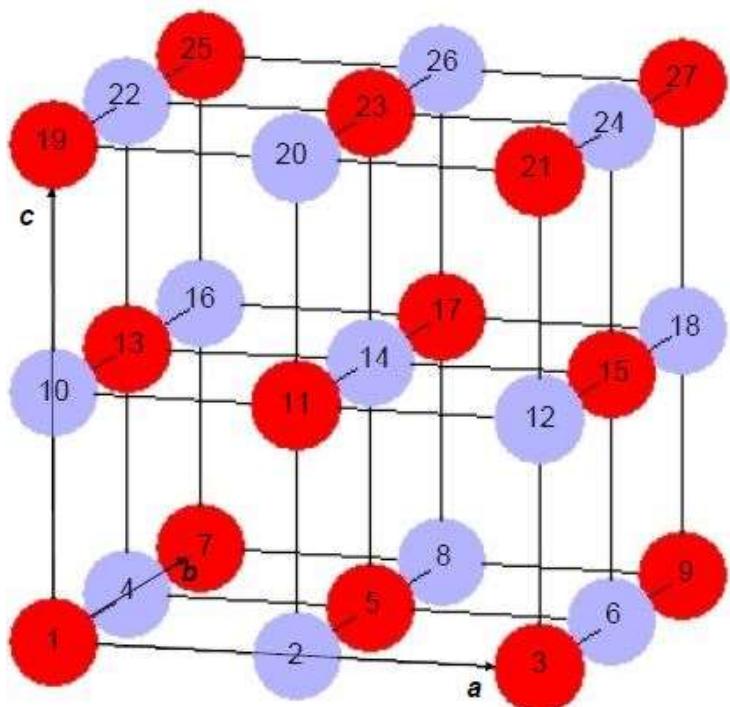


Figure 1. The structure of NaCl crystal