UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

Crystallography (*winter term 2015/2016*)

Lecturer: **Dr Semën Gorfman (**ENC B-011)

Exercise tutor: **Hyeokmin Choe** **(**ENC B-015)

Exercise sheet 1: Operation with vectors, crystal lattice, unit cell (16 points)

1. Exercise on operations with vectors in crystallography (5 points).

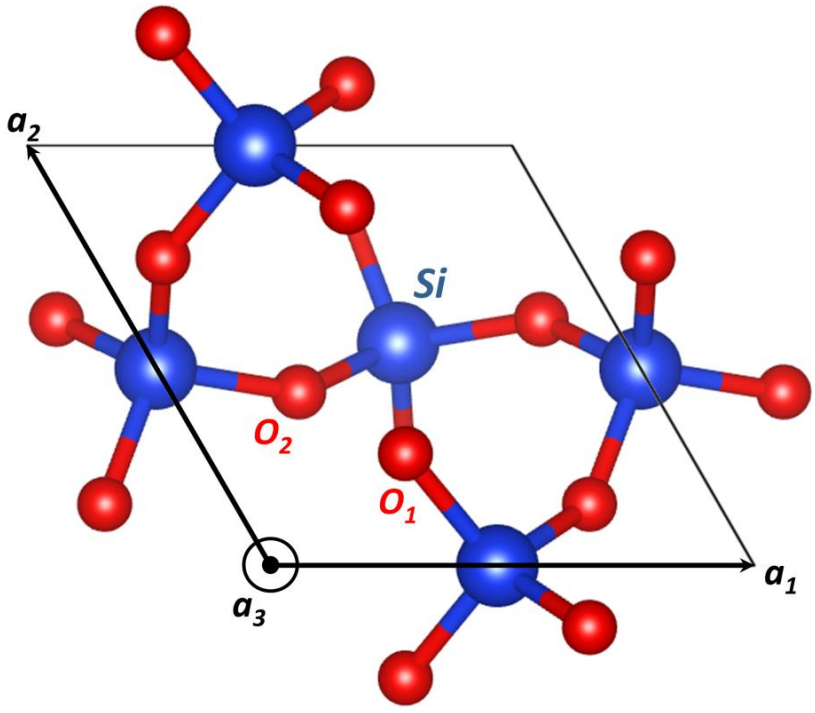
The structure of α-quartz (SiO_2) has the following lattice parameters:

a = b = 4.9 Å, c = 5.405 Å, α = β = 90°, γ = 120°. The positions of three atoms in the unit cell are given:

Si : [0.53 0.53 0.33]

O_1 : [0.41 0.27 0.12]

O_2 : [0.27 0.41 0.54]



Calculate the bond distances Si – O_1, Si – O_2 and bond angles O_1 – Si – O_2 by implementing the operation of dot product between vectors. Use the expressions for the dot product $\boldsymbol{A} \cdot \boldsymbol{B} = A_i B_j G_{ij}$ and the metric tensor $G_{ij} = \boldsymbol{a}_i \cdot \boldsymbol{a}_j$.

2. Exercise on visualizing crystal structures (4 points).

The lattice parameters of *GaAs (zinc blende structure)* crystal are: a = b = c=5.65 Å, $\alpha = \beta = \gamma = 90$ °. The unit cell is composed of 8 atoms, whose fractional positions are:

Ga [0 0 0] Ga [0 1/2 1/2] Ga [1/2 0 1/2] Ga [1/2 1/2 0]

As [1/4 1/4 1/4] As [1/4 3/4 3/4] As [3/4 1/4 3/4] As [3/4 3/4 1/4].

Find the position of all atoms inside a parallelepiped, containing two unit cells in each of $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$ direction (4 crystallographic unit cells in total) and 1 unit cell in $\boldsymbol{a}_3$ direction. Plot the resulting structure in projection along one of the crystallographic $\boldsymbol{a_3}$ axis.

3. Mass density of crystals from the structural data (2 points).

Calculate the mass density ([g/cm^3]) of GaAs material (the structure is described in the task 2).

4*. Geometrical properties of crystal lattice (6 points).

Find the coordinates of the points inside the hexagonal crystallographic unit cell (a =b, α=120°) that are most remote from a lattice point.

Please return on 02/11/2015