Solid state physics (*winter term 2015/2016*)

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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 quartz has the following lattice constants:

a = b = 4.9, c = 5.405 Å, α = β = 90°, γ = 120 °.

The positions of three atoms in the unit cell are given:

Si: [0.45, 0, 0.5]

O_1: [0.41, 0.26, 0.41]

O_2: [0.73, 0.14, 0.71]

Calculate the bond distances Si – O_1, Si – O_2 (in Å) and bond angles O_1 – Si – O_2 (in degrees), by using operation of dot product in crystallographic coordinate system.

2. Exercise on visualizing crystal structures (4 points)

The <u>lattice constants</u> of *GaAs* crystal are:

a = b = c = 5.65 Å, α = β = γ = 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]

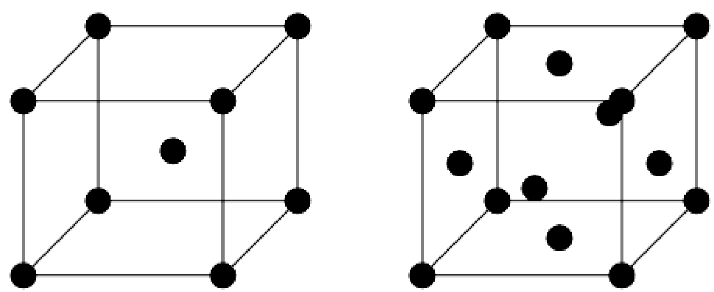
As [1/4, 1/4, 1/4], As [1/4 3/4 3/4], As [3/4 1/4 3/4], As [3/4 3/4 1/4].

1. Find the position of atoms inside a parallelepiped, containing 2 unit cells in each direction (8 crystallographic unit cells in total).

2. Plot the resulting structure in projection along one of the crystallographic axis (**a**, **b** or **c**).

3. FCC and BCC structures of iron (4 points)

Fe crystallizes in two phases, face-centred cubic (FCC) and Body-centred cubic (BCC) phase.



bcc fcc

1. Calculate the packing density of both phases. Atoms can be approximates by a hard sphere shape with constant radius.
2. Indicate the closest distance between two neighbour atoms in the FCC and BCC structure.
3. Calculate the packing density defined as the ratio:

$$P = Number^{sphere}\frac{Volume^{sphere}}{Volume^{unit\ cell}}$$

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

Calculate the <u>mass density ([g/cm^3])</u> of GaAs material (structure is described in the task 1), diamond and graphite.

Please return on 28/10/2015