UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

Crystallography (*winter term 2015/2016*)

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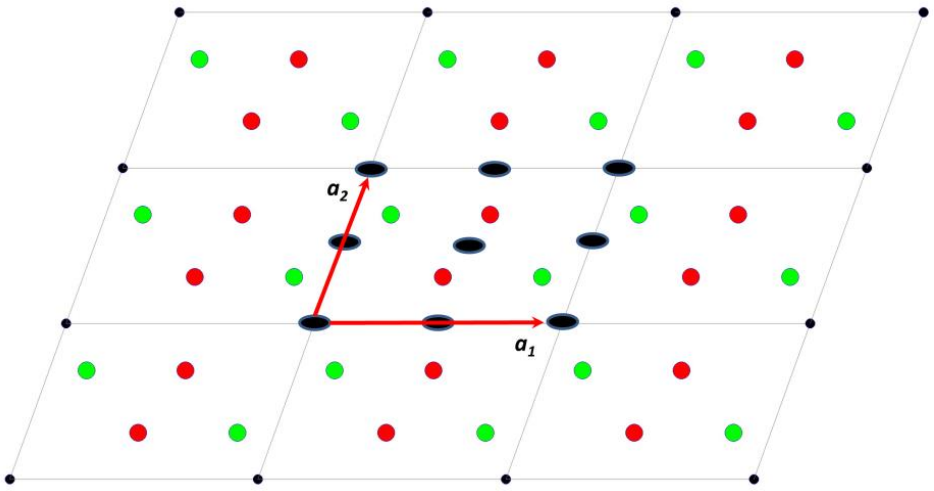
Exercise sheet 8: Space groups and structure types.

1. Non-centred symmetry operations (5 points)

The structure of a 2D crystal has 2-fold symmetry. The two fold symmetry axes intersect the following points in the unit cell a) [1/2 0]; b) [0 1/2]; c) [1/2 1/2]. Express the corresponding symmetry operations, using the matrix and the 'x,y' format. Explain why these symmetry operations can be reduced to the combination of a) lattice translation and b) 2-fold axis intersecting the point [0 0].



Hint: Draw the basis vectors of the new coordinate system by 'rotating' the basis vectors of old coordinate system around the corresponding axis. Find the rotation matrix / displacement vector and convert them to the 'x, y' format.

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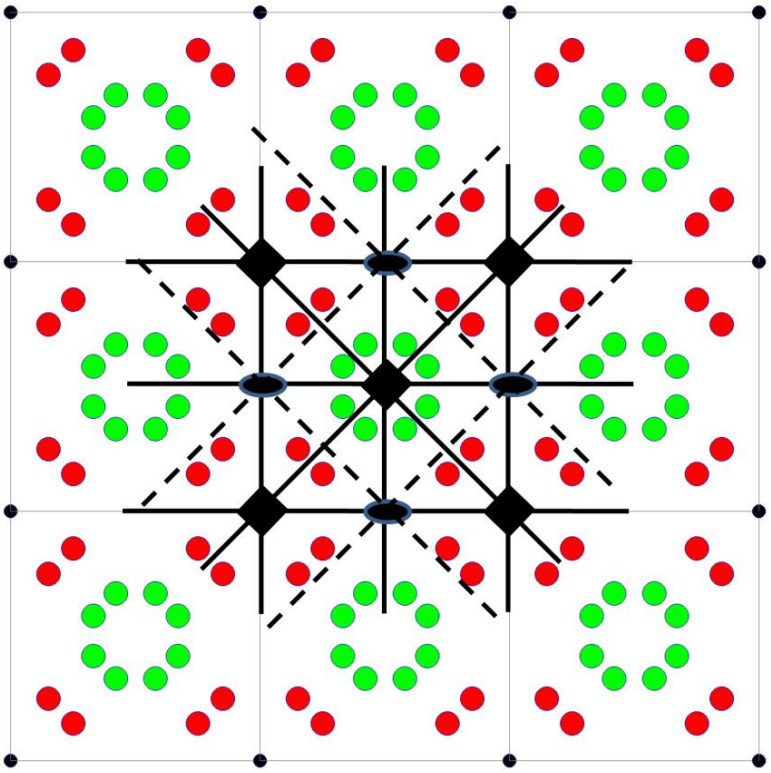
2. Non-centred symmetry operations (5 points)

The structure belongs to the planar space group *p4mm*. Show that the combination of the symmetry operations (see the lectures) with the lattice translation produces the following symmetry elements

a) 4-fold axis intersecting the point [1/2 1/2]

b) Glide plane passing through the points [1/2 0] and [0 1/2]



3. Wyckoff positions (4 points)

A crystal belongs to the space group a) $P222_1$ b) *Cm* c) *Amm2* d) $I\bar{4}2d$

Use Bilbao Crystallographic Server (http://www.cryst.ehu.es/) to calculate the crystallographic orbit (single unit cell) corresponding to the position [0.3 0.5 0.4].

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4. Structure types (5 points)

The $ZnSiP_2$ crystal (chalcopyrite structure type) belongs to the tetragonal space group $I\bar{4}2d$. Symmetry independent atoms in the unit cell are

Zn: [0 0 0] Si : [0 0 1/2] P : [1/4 1/4 1/8]

Which Wyckoff positions do they belong to? Give the total number of atoms in the crystallographic unit cell and calculate their positions. Draw the structure, using VESTA program and explain the coordination of Zn, Si and P atoms. The lattice parameters are a = 5.399 Å, c=10.435 Å.

5. Perovskite (5 points)

Perovskite structure type is adopted by the wide range of materials. Their general chemical formula is ABX_3 (e.g. $CaCO_3$, $SrTiO_3$, $BaTiO_3$, $PbZrO_3$). The structure of a cubic perovskite belong to the space group $Pm\bar{3}m$. The lattice parameter a=4 Å. The positions of symmetry independent atoms are

A: [0 0 0] B: [1/2 1/2 1/2] X: [1/2 1/2 0]

What is the total number of atoms in the unit cell? Draw the structure, using VESTA program, explain the coordination of each atoms: how many next nearest neighbours does each atoms have?

Please return on 18.01.2016