Crystallography (*winter term 2015/2016*)

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Exercise sheet 7: Unit cell, space symmetry operations

General remark 1: Space symmetry operation combines a point symmetry operation (rotation, reflection, inversion) and a displacement. It is mathematically expressed by a) transformation matrix, $\boldsymbol{S}$ and b) displacement vector, $\boldsymbol{d}$. **One typical space symmetry operation is a crystal lattice.** N elements in a space symmetry group mean that there are N symmetry equivalent basis sets $\left\{\boldsymbol{a}_i^{(1)}, \boldsymbol{d}^{(1)} = \boldsymbol{0}\right\}$, $\left\{\boldsymbol{a}_i^{(2)}, \boldsymbol{d}^{(2)}\right\}$, ..., $\left\{\boldsymbol{a}_i^{(N)}, \boldsymbol{d}^{(N)}\right\}$, each one is described by the transformation matrix (axes orientation) and displacement vector (origin). The columns of $\boldsymbol{S}^{(n)}$ represent the coordinates of the vectors $\boldsymbol{a}_i^{(n)}$ relative to $\boldsymbol{a}_i^{(1)}$. The column $\boldsymbol{d}^{(n)}$ represents the origin of the corresponding coordinate system $\boldsymbol{a}_i^{(n)}$. The transformation of the coordinates from the coordinate system $\boldsymbol{a}_i^{(n)}$ to the coordinate system $\boldsymbol{a}_i^{(1)}$ must go via:

$$\begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix} \begin{pmatrix} x_1^{(n)} \\ x_2^{(n)} \\ x_3^{(n)} \end{pmatrix} + \begin{pmatrix} d_1^{(n)} \\ d_2^{(n)} \\ d_3^{(n)} \end{pmatrix} \qquad (1)$$

General remark 2: This symmetry operation (transformation matrices and displacement vectors) are typically presented in the CIF-files (Crystallographic Information file) using more 'text-friendly' format: x,y,z -x, -y, z, etc.

Tasks:

1. Combination of space symmetry operations through matrices (3 points)

Using matrices and vectors for the representation of symmetry has clear benefits: knowing the transformation matrix and displacement vector of any two symmetry operation makes it possible to derive their combinations. Assume that two symmetry operations exist: their transformation matrices and displacement vectors are $\boldsymbol{S}^{(1)}, \boldsymbol{d}^{(1)}$ and $\boldsymbol{S}^{(2)}, \boldsymbol{d}^{(2)}$. Find the symmetry operations, which combine both of them.

2. Building the crystallographic unit cell (5 points)

The 2D structure crystal has 3-fold rotation axis. Which Bravais type of the lattice does it have? The position of four **symmetry independent atoms** in the conventionally chosen crystallographic unit cell are given by

a) [0.2,0.1]; b) [1/3,2/3]; c) [1/3,1/7]; d) [0.3,0.7]

Please, give the positions of **all the other atoms** in the *crystallographic unit cell*.

3. Building the crystallographic unit cell (5 points).

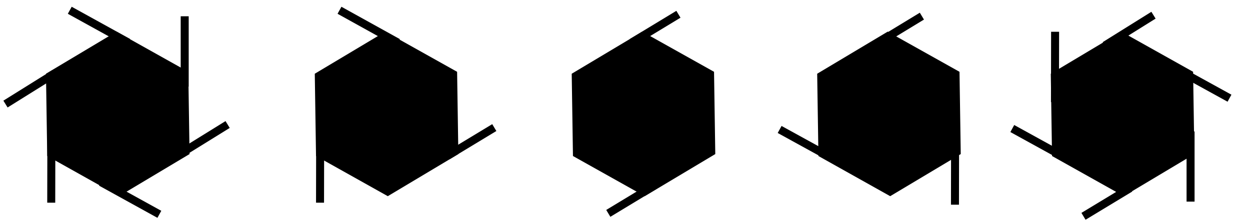
The structure of 2D crystal has one mirror plane. It is also described by a centered rectangular Bravais lattice, so that the mirror plane is parallel to the axis $\boldsymbol{b}$. The position of four symmetry equivalent atoms $\boldsymbol{A}$ in crystallographic unit cell are given by a) [0.2,0.1]; b) [0,0]; c) [0.25,0.25]; d) [0.3,0.7]

Please, derive the positions of all other atoms (symmetry equivalent to $\boldsymbol{A}$) in the *crystallographic unit cell.*

4. Screw axes (10 points).

A crystal has one of the five possible 6-fold screw axes. Calculate the transformation symmetry matrices and displacement vectors of all the possible symmetry operations. Present these operations in the CIF format

6_1 6_2 6_3 6_4 6_5



5. CIF-format of symmetry cards (6 points).

The symmetry operations (as given in a CIF-file of a rhombohedral crystal) are the following:

1) x,y,z 2) -y,x-y,z 3) -x+y,-x,z

4) -y,-x,z+1/2 5) -x+y,y,z+1/2 6) x,x-y,z+1/2

7) x+2/3,y+1/3,z+1/3 8) -y+2/3,x-y+1/3,z+1/3 9) -x+y+2/3,-x+1/3,z+1/3

10) -y+2/3,-x+1/3,z+5/6 11) -x+y+2/3,y+1/3,z+5/6 12) x+2/3,x-y+1/3,z+5/6

13) x+1/3,y+2/3,z+2/3 14) -y+1/3,x-y+2/3,z+2/3 15) -x+y+1/3,-x+2/3,z+2/3

16) -y+1/3,-x+2/3,z+1/6 17) -x+y+1/3,y+2/3,z+1/6 18) x+1/3,x-y+2/3,z+1/6

Identify the transformation matrix and displacement vector for each of these operations. *Hint: use the equation (1) and the lecture materials.*

Please return on 04/01/2016

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