UNIVERSITÄT SIEGEN FESTKÖRPERPHYSIK

Crystallography (*winter term 2015/2016*)

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Exercise sheet 6: Transformations, matrices and symmetry operations

General remarks 1: It is a common practice in crystallography to describe a crystal structure using different sets of basis vectors (settings). The transformation between two different settings is given by the transformation (orientation) matrix.

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} = (\boldsymbol{A}_1 \quad \boldsymbol{A}_2 \quad \boldsymbol{A}_3) \tag{1}$$

This matrix is defined in the simple and intuitive way: three **columns** of the matrix are the coordinates of the vectors of the new coordinate system $\{\boldsymbol{A}_i\}$ relative to the old coordinate system $\{\boldsymbol{a}_i\}$, so that $\boldsymbol{A}_i = A_{ji}\boldsymbol{a}_j$. It is easy to show that the transformation of coordinates between these two different coordinate systems is done via the transformation matrix. More specifically: a point (atom, direction, etc) which has the coordinates $U_1U_2U_3$ relative to the new coordinate system would have the coordinates $u_1u_2u_3$ relative to the old coordinate system:

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \\ U_3 \end{pmatrix}, \quad u_i = A_{ij}U_j \tag{2}$$

General remarks 2: Transformation matrices are the mathematical representations of symmetry. Assume that there is the set of N movements (transformations of coordinate systems), each leaving the crystal structure unchanged. This is reflected as the existence of N *symmetry equivalent sets of basis vectors.* $\left\{\boldsymbol{a}_i^{(1)}\right\},\left\{\boldsymbol{a}_i^{(2)}\right\},\ldots,\left\{\boldsymbol{a}_i^{(N)}\right\}$. The symmetry equivalence of these basis sets means that everything (e.g. atomic coordinates, physical properties) looks exactly the same on in any of these coordinate systems. It is common to express these new coordinates systems using the transformation matrices $A^{(1)} = I$, $A^{(2)}$,..., $A^{(N)}$. The columns of the $A^{(n)}$ matrix represent the coordinates of $\left\{\boldsymbol{a}_i^{(n)}\right\}$ relative to $\left\{\boldsymbol{a}_i^{(1)}\right\}$.

0. Combination of the symmetry operation (3 points)

The benefit of using matrices for symmetry operations is the easy way to combine the two different symmetry operations to check if the new operation is produced. Please show / prove that if the $A^{(n)}$ and $A^{(m)}$ are symmetry operations, then both matrix products $A^{(n)}A^{(m)}$ and $A^{(m)}A^{(n)}$ are also the symmetry operations!

1. The transformation of the reciprocal basis vectors (5 points)

It is also very important to transform reciprocal coordinate system, together with the direct coordinate system. In this task you will *learn how to do it*. The sets of three basis vectors are transformed from $\{\boldsymbol{a}_i\}$ to $\{\boldsymbol{A}_i\}$. The transformation matrix (defined according to the equation (1)) is A. Find the matrix A^*, which transforms the corresponding reciprocal lattice vectors from $\{\boldsymbol{a}_i^*\}$ to $\{\boldsymbol{A}_i^*\}$.

Hint: Assume that the transformation of the direct basis vectors is expressed $\boldsymbol{A}_k^* = A_{lk}^*\boldsymbol{a}_l^*$ *. Remember that* $\boldsymbol{A}_i \cdot \boldsymbol{A}_k^* = \delta_{ik}$

2. The concept of a symmetry group (3 points)

What is meant by the symmetry group? How many crystallographic point symmetry groups do you know? Why is there finite number of groups only?

3. Assembling point symmetry operations into groups (6 points)

A crystal has the following symmetry elements: a 2-fold axis $\parallel \mathbf{a}_2$ and a 4-fold rotoinversion axis $\parallel \mathbf{a}_3$. Find the symmetry group of this crystal. List all the symmetry elements of the group and plot the symmetry diagram of the object, using graphical symbols of different symmetry elements.

4. Assembling point symmetry operations into groups (6 points)

A crystal has the following symmetry elements: a 2-fold axis $\parallel \mathbf{a}_1$ and a 2-fold axis $\parallel$ a_3. Find the complete symmetry group of this crystal, list all the symmetry elements and plot the symmetry diagram by using graphical symbols of different symmetry elements. *Hint: find the matrices of these two symmetry (A_1, A_2) operations above and find all the possible new symmetry elements, by finding all the possible products such as A_1A_2, A_2A_2, $A_1A_2A_2$ until you form a group)*

Please return on 14/12/2015