Crystallography (*winter term 2015/2016*)

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<u>Exercise sheet 1: Cross and mixed products. Reciprocal basis.</u>

1. Octahedron (5 points).

Octahedron is a three-dimensional figure, which is typical in many crystal structures (for example perovskites). Those structures are organized in such a way that some of their atoms sit in the corners of octahedra (see the Figure). An octahedron has 6 corners and 8 faces (each of the faces is a triangle). The coordinates of the corners of an octahedron are given below:

1: [0 0.5 0.5]

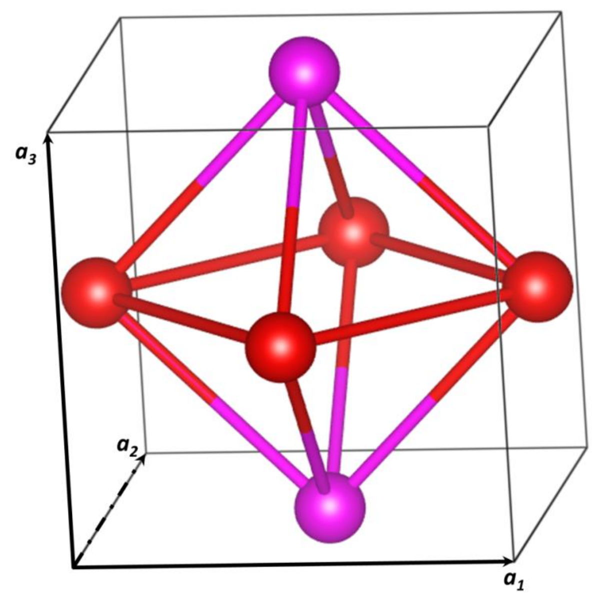
2: [0.5 0 0.5]

3: [0.5 0.5 0]

4: [1 0.5 0.5]

5: [0.5 1 0.5]

6: [0.5 0.5 1]



Please, choose <u>any</u> two octahedron faces and calculate a) The normal vectors to these faces; b) the areas of these faces (i.e. the areas of the triangles).

2. Tetrahedron (5 points).

Tetrahedron is another three-dimensional geometrical figure. It has 4 corners and 4 faces (where each face is also a triangle). The coordinates of the corners of a regular tetrahedron are given below. The coordinate of an atom in the centre of the tetrahedron is also given.

Corners (Red)

1: [0 0 0]

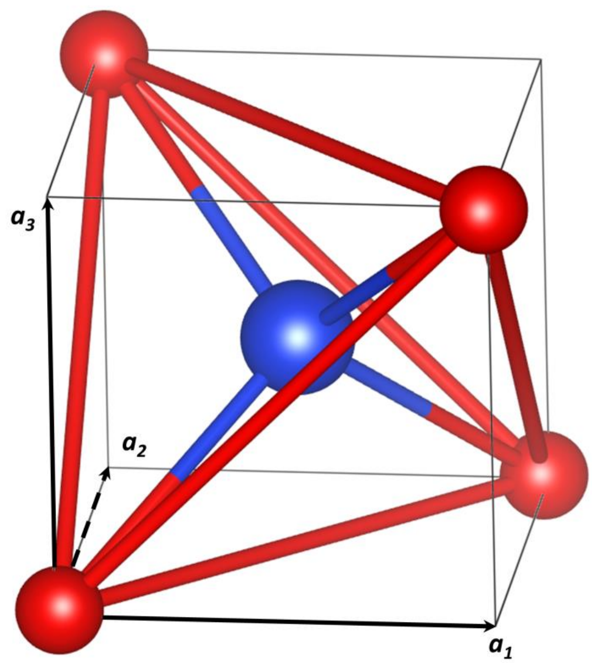
2: [0 1 1]

3: [1 0 1]

4: [1 1 0]

Centre (Blue)

5: [0.5 0.5 0.5]



Choose <u>any</u> two tetrahedron faces and calculate a) The normal vectors to these faces; b) The area of these faces (i.e. the areas of the triangles) Also, please, calculate the normal vector to one of the Corner-Centre-Corner plane and the area of the corresponding triangle.

Hint to the Tasks 1 and 2: Use the operation of cross product between vectors. Remember that a cross product represent the normal to the plane of vectors, while the length of the cross product is numerically equal to the area of the parallelogram, based on these vectors. Assume that the coordinate system is Cartesian.

3. Reciprocal lattice vectors (8 points)

Reciprocal basis vectors form an elegant mathematical tool, which simplifies the vector calculations in non-Cartesian coordinate systems significantly. Reciprocal lattice is the key concept of (X-ray) crystallography. For a 3D space, reciprocal basis vectors, $\boldsymbol{a}_1^* \ \boldsymbol{a}_2^* \ \boldsymbol{a}_3^*$, are defined by three equations:

$$\boldsymbol{a}_1^* = \frac{1}{V_a}[\boldsymbol{a}_2 \times \boldsymbol{a}_3]\,, \quad \boldsymbol{a}_2^* = \frac{1}{V_a}[\boldsymbol{a}_3 \times \boldsymbol{a}_1], \quad \boldsymbol{a}_3^* = \frac{1}{V_a}[\boldsymbol{a}_1 \times \boldsymbol{a}_2],$$

with $V_a = (\boldsymbol{a}_1\boldsymbol{a}_2\boldsymbol{a}_3) = \boldsymbol{a}_1 \cdot [\boldsymbol{a}_2 \times \boldsymbol{a}_3]$ is the mixed product between the basis vectors (also defining the volume of the corresponding unit cell).

Show that the triples of vectors $\boldsymbol{a}_1^* \ \boldsymbol{a}_2^* \ \boldsymbol{a}_3^*$ and $\boldsymbol{a}_1 \ \ \boldsymbol{a}_2 \ \ \boldsymbol{a}_3$ are <u>reciprocal to each other</u>. In other words, show that the following equations are also true:

$$\boldsymbol{a}_1 = \frac{1}{V_a^*}[\boldsymbol{a}_2^* \times \boldsymbol{a}_3^*], \boldsymbol{a}_2 = \frac{1}{V_a^*}[\boldsymbol{a}_3^* \times \boldsymbol{a}_1^*], \quad \boldsymbol{a}_3 = \frac{1}{V_a^*}[\boldsymbol{a}_1^* \times \boldsymbol{a}_2^*],$$

with $V_a^* = (\boldsymbol{a}_1^*\boldsymbol{a}_2^*\boldsymbol{a}_3^*) = \boldsymbol{a}_1^* \cdot [\boldsymbol{a}_2^* \times \boldsymbol{a}_3^*]$.

Hint 1: Use the famous expression for the double dot product

$$\big[\boldsymbol{A} \times [\boldsymbol{B} \times \boldsymbol{C}]\big] = \boldsymbol{B}(\boldsymbol{A} \cdot \boldsymbol{C}) - \boldsymbol{C}(\boldsymbol{A} \cdot \boldsymbol{B})$$

Hint 2: Start solving this task by proving that $V_a^* = \frac{1}{V_a}$

Please return on 09/11/2015