YFX1120-Solid States Physics and Semiconductors Physics

First, a few words about the content of our course, it consists of two parts. The first is solid state physics and the second is semiconductor physics, which will begin in November. In the last week of November, we will run a test. A week before that, I will ask everyone one question from the topics of our part of the course. After that, you will have a week to prepare a detailed answer to the question asked. The final mark for the exam will be set based on the discussion of the topic of the question.

You can find more information about our course here: parsek.yf.ttu.ee/~physics/ssp.

As part of our course, we look at simple models. But, despite the simplicity of the models, we will try to calculate the real properties of crystals, for example, the heat capacity of crystals, and so on. A separate part of our course is the use of software packages (VASP https://www.vasp.at/ , Phonopy https://phonopy.github.io/phonopy/) for calculating the basic properties of simple crystals such as optimization of stricture, calculation of elastic properties and phonons spectrum, calculation of band gap by different ab-initio methods, calculation of optical properties.

The textbooks you can find in our library or in internet:
1. Ch. Kittel, "Introduction to Solid State Physics"
2. Ashcroft, N.W., Mermin, N.D. "Solid State Physics"
3. A. Anselm, "Introduction to the theory of semiconductors"

We will begin from the short review of the symmetry properties of perfect crystals.

We will begin from the short review of the symmetry properties of perfect crystals. But what does it mean - the "perfect crystal". We assume that the ideal crystal is perfect if it have the infinite periodic structure without any defects of lattice and the atoms are in their equilibrium position - crystal temperature is equal to zero.

§1.1 Crystals point symmetry transformations.
Point symmetry operations. Proper rotations, reflection, inversion, improper rotations. Point groups. Translation symmetry. Translation vectors. Allowed to point groups (some examples). Base vectors. Elementary cell. Primitive cell. Space groups. Classes. Reciprocal lattice. Wigner-Seitz cell. Miller indices.

What we can said about the point symmetry properties of molecules and crystals? What does it means? This means that there are a set of symmetry operations (transformations) such that the atomic or molecular structures remains invariant under that transformations (the macroscopic properties of a crystal would look exactly the same before and after any of the symmetry operations, body coincide with itself). What kinds of symmetry transformations we can apply to the molecules and lattices to stay its invariant (do not forget that the molecules is nt a periodic structure)?

Proper rotation (denotes as C) around some symmetry axes or "proper" rotations.
Besides the rotation we can use the other symmetry operations such as:
Reflections (denotes as σ) in some vertical or horizontal mirror plane. There is two different types of reflection planes **σ$_h$** - axis of rotation **C$_n$** is perpendicular to this plane, **σ$_v$** - axis of rotation **C$_n$** is in the plane **σ$_v$.**
Inversion(denotes as I) through a point (center of symmetry) and their any combinations.
Rotary-reflection(Improper rotation S) transformation (axis) is defined as a sequential application of two operations   **C$_n$** and **σ$_h$.**

A good description of point transformations with 3d illustrations you can find here
http://symmetry.otterbein.edu.
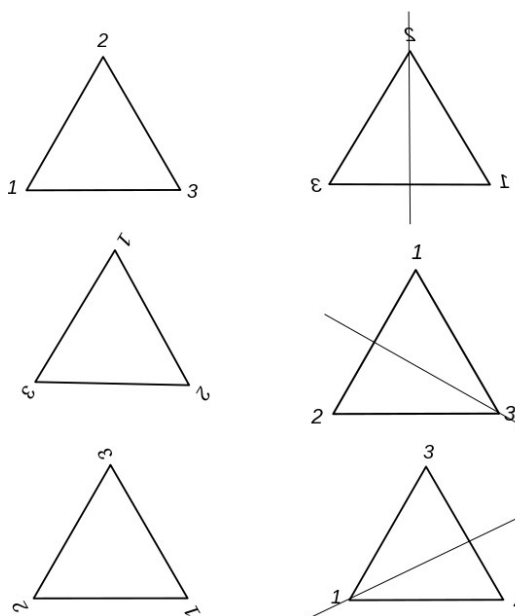
Example 1

We need to consider the group of symmetry elements of regular triangle (figure om left). A triangle can be represented as a molecule with three equivalent atoms located at each vertices of the triangle. As you see we can define the next symmetry transformations for this molecules (regular triangle):

1. Rotations around vertical axes through angles 0, 120, 240 and 360 degrees. It is clear that the first and last transformation are identical (because these rotations are do not change the order of vertices numbering). The non zero minimal allowed angle of rotation is 120 degree can be written as $2\pi/3$ or by other words we have the 3-fold (3-th order) symmetry axis. For n-fold rotational axis the minimal allowed angle can be denoted as $2\pi/n$.

In our case the symmetry transformations associated with rotations vertical symmetry axis can be respectively denoted as $C_3^0, C_3^1, C_3^2, C_3^3 = C_3^0$. Here the down index denote the order of symmetry axis (in our case is 3) and upper index define the 1,2 or 3-fold rotations on minimal angle ($C_3^0 = 0$, $C_3^1 = 120$, $C_3^2 = 240$, $C_3^3 = C_3^0 = E = 0$ or 360) E-identity transformation.

2. Rotation around horizontal 2-fold axis C_2^1 (total number is 3) or reflections in vertical planes σ_v (total number is 3). In this case does not matter is we use the rotations or reflections because the rotation around the 2-fold horizontal axis and the reflection in the vertical plane change the order of the numbering of the vertices in the same way.

*I have to mark that all above mentioned symmetry transformations leave a central point fixed so they called by **point symmetry** elements*. All symmetry elements of given crystal are form the group of symmetry elements $\{E, C_3^1, C_3^2, 3C_2\}$ or $\{E, C_3^1, C_3^2, \sigma_v^1, \sigma_v^2, \sigma_v^3\}$ here $C_3^0 = C_3^3 = E$. But what does it means , group of symmetry elements?

The group definition:

The some elements are form the group if they are obey to the following rules:

1. If A and B are elements from group , so their multiplication A*B is the element from the same group.
2. (Associativity) for elements A,B and C (A*B)*C=A*(B*C)
3. (Identity element) There is an element E in the group so that for every element A, A*E=A.
4. (Inverse element) For each element A from group G exist inverse element A^{-1} so that A* A^{-1}=E

In our case additionally i want to do one important remark. *If we numirate all the vertices of a triangle a complete group of symmetry transformations must realize all possible and allowed options of the numbering of the vertices.* In our case (triangle) the number of these possibility is 6 and all options can be realised by 6 symmetry transformations. The result of multiplication of any two elements from this group give the element from the same group.

Example 2 molecules of water. Water molecules consist from 2 hydrogen and 1 oxygen. The angle between O-H bonds is equal to 104,46 degree. It is clear that these atoms form a triangle. How about a complete set of symmetry transformations? *You have to find all non equivalent symmetry transformations for this object.* Can use **http://symmetry.otterbein.edu**.

Example 3 Symmetry of square molecules. On left figure all vertices are equivalent, since all sides
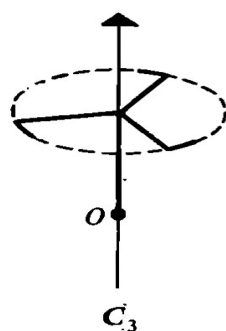
are of the same length. On right figure atoms are pairwise identical. _You have to find all non equivalent symmetry transformations for these two molecules._
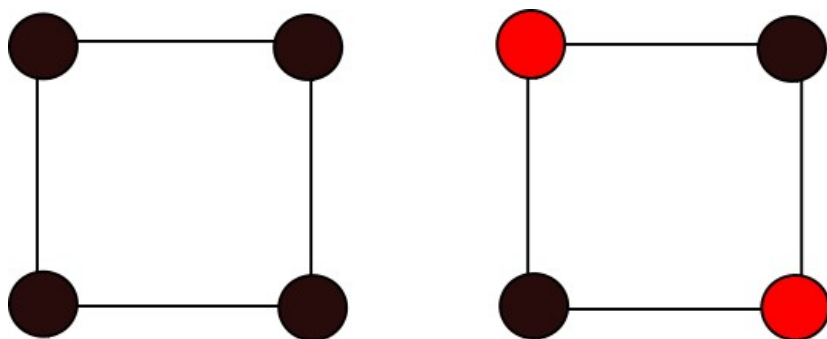
Examples of some simple point groups:
rotation through 180 degree about the height
1. C_n group

These groups consist only a symmetry axis of the order n, i.e., the body coincides with itself if it was rotated around the axis through an angle **2*pi/n**, This group consists of n elements, only rotations $C_n = \{C_n^1, C_n^2 ... C_n^n = E\}$

The object on the left has a symmetry group **$C_{3=}$\{ E, C_3^1, C_3^2\}.**
The symmetry of **Hydrogen peroxide H_2O_2** is **C_2.**

Some additional examples for molecules with that type of symmetry you can find here: https://symotter.org/gallery
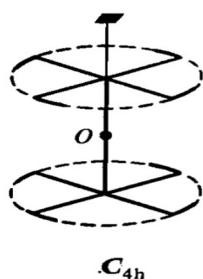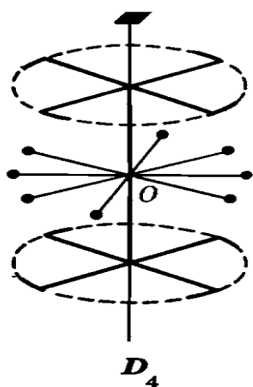
2. C_{nv} group
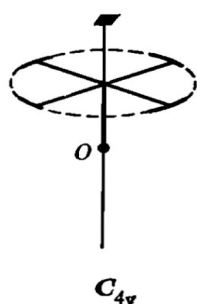
This group can be presented as a   sum of group of pure rotations C_n and reflections in vertical planes $C_{nv} = C_n + \sigma_v$.

The object on the left has a symmetry group   **$C_{4v} = \{E, C_4^1, C_4^2, C_4^3, \sigma_v^1, \sigma_v^2, \sigma_v^3, \sigma_v^4\}$.**This group consist four rotations about vertical axes through pi/2 degree and reflections in vertical planes.

The symmetry of Water molecules **H_2O** is **C_{2v}.**

Some additional examples for   molecules with that type of symmetry you can find here: https://symotter.org/gallery

3. C_{nh} group

This group can be presented as a   sum of group of pure rotations C_n and reflections in horizontal planes $C_{nv} = C_n + \sigma_h$.

The object on the left has a symmetry group **$C_{4h} = \{E, C_4^1, C_4^2, C_4^3, \sigma_h\}$**
This group consist four rotations about vertical axes through 90 degree and planes perpendicular to a symmetry axes order 4.

Some practical examples for   molecules with that type of symmetry you can find here: https://symotter.org/gallery

4. D_n (dihedral group)

If we add the horizontal symmetry axis C_2 perpendicular to a vertical symmetry axis C_n so we get the new group of symmetry D_n (C_n axis is bilateral).

The object on the left has a symmetry group $D_4 = \{E, C_4^1, C_4^2, C_4^3, u_1, u_2, u_3, u_4\}$
This group consist four rotations about vertical axes through pi/2 degree and 4 2-fold symmetry axes perpendicular to a symmetry axes order 4.

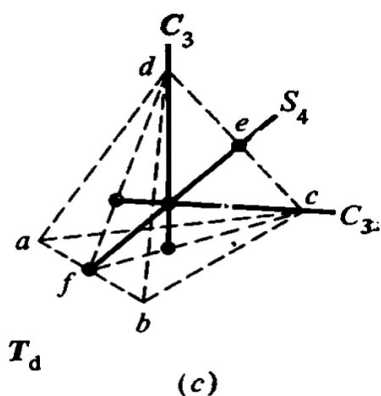Some practical examples for molecules with that type of symmetry you can find here: https://symotter.org/gallery

5. D_{nh} group

This group can be presented as a sum of group D_n and the reflection in horizontal plane σ_h.
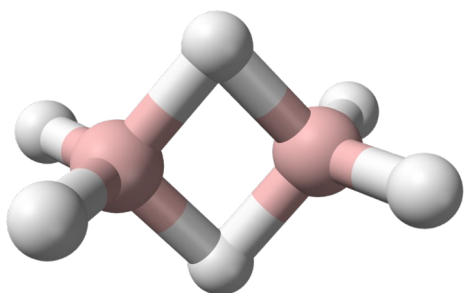
The diborane molecules B_2H_6 **has a** symmetry properties describe the group of symmetry $D_{2h} = \{E, 3C_2, I, \sigma_h^1, \sigma_h^2, \sigma_h^3\}$.

Some additional practical examples for molecules with that type of symmetry you can find here: https://symotter.org/gallery

6 . T_d group (tetrahedron complete group of the symmetry transformations)

$T_d = \{E, 4C_3^1, 4C_3^2, 3C_2, 6\sigma_d, 3S_4^1, 3S_4^3\}$ total number of a symmetry elements is 24

Some practical examples for molecules with that type of symmetry you can find here: https://symotter.org/gallery.

You can find a description of all symmetry elements at https://symotter.org/gallery.

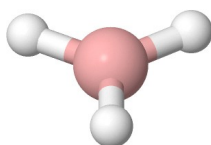## 7. Oh group (complete set of the symmetry transformations for Cube)

$O_h = \{E, 6C_2, 4C_3^1, 4C_3^2, 3C_4^1, 3C_4^2, 3C_4^3, 3\sigma_h, 6\sigma_d, 3S_4^1, 3S_4^3, 4S_6^1, 4S_6^5, I\}$ total number of symmetry elements is 48.

You can find a description of all symmetry elements at https://symotter.org/gallery.

Some additional practical examples for molecules with that type of symmetry you can find here: https://symotter.org/gallery

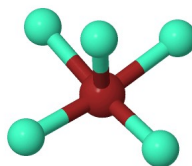**8,9,10**   **the last 3 examples of the simple molecules.**

      BH BrF_5 Benzene
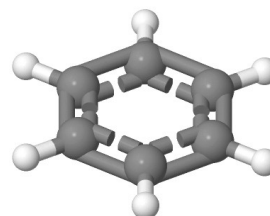
Point Group = D_{3h} Point Group = C_{4v} Point Group = D_{6h}

You have to find and describe the complete symmetry properties of the presented molecules !!!
A complete description can be founded here: http://symmetry.otterbein.edu.

So, we have the next symmetry transformations describing the point symmetry properties of perfect crystals. First one is proper rotations the next is reflections, inversion and improper rotations.

The second type of symmetry properties of ideal crystals is associated with the displacement of the crystal as a whole by a certain translation vector R. This property of symmetry is called the **translation symmetry** of the lattice.

Not all possible displacements are lattice symmetry transformations, but only those that leave the crystal unchanged (invariant transformations). Any vector of lattice displacement (translation) in 3d space can be presented in the next form:

$$\vec{R}=n_1 \cdot \vec{a}_1 + n_2 \cdot \vec{a}_2 + n_3 \cdot \vec{a}_3, \text{ here } n_1, n_2, n_3 \text{ coordinates of vector } \vec{R}, \text{ are real numbers } . \qquad (1)$$

The **a₁,a₂,a₃** are the so called **basis vectors** of lattice. The choice of base vectors is completely free and ambiguous. For 2d lattice the possible choice is looks like so as presented at figure 1. Parallelepiped built on the basis vectors is called the unit cell (figure 2). It is clear that the unit cells, in figure 2, fill the entire lattice without gaps (and all unit cells are equivalent). Uncertainty of choice of basis vectors can be avoided by applying additional rules for basis vectors:

 1. Choice the vectors with minimal possible length,
 2. Keeping in mind that the displacement of lattice on any basis vector **a$_i$** or any their   (2)
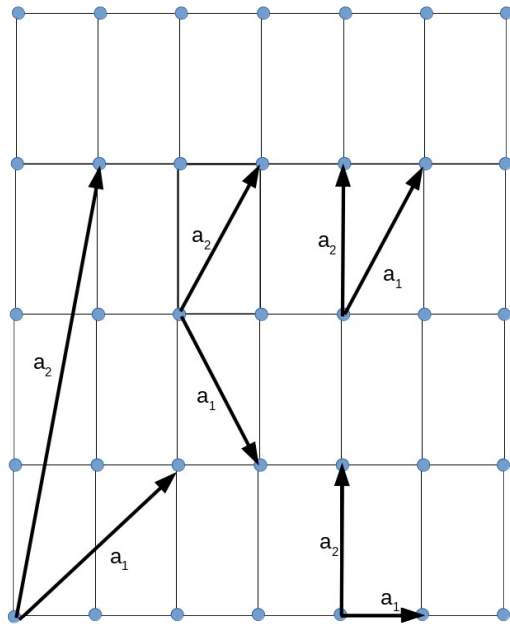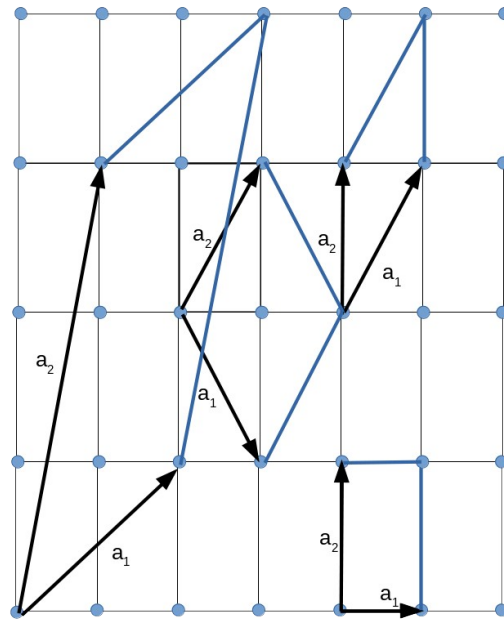 combination (1) must be invariant.
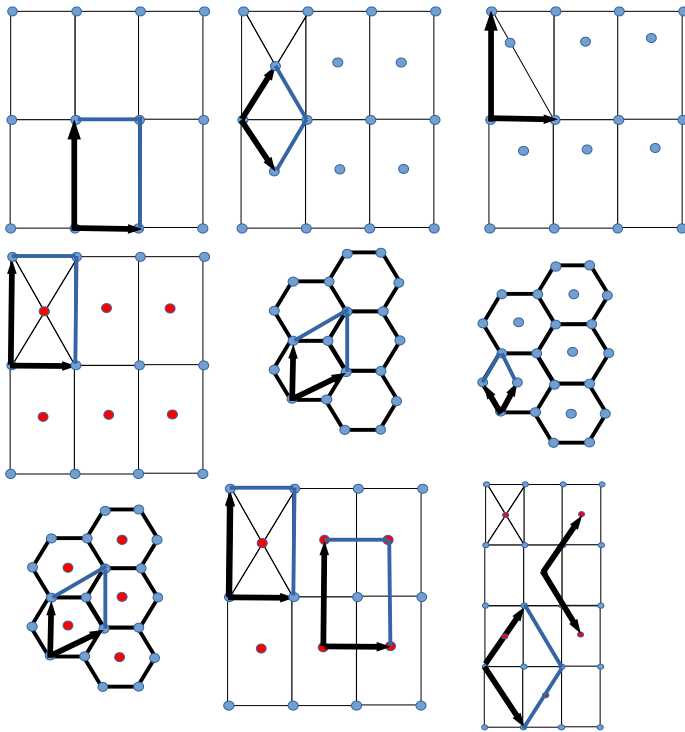
figure 1

figure 2

figure 3

At figure 1 and 2 you can see the possible choice for basis vectors and corresponding unit cells. At figure 3 represented the basis vectors for 2d lattices satisfied to conditions (2). The corresponding unit cell have the name – **primitive unit cell**. It is clear that for the basis vectors satisfying (2) (primitive unit cell), the coordinates of the translation vector (1) must be an integer and can play the role of a unit cell number.

The translation vector has very useful and practical applications for determining the position of any atom in a crystal lattice. The position of atom type **s** in unit cell with coordinates (n_1, n_2, n_3) could be presented as follows:

$$\vec{R}^s_{n_1, n_2, n_3} = \vec{R}_{n_1, n_2, n_3} + \vec{r}^s \tag{3}$$

$\vec{r}^s$ -is vector of position of atoms inside of any unit cell (all cells are equivalent). On figure 4 presented some examples of 3d lattices. The detailed description you can find below.
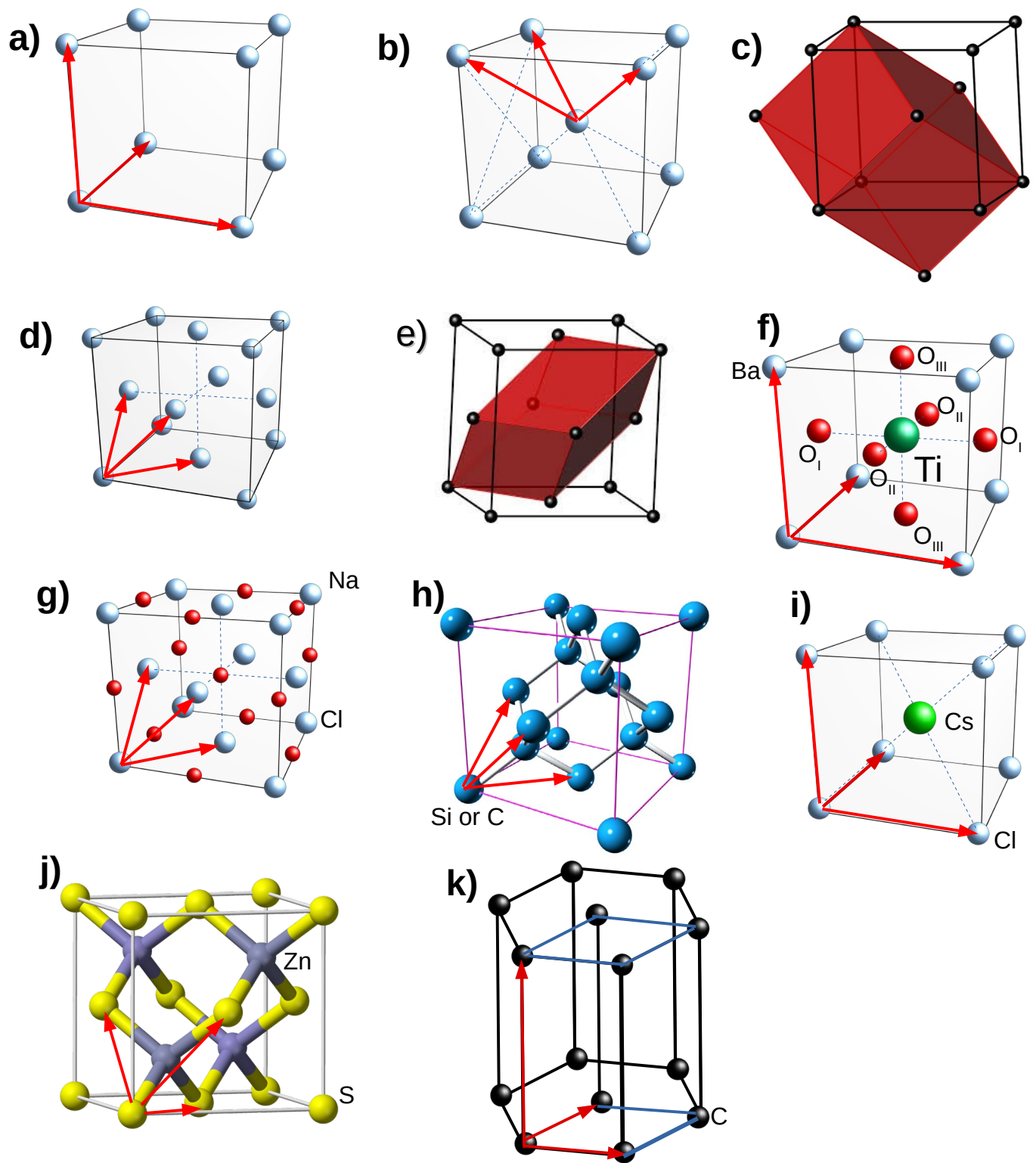
a)

b)

c)

d)

e)

f) Ba, O_{III}, O_{II}, O_I, O_I, O_{II}, Ti, O_{III}

g) Na, Cl

h) Si or C

i) Cs, Cl

j) Zn, S

k) C

figure 4

a) Basis vectors for simple cubic unit cell Γ_c. Primitive unit cell is cubic and simple (contains 1 atom).

b) Basis vectors for volume centered cubic unit cell (BCC – or body centered cell) Γ_c^v.

c) Primitive unit cell for Γ_c^v unit cell is simple (contains 1 atom).

d)Basis vectors for face centered cubic unit cell (FCC – face centered cell) Γ_c^f.

e) Primitive unit cell for Γ_c^f unit cell is simple (contains 1 atom).

f) Lattice structure and basis vector for barium tinatate ferroelectric crystal (BaTiO$_3$). Primitive unit cell is a simple cubic and contains 5 atoms Ba-1 atom, Ti-1 atom, O-3 atoms. Despite the oxygen atoms are equal form chemical point of view but they are crystallographically different . The whole crystal can presented as a combination of five Γ^c sublattices: Barium,Titanium and 3 Oxygen.

g) Lattice structure and basis vector for rock salt crystal (NaCl). Primitive unit cell is a face centered cubic and contains 2 atoms Na-1 atom, Cl-1 atom. The whole crystal can presented as a combination of two Γ_c^f sublattices: natrium and chlorine. The entire NaCl crystal can be represented as a combination of two Γ_c^f sublattices, with one sublattice shifted relative to the other by a half of the side length of cube.

h) Lattice structure and basis vector for silicon,dimond or germanium crystals (Si,C,Ge). Primitive unit cell is a face centered cubic and contains 2 silicon atoms. The entire Si crystal can be represented as a combination of two Γ_c^f sublattices, with one sublattice shifted relative to the other by a quarter of the main diagonal length.

i) Lattice structure and basis vector for cesium chlorine crystal (CsCl). Primitive unit cell is a simple cubic and contains 2 atoms Cs-1 atom, Cl-1 atom. The entire crystal can presented as a combination of two Γ^c sublattices,with one sublattice shifted relative to the other by a half of the main diagonal length.

j) Lattice structure and basis vector for Zinc Sulfide or Gallium Nitride crystal (ZnS, GaN). This option is similar to the Si crystal.
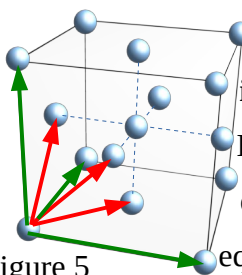
k) Lattice structure and basis vector for graphite crystal. Primitive unit cell is a hexagonal.

I want to emphasize that there is no need to always use a primitive unit cell to describe the physical properties of a crystal (do not forget that all unit cells are equivalent). This choice simply minimizes the number of objects to explore -

figure 5

number of atoms (red vectors). For example, for the Γ_c^f (figure 5) lattice, it is necessary to take into account only one atom located in a primitive unit cell. For a non-primitive unit cell (just a unit cell,

green vectors), the number of atoms should be increased from 1 to 5. Sometimes, for example, to study the properties of defects in solids, instead of one primitive unit cell, it is necessary to use a **supercell** consisting of several primitive cells or just unit cells (the green vectors) .

As you see the crystal has two different kind of symmetry transformations: the point symmetry transformations and translations. The combinations of all elements of the different point-groups with the allowed displacements (translations) of lattice give us all possible symmetry transformations of lattice or **space group of crystal.** But we know that the number of different point groups is infinite.

In 1919 Paul Niggly demonstrate that for simple lattices there are only seven point groups symmetry transformations compatible with translations of crystals. Only 7 groups from the infinite number of point groups can be used for the building of any real lattices. If we inspect all points groups we will establish that only these groups are compatible with the translations of crystals: S_2 C_{2h} D_{2h} D_{3d} D_{4h} D_{6h} O_h . This give a very useful ability for classification of different crystal lattices. The seven point groups specified above constitute **seven crystal systems**, the designation for them being:
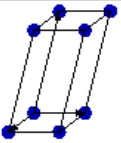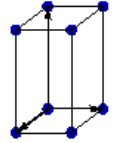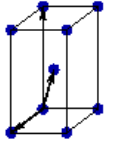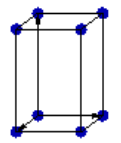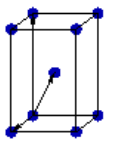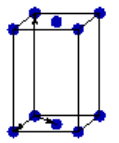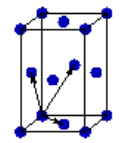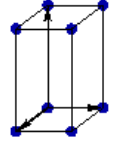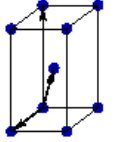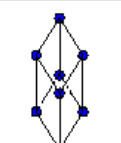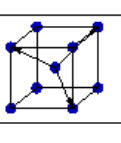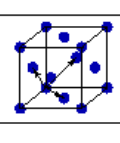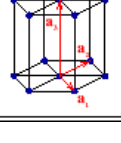
1) triclinic (S_2)
2) monoclinic (C_{2h})
3) orthorhombic (D_{2h})
4) tetragonal or quadratic (D_{4h})
5) rhombohedral or trigonal (D_{3d})
6) hexagonal (D_{6h})
7) cubic (O_h)

Auguste Bravais demonstrated that there are altogether 14 types of simple lattice (Bravais lattice) corresponding to the seven systems (tables 1 and 2).

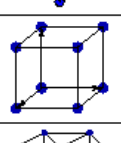|	α β γ	The lengths of basis vectors a_1 a_2 a_3	Bravis lattice
Triclinic	$\alpha \neq \beta \neq \gamma$	$a_1 \neq a_2 \neq a_3$	Γ_t
Monoclinic	$\alpha \neq \beta = \gamma = 90$	$a_1 \neq a_2 \neq a_3$	Γ_m, Γ_m^b
Orthorhombic	$\alpha = \beta = \gamma = 90$	$a_1 \neq a_2 \neq a_3$	$\Gamma_o, \Gamma_o^b, \Gamma_o^v, \Gamma_o^f$
Tetragonal	$\alpha \neq \beta = \gamma = 90$	$a_1 = a_2 \neq a_3$	Γ_q, Γ_q^v
Rhombohedra	$\alpha \neq \beta = \gamma \neq 90$	$a_1 = a_2 = a_3$	Γ_{rh}
Hexagonal	$\alpha = 120 \beta = \gamma = 90$	$a_1 = a_2 \neq a_3$	Γ_h
Cubic	$\alpha = \beta = \gamma = 90$	$a_1 = a_2 = a_3$	$\Gamma_c, \Gamma_c^v, \Gamma_c^f$

Table 1 Bravais lattices.

Table 2

Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

   Any possible crystal lattices we can build by using only 14 Bravais lattices or as a combination of a few Bravais lattices from the same class.

Some additional examples of real 3d structures:

1. Li,Na,K,Rb,Cs,Ba= Γ_c^v

2. Cu,Ag,Au,Al,Pb,Fe,Ni,In,Pt=Γ_c^f

3. Be,Mg,Zn,Cd= Γ_h

4. Lattices with the structure of NaCl =Γ_c^f

 NaCl   sodium clorine, The following substances are crystallized in this structure,this is a prototype of such lattices.

LiH, NaF, NaBr, NaI, Kcl, RbBr, MgO, SrO, BaO, AgBr

5. Lattices with the structure ZnS Zinc-Blend (zinc sulphide)=Γ_c^f

SiC, GaP, InP, CuCl, CuBr, CuI, GaN

6. Lattices with the structure of Wurzite =Γ_h

BeO,CuI,ZnO,AgI

7. Lattices with the structure of Diamond =Γ_c^f

Ge,S,C

8. Lattices with the structure of CsCl =Γ_c

CsBr,CsI,lCl...

*9. Lattices with the structure of BaTiO3 =Γ_c*

PbTiO ,SrTiO3

If we take into account all possible point group symmetry elements, translations, glide planes and screw axes we will see that there is only 230 possible space groups (crystal systems) describing any symmetry properties of the any crystal at nature.

As you can see, the choice is finite https://en.wikipedia.org/wiki/Space_group. There is a very useful resource on lattices symmetry properties (Bilbao server) https://www.cryst.ehu.es/. And open database with describing of different crystal lattices http://www.crystallography.net/cod/. The crystals structures here presented in **.cif** files and can be visualized by VESTA free software https://jp-minerals.org/vesta/en/.

It is clear that the volume of unit cell we can calculate as mixed multiplication of basis vectors:

$$V_0 = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \qquad (4)$$

§1.2 Wigner-Seitz cell
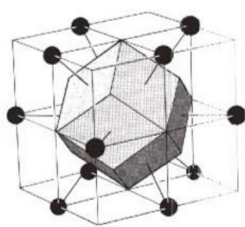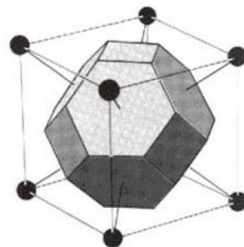
f.c.c Wigner-Seitz cell   b.c.c Wigner-Seitz cell

There are different ways of choosing a primitive unit cell. One of these ways is the Wigner-Seitz-cell.
A unit cell built on the basis vectors for a primitive cell does not always reflect all the symmetry properties of the lattice. Compare d) and e). The Wigner-Seitz cell has all the symmetries of the crystal.

It is constructed by choosing one atom (e.g. bcc: central atom). Then draw lines to the nearest neighbours and cut all the lines in half with a plane. The Wigner-Seitz cell consists of all points that can be reached from the central atom without crossing one of those planes. It also has the same volume as any other primitive unit cell and can also be stacked on the Bravais-lattice to construct the whole crystal.

Example. We consider the Γ_c^f cubic Bravais lattice.
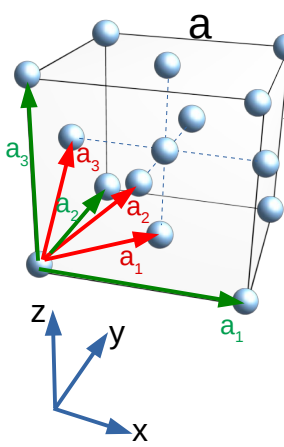
1. For cubic unit cell (the green basis vectors) basis vectors can be presented as follows: $a_1=(a,0,0)$; $a_2=(0,a,0)$; $a_3=(0,0,a)$. The volume of unit cell is equal to $V_0=a^3$.

2. For primitive unit cell : $a_1=(a/2,a/2,0)$; $a_2=(a/2,0,a/2)$; $a_3=(0,a/2,a/2)$. By using (4) we will get $V_0=a^3/4$.

§1.3 Reciprocal lattice

As we know, a unit cell is the smallest part of a crystal that can be used to restore an entire crystal. This means that it is sufficient to calculate any physical property in only one unit cell. Because all elementary cells are equivalent. This means that the function describing some physical property of the crystal is a periodic function with the periodicity of the basis vectors. But any periodical function could be expand into a Fourier series:

$$U(\vec{r})=\sum_{\vec{b}} U_{\vec{b}}\cdot e^{i\cdot \vec{b}\vec{r}}=\sum_{\vec{b}} U_{\vec{b}}\cdot e^{i\cdot(b_x x+b_y y+b_z z)} \tag{5}$$

Here

$$\vec{b}=g_1\vec{b}_1+g_2\vec{b}_2+g_3\vec{b}_3 \tag{6}$$

is a vector in reciprocal space and $\vec{b}_1,\vec{b}_2,\vec{b}_3$ basis vectors in reciprocal space. Why is such a strange name? The answer is r -vector have dimension meter and b-vector 1/m, reciprocal meter. Due to the periodicity of the lattice with the periodicity vector (1):

$$U(\vec{r})=U(\vec{r}+\vec{R}_n) \tag{7}$$

After substitution (5) to (7)

$$U(\vec{r})=U(\vec{r}+\vec{R}_n)=\sum_{\vec{b}} U_{\vec{b}}\cdot e^{i\cdot \vec{b}\vec{r}}=\sum_{\vec{b}} U_{\vec{b}}\cdot e^{i\cdot \vec{b}\vec{r}} e^{i\cdot \vec{b}\vec{R}_n} \tag{8}$$
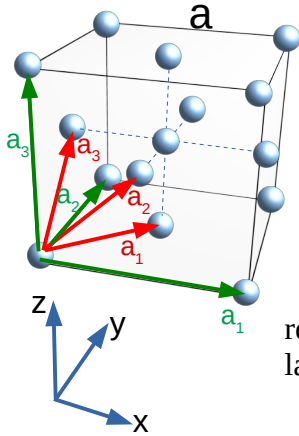
But this is possible only if : $e^{i\cdot \vec{b}\vec{R}_n}=1$ and $n_1\cdot\vec{b}\cdot\vec{a}_1+n_2\cdot\vec{b}\cdot\vec{a}_2+n_3\cdot\vec{b}\cdot\vec{a}_3=2\cdot\pi\cdot$ some integer number.

It can be shown that it is possible if basis vectors of reciprocal lattice $\vec{b}_1;\vec{b}_2;\vec{b}_3$ and basis vectors of

unit cell $\vec{a}_1 ; \vec{a}_2 ; \vec{a}_3$ are related as follows:

$$\vec{b}_1 = \frac{2\pi}{V_o}(\vec{a}_2 \times \vec{a}_3)$$

$$\vec{b}_2 = \frac{2\pi}{V_o}(\vec{a}_3 \times \vec{a}_1) \quad V_o\text{- volume of unit cell.} \tag{9}$$

$$\vec{b}_3 = \frac{2\pi}{V_o}(\vec{a}_1 \times \vec{a}_2)$$

Example. We consider the FCC (Γ_c^f) cubic Bravais lattice.

1. For cubic unit cell (the green basis vectors) basis vectors can be presented as follows: $a_1=(a,0,0)$; $a_2=(0,a,0)$; $a_3=(0,0,a)$. The volume of unit cell is equal to $V_0=a^3$. The basis vector for reciprocal lattice could be calculated by (9): $b_1=2\pi(1/a,0,0)$; $b_2=2\pi(0,1/a,0)$; $b_3=2\pi(0,0,1/a)$.

2. For primitive unit cell : $a_1=(a/2,a/2,0)$; $a_2=(a/2,0,a/2)$; $a_3=(0,a/2,a/2)$. By using (4) we will get $V_0=a^3/4$.
$b_1=2\pi/a^3(1,-1,-1)$; $b_2=2\pi/a^3(-1,1,-1)$; $b_3=2\pi/a^3(1,-1,-1)$.
To this set of basis vectors there corresponds BCC unit cell. It means that the reciprocal lattice for FCC crystal is BCC lattice. And vice versa the reciprocal lattice for BCC crystal is FCC lattice.

§ 1.4 Symmetry of the physical tensors.

§ 1.4.1 Tensor of conductivity.

Generally the Ohm low in tensor presentation is looks like so:

$$j_\alpha = \sigma_{\alpha,\beta} \cdot E_\beta \tag{10}$$

j- vector of the density of currant, E-strength vector of electric field, σ-second rank conductivity tensor. It is clear that any symmetry transformations (rotations, reflections, etc.) of the Crystal do not change its physical properties. For a cubic crystal, we take into account only rotations around the axis of symmetry of the 4th order (do not forget that the total number of elements of the point symmetry group for a cube O_h is 48). If R is the crystal symmetry transformation matrix then:

$$R \cdot \vec{j} = R \cdot \sigma \cdot \vec{E} = R \cdot \sigma \cdot R^{-1} \cdot R \cdot \vec{E} \tag{11}$$

symmetry transformation should not change the conductance tensor(the physical property):

$$\sigma = R \cdot \sigma \cdot R^{-1} \tag{12}$$

The matrix of rotations around the x,y and z axes by an angle Θ is:

$$R_x(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}$$ (13)

$$R_y(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}$$

$$R_z(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The matrix of transformation for C_4^1 rotation around z axis is looks like so:

$$C_4^1 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad C_4^2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

$$(C_4^1)^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (C_4^2)^{-1} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$ (14)

Combination of matrices according to (12):

$$C_4^1 \cdot \sigma \cdot (C_4^1)^{-1} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \sigma_{yy} & -\sigma_{yx} & -\sigma_{yz} \\ -\sigma_{xy} & \sigma_{xx} & \sigma_{xz} \\ -\sigma_{zy} & \sigma_{zx} & \sigma_{zz} \end{pmatrix}$$ (15)

Comparing the result of multiplication with the original σ matrix we will see that:

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$ (16)

Applying another symmetry transformations will give the following final result for σ:

$$\sigma_{\alpha,\beta} = \sigma \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$ (17)

It means that to describe the properties of conduction for cubic crystal we need to know not all nine members of the conduction matrix but only one. Due to the symmetry properties this matrix is diagonal. As you can see, knowledge of the crystal symmetry can help to reduce the number of parameters describing the physical properties of the research object.

§ 1.4.2 The stiffness tensor (https://en.wikipedia.org/wiki/Linear_elasticity)

The equation for Hooke's law is:

$$\sigma_{\alpha,\beta} = C_{\alpha,\beta,\gamma,\delta} \cdot \epsilon_{\gamma,\delta} \qquad (18)$$

here: σ-stress tensor, C-stiffness tensor (rank 4), ε-strain (deformation) tensor. In the same way, for a cubic crystal, it can be shown that instead of 81 stiffness tensor terms, it is sufficient to determine only 3 of them: $C_{xxxx}=C_{11}$, $C_{xxyy}=C_{12}$, $C_{yzyz}=C_{44}$.

§ 1.5 Miller indices (https://en.wikipedia.org/wiki/Miller_index)

§ 1.6 X-ray crystallography (XRD method)(https://en.wikipedia.org/wiki/X-ray_crystallography)

Questions:

1. Do integers form a group with respect to addition and multiplication operations? Proof it.This group is finite?
2. Do real numbers form a group with respect to addition and multiplication operations? Proof it.This group is finite?
3. What does Abel's group mean? Do square matrices form an Abel group? Proof it.This group is finite?
4. There is a group for 3d vectors with respect to summation? Proof it. This group is finite?
5. Present and describe all elements for point group C_{3v}.
6. Present and describe all elements for point group C_{6h}.
7. Present and describe all elements for point group D_{3h}.
8. How is looks like $3S_4^1$ transformation if T_d group. Why are there 3.
9. Write the transformation matrix for C_3^1 and C_3^2 elements of C_3 group.
10. Write the transformation matrix for C_3^1 and σ_h elements of C_{4h} group.
11. How is looks like transformation matrix for inversion for O_h group.
12. Define the basis vectors of primitive unit cell for crystal MgO. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell. Calculate the volume of primitive unit cell.
13. Define the basis vectors of primitive unit cell for crystal GaN. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group.
14. Define the basis vectors of primitive unit cell for crystal CsCl. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell.
15. Define the basis vectors of primitive unit cell for crystal CuI. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell.
16. Define the basis vectors of primitive unit cell for **graphite** crystal. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell.
17. Define the basis vectors of primitive unit cell for crystal $SrTiO_3$. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell.
18. Define the basis vectors of primitive unit cell for crystal CuCl. What Bravais lattice is in the basis

of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell.

19. Define the basis vectors of primitive unit cell for crystal TiC. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell.

20. Define the basis vectors of primitive unit cell for crystal $CuSO_4$. What Bravais lattice is in the basis of this lattice? Define the cartesian coordinates of basis vectors and all atoms inside of primitive unit cell. Define the number of space group. Calculate the volume of primitive unit cell.

21. Calculate the basis vectors for reciprocal Γ_h Bravais lattice.

22. Draw the planes for $<111>$, $< \frac{1}{2},\frac{1}{2},\frac{1}{2} >$, $< 0,\frac{1}{2},\frac{1}{2} >$, $< 0,\frac{1}{4},\frac{1}{4} >$, $< 0,0,\frac{1}{4} >$ Miller indices in Γ_c lattice.

23. The basis understanding of XRD. Bragg's law. What useful information about crystal could be obtained by XRD method?