

REGARDING THE STUDY OF CRYSTAL STRUCTURES OF SUBSTANCES

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ABSTRACT

This tutorial on defects in crystalline solids and their magnetic properties is one of the main parts of solid state physics, in undergraduate courses in physics, physics teaching methodology, vocational education, electronics and microelectronics. designed for students and masters. In it, the current achievements and current problems of solid state physics are partially described.

The educational materials, tables and drawings given in the educational manual were chosen with a specific purpose, that is, as auxiliary factors in the analysis of the problem being studied. Due to the limited size of the book, the methods of checking the structures and their physical properties were not fully described; we limited ourselves only to the X-ray diffraction method in the crystal lattice.

However, the explanation of many physical investigation methods allows the student to understand and imagine enough to analyze the next chapters of the physics of solid bodies.

Keywords: phonon, quantum mechanics, volume centered, atomic, elementary, crystalline structures, crystallization, crystal, solids.

A crystal can be considered as a collection of the same elementary (simple) structural units - crystal elementary cells, periodically located in space.

In general, the elementary cell is described as a curved parallelepiped. All atoms located in it are considered as the base of the crystal unit cell. There are specific rules for the construction of the elementary cell and base, in particular, its degree of symmetry determines most of the electrical, magnetic and mechanical properties of the crystal. An elementary cell can contain one or several atoms. For example, in many metals, such as iron, chromium, copper, silver, it covers only one atom. If the crystal consists of several chemical elements, for example, sodium and chlorine, then the unit cell contains at least two atoms: sodium and chlorine. Also, the elementary cell is composed of a group of molecules connected to each other, for example, an ice crystal or a series of magnetic materials. There are also single-cell crystals, for example, blind molecular compounds, consisting of molecules consisting of several thousand atoms.

Elementary cell. In general, after choosing the description of the elementary cell, the structure of an arbitrary crystal can be described. Naturally, one crystal unit cell can be selected in several ways (Fig. 1.1). In such a selection, the simplest cell shape, in particular, the number of right angles is as large as possible, and the size is chosen to be as small as possible (minimum). The cell with the smallest volume is called a primitive (simple) elementary cell. However, many In most cases, the largest, most shaped unit cell is selected, which consists of several atoms that form the basis of the unit cell. Figure 1.1 shows the crystal lattice of iron. This lattice is filled with cubes in the corners (1) and centers (2) of iron atoms. can be considered as an expanded space. Such a common spatial grid is called a volume-centered cube (HMK). In this case, the elemental cell can be obtained in the form of a parallelepiped (b) with a square base and oblique angles. However, as an elemental cell, the volume is 2 times larger, but It is convenient to choose a right-angled (a) cell, because it fully ensures symmetry in the arrangement of atoms, and the t of the problem makes it easier.

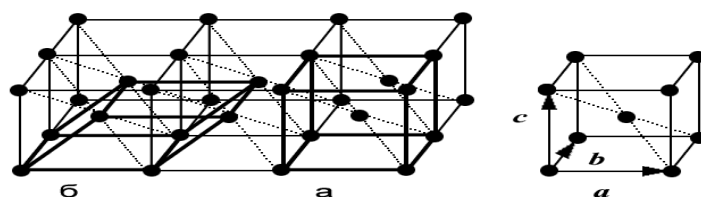


Figure 1.1. Selection of the elementary cell of the volume-centered cubic lattice.

There are three elementary cells selected $\vec{a}, \vec{b}, \vec{c}$ characterized by basic translation vectors. These vectors meet at a point and are directed along cell edges. \vec{r} and \vec{r}' two points with a radius vector are mutual $\vec{r}' = \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$ connected with the relationship, here n_1, n_2, n_3 - integers. In this case, it is convenient to describe the basic atoms at the boundary of the elementary cell, because the entire structure of the crystal can be translated into this cell, i.e. $\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$ can be created by parallel transfer to translation vectors. To fully describe the crystal structure: from one point T the vector must be given a spatial grid and a basis formed by parallel displacements.

Usually the spatial grid is three a, b, c lengths (crystal lattice constants) are known $\vec{a}, \vec{b}, \vec{c}$ vectors and between them α, β, γ is built using angles.

The basis is all atoms located in the same unit cell $\vec{r}_i = x_i\vec{a} + y_i\vec{b} + z_i\vec{c}$ is described using a set of radius vectors, here x_i, y_i, z_i endings $\vec{a}, \vec{b}, \vec{c}$ gives selected states in proportion of vectors.

It is convenient to calculate the number of atoms in the base by adding up the whole and "half", "quarter" and "one-eighth" atoms that are cut by the sides of the cell and are located inside it. The cell depicted in Figure 1.1-b contains 8 "one-eighth" atoms and atoms located in the corners, and such a basis is considered to be 1-atomic.

In crystallography, the coordinates of atoms are represented by middle brackets, because curved brackets represent crystal planes. In the case of a volume-centered cubic lattice (Fig. 1.1(a)), the cell contains one central and 8 one-eighth "corner" atoms. As a result, the basis consists of two coordinate atoms: one and the other.

Structures of polynomial compounds ($\text{CsCl}, \text{FeCo}, \text{CuZn}$ and others) is similar to the above: state 1 is occupied by atoms of one element, and state 2 is occupied by atoms of another element (Fig. 1(a)), they differed only by the lengths of the cube edges - the period of the cubic crystal lattice. Such unit cells are known as chlorinated cesium type structures.

Crystal lattice symmetry. The crystal lattice of many bodies has several symmetry elements. A symmetry operation is associated with a symmetry element. Under the influence of this operation, the spatial grid changes to itself - its shape remains unchanged. As elements of symmetry $2\pi/2; 2\pi/3; 2\pi/4; 2\pi/6$ corner-turning torsion axes are examples and are referred to as 2nd, 3rd, 4th, and 6th order torsion axes, respectively. The grids presented in Figures 1.1 (a)- and 1.2 have symmetry axes of the second, third and fourth order. Also, the plane of symmetry (usually a mirror plane) and the center of symmetry (or inversion) can be elements of symmetry.

Three symmetry planes parallel to the sides of the cubic lattice (Fig. 1.2), six diagonal symmetry planes perpendicular to the diagonal sides, four third and six second and four third order symmetry axes, as well as symmetry located at the center of the cube has a center.

Crystal lattice types. With the help of group theory, at the same time, it was proved that various structural forms of crystals can be determined by 14 types of lattices (Brave lattices) (Fig. 1.1). They form seven systems that differ in their elementary cell, including: triclinic, monoclinic, rhombic, tetragonal, trigonal, hexagonal and cubic systems. Some of them can be: -, primitive (simple), -centered in size, -centered sides, and -centered pairs of opposite sides.

So, if the elementary cell is directed along the sides of the parallelepiped connecting at one point and the nearest neighboring nodes tutashtiruvchi uchta $\vec{a}, \vec{b}, \vec{c}$ characterized by basic translation vectors, then the spatial grid $\vec{a}, \vec{b}, \vec{c}$ lengths of vectors (they are called crystal lattice constants) and between adjacent vectors

α, β, γ characterized by angles. Of course, in the information about crystals, these quantities are given quantitatively.

Now let's describe the classes of crystals in order.

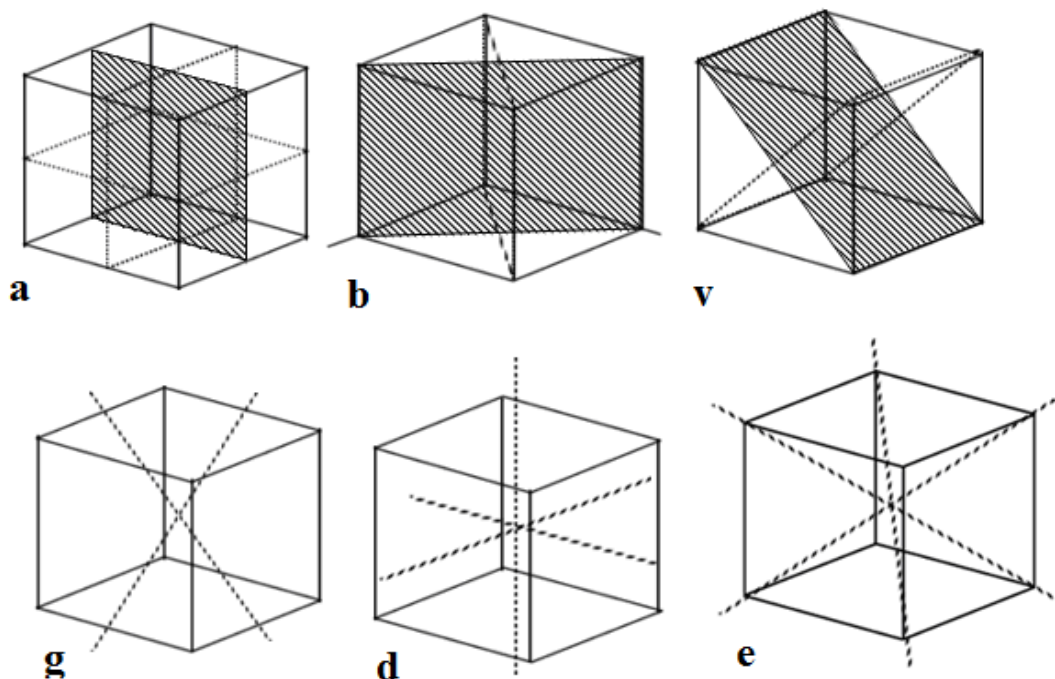
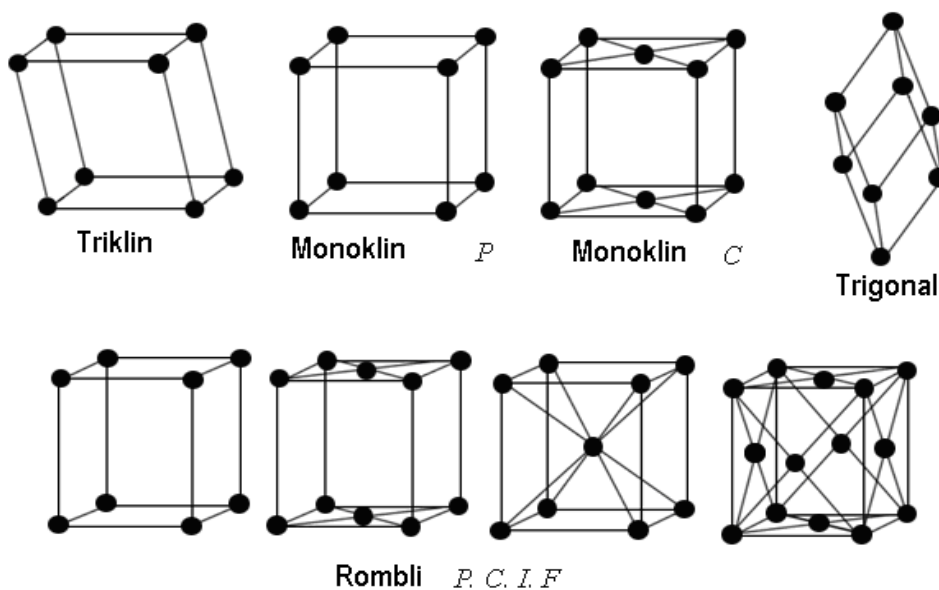
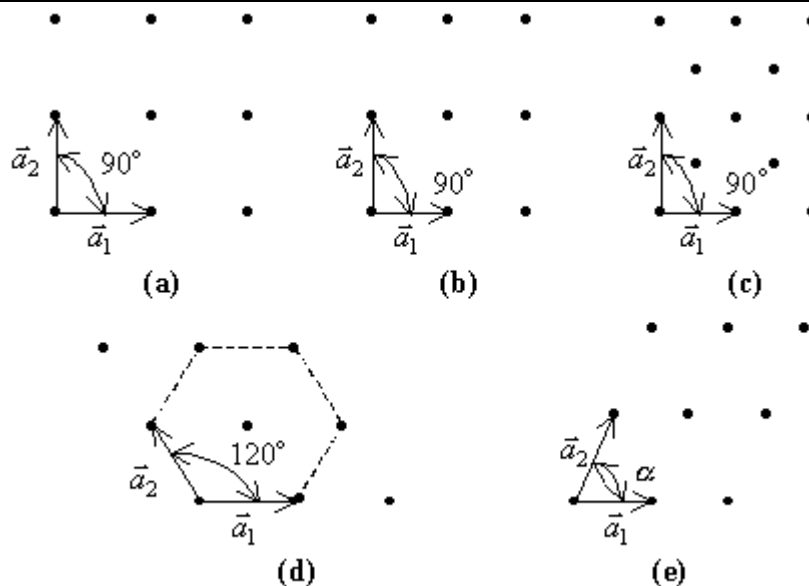


Figure 1.2. Some symmetry elements of the cube:

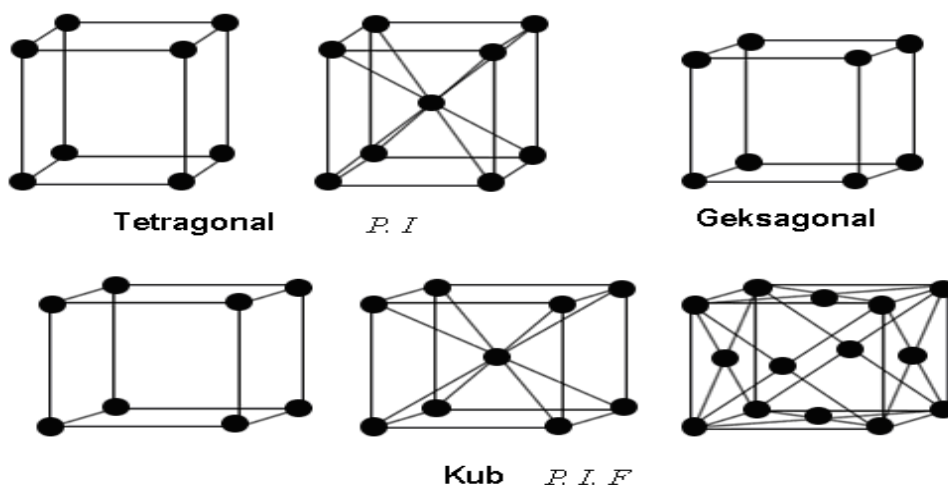
a) 3 symmetry planes perpendicular to the edges of the cube; b, c) 4 of the 6 symmetry planes perpendicular to the diagonals of the cube sides; g) 2 of the 6 symmetry axes of the 2nd order passing through half of the opposite edges of the cube and parallel to the diagonals of the sides; d) 3 axes of symmetry of the 4th order perpendicular to the sides of the cube and passing through their center; e) 4 axes of symmetry of the 3rd order parallel to the diagonals of the cube and passing through the vertices.





1.3-a rasm. Brave panjarasi.

1. Triklin system $\vec{a}, \vec{b}, \vec{c}$ the lengths of the vectors are not equal to each other, but between the adjacent sides α, β, γ angles are equal to each other. Such a lattice has a center of symmetry located at the center of the elementary cell.
2. The monoclinic system is in the form of a cell, and the lengths of its edges are different. Nest C and P it can be in the form of a prism. Symmetry elements such as a plane of symmetry parallel to the base plane of a right prism and a second-order torsion axis are added to such a grid.
3. In the rhombus system, the lengths of the edges of the cells are in the form of parallelepipeds with different right angles. The nest is mentioned above P, I, F, C includes parallelepipeds. In such a grid, the following symmetry elements are added: three symmetry planes parallel to the legs and three second-order torsion axes directed along the straight line connecting the nodes of the parallelepiped center and opposite sides.
4. In the tetragonal system, the cell is in the form of a rectangular parallelepiped with a square base, and its size can be centered. Also, in contrast to the rhombus system, a fourth-order torsion axis passing through the centers of the opposite sides of the parallelepiped and some symmetry planes additionally appear.
5. The cube system is in the form of a nested cube, and its sides and volume can be in the form of a centered cube. Such type of grids have high symmetry.



1.3-b rasm. Brave panjarasi.

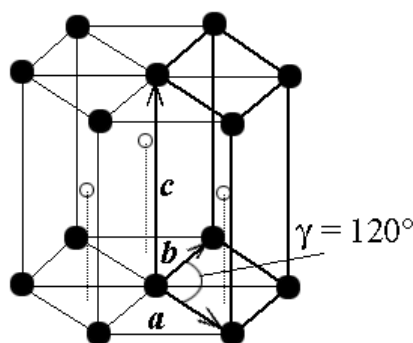


Figure 1.4. An elementary cell of a hexagonal lattice.

6. In the hexagonal system, the slot is in the form of a right prism with a 60-degree rhombus base, and is viewed as a triple slot (Fig. 1.4a). In order to analyze this cell, a hexagonal prism with a sixth-order torsion axis connecting the centers of the hexagonal bases is introduced.

7. In the trigonal system, the cell is in the form of a rhombohedron, and all its sides are the vertex angle $\neq 90^\circ$ is made up of identical rhombuses. If a grid is chosen in the form of a cube centered on , sides and volume, then the grid can be divided into elementary trigonal cells of 4 and 2 times smaller size than the selected cube volume, respectively.

All other "types" of lattice types can also be encountered. For example, the grid "b" with a square base depicted in Figure 1.1 is another type of grid that leads to the above-mentioned type of grid. $\vec{a}, \vec{b}, \vec{c}$ can be described by vectors.

The symmetry of the grid determines the anisotropy of physical properties, that is, the characteristic values take a value depending on the selected direction. The anisotropy of some physical quantities is characterized by the shape of the unit cell in the crystal. For example, rhombic, monoclinic and triclinic lattice crystals usually have a small number of symmetry elements, and anisotropy is observed in their series of properties, such as relative electrical conductivity and thermal conductivity coefficient. These quantities are usually expressed using matrices of the second order. In crystals with a symmetric cubic lattice, these quantities are scalar; in crystals with a tetragonal or hexagonal lattice become single-valued quantities in the planes perpendicular to the edges. Thus, the symmetry properties of tensors of physical quantities are determined by the symmetry of the crystal lattice.

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