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ATOMIC STRUCTURE OF THREE-DIMENSIONAL CRYSTALS

Abstract: If the arrangement of atoms or molecules in crystals is preserved throughout the crystal, such crystals are called monocrystals. All single crystals have anisotropy, that is, their physical properties differ in certain directions. In crystalline solids, the atoms and molecules that make up them are arranged in a certain order. If this order is maintained up to distances several times greater than the distance between two neighboring atoms or molecules, we call it a long order.

Key words: Crystal, electron microscope Polycrystals, macroscopic fragments of monocrystals, electron diffraction, interaction between atoms on the surface, physical properties of single crystals, Three-dimensional crystal lattices.

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АТОМНАЯ СТРУКТУРА ТРЕХМЕРНЫХ КРИСТАЛЛОВ

Аннотация: Если расположение атомов или молекул в кристаллах сохраняется по всему кристаллу, такие кристаллы называются монокристаллами. Все монокристаллы обладают анизотропией, то есть их физические свойства различаются в определенных направлениях. В кристаллических твердых телах атомы и молекулы, входящие в их состав, расположены в определенном порядке. Если этот порядок сохраняется до расстояний, в несколько раз превышающих расстояние между двумя соседними атомами или молекулами, мы называем его длинным порядком.

*Ключевые слова: Кристалл, электронный микроскоп
Поликристаллы, макроскопические фрагменты монокристаллов,
дифракция электронов, взаимодействие атомов на поверхности,
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решетки.*

In crystalline solids, the atoms and molecules that make up them are arranged in a certain order. If this order is maintained up to distances several times greater than the distance between two neighboring atoms or molecules, we call it a long order. If the arrangement of atoms or molecules in crystals is preserved throughout the crystal, such crystals are called monocrystals [1]. All single crystals have anisotropy, that is, their physical properties differ in certain directions. There are very few single crystals in nature, therefore polycrystalline materials are converted into liquid and monocrystals are grown based on special technologies. Crystals formed by the irregular joining of macroscopic particles of monocrystals are called polycrystals. Since polycrystals are composed of irregular arrangement of single crystal cells, their physical properties are the same in all directions. Such bodies are called isotropic bodies [2].

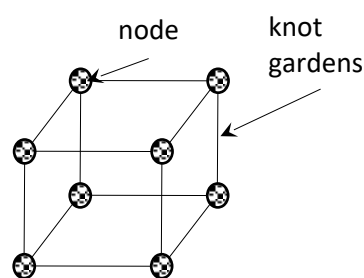


Figure 1.1. View of crystal lattice nodes and node bonds

Particles that make up crystals vibrate at their equilibrium point. These balance points are called crystal lattice nodes. The threads that connect the knots are called knot ties [3].

The distance between nodes is 1-5 Å. The distance between the nodes in one direction may differ from the distance between the nodes in another

direction, depending on the crystal structure of the body, we can distinguish one type or different types of crystal lattices. For example, Si atoms are located in all the nodes of silicon crystals, while GaAg crystals have Ga in one node and Ag in another node [4]. The smallest part that preserves the structure of the crystal lattice is called an elementary cell. Usually, the elementary cell crystal consists of a parallelepiped shape, we direct 1 2 3 vectors along the 3 edges of this parallelepiped, the length of these vectors should be equal to the length of the edge of these parallelepipeds, such vectors are called basic translation vectors (or periods) [5]. The main property of translation vectors is that infinitely large crystals can be formed using these vectors. The simplest parallelepiped crystal is as follows:

$$R = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

where n_1, n_2, n_3 are integers, R is the size (size) of the crystal lattice

If all of these elementary cells are moved on top of each other, a crystal lattice is formed. Such a repeating group of atoms is called a base

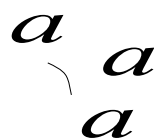


Figure 1.2. The view of the elementary cell

If the basis and translational size of an arbitrary crystal is determined, then this crystal lattice is determined [6].

In general, crystals have a certain point symmetry, which means that certain rotations of this lattice can be brought back to its place by reflection. Symmetry is determined using a scanning electron microscope. Depending on this point, it is possible to determine the physical properties of monocrystals by turning them to azimuths or polar angles in order to determine whether they have the property of anisotropy [7].

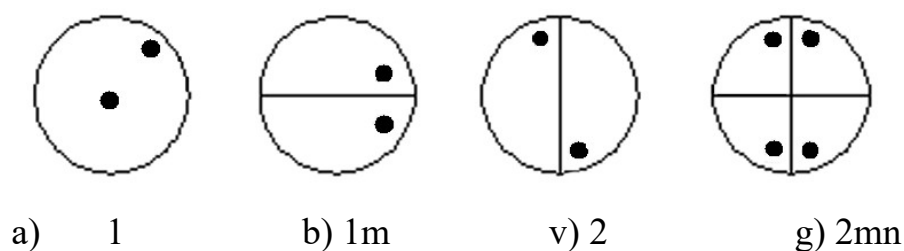


Figure 1.3. Appearance of symmetries

a) the figure shown in the picture does not have symmetry with respect to the given axis or plane, this figure overlaps with itself only when it is turned through an angle of 360° , the circular designation of objects with such lower symmetry is accepted as 1.

The shape in b) is represented by a long line, so it is symmetrical about the plane. Such a form is designated as 1m [8].

c) in the figure, when turning 180° degrees, the symmetry overlaps each other. And when it turns 360° degrees, it falls on top of each other on March 2. Such symmetry has a 2-order symmetry bar and is denoted by the number 2. The last symmetry is defined as 2 mm because it is symmetrical about the plane and the torsion axis.

Crystal lattices can be considered to be formed by stacking, twisting (rotating) or reflection of elementary cells. So, the crystal lattice consists of a set of elementary cells arranged in a certain order [9].

In general, crystal lattices have a certain point symmetry. that is, this grid can be brought back to its place (its state) through certain rotations and reflections.

The sum total of rotations and reflections that keep the given configuration (shape) of geometric points invariant forms a certain group. Such groups are called point groups [10].

Three-dimensional crystal lattices can be divided into 7 different point groups. They are called halohedral point groups. One crystal system corresponds to each halohedral group. There are 7 different crystal systems, which make up

14 different types of lattices. These grids are called Bravais lattices. They are given in Table 1.1 [11].

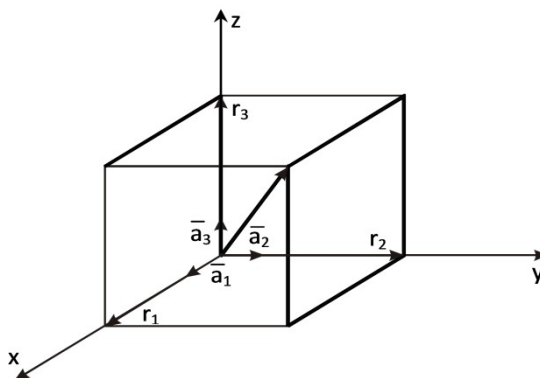


Figure 1.4. Drawing view of primitive grid. - unit vectors, - integer coefficients.

It can be seen from the table that one or more Bravais lattices are suitable for each system.

1.1 – table Symmetry groups of three-dimensional crystals

t/r	Crystal system	Bravais lattice
1	Triclinic	Simple
2	Monoclinic	Simple, the base is centered
3	Orthorhombic	Simple, base-centered, volume-centered, side-centered
4	Trigonal	Simple
5	Tetragonal	Simple, the base is centered
6	Hexagonal	Simple
7	Cubic	Simple, base-centered, volume-centered, side-centered

In addition to translational symmetry, crystal lattices are characterized by other symmetry properties. These are called point groups and spatial groups of directions. Point groups of directions are divided into 32 types. Each of these groups corresponds to one crystal class. The number of spatial groups is 230. We will not consider the point group and spatial groups [12,13].

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