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CRYSTAL STRUCTURE OF METALS

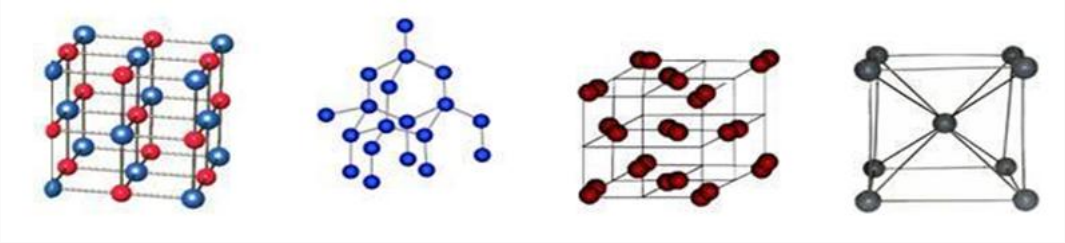
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Abstract: In this article, the types of bonding of metals, crystal lattice shapes, Miller indices, crystalline iodine, sulfur, white phosphorus, carbon dioxide, crystal structure of methane elements, types of crystal lattices of some metals and their parameters, the main types of crystal lattices and sodium chloride crystal Information such as structure is widely covered.

Key words:crystal, Miller indices, carbon dioxide, methane, parameter, sodium chloride, fluorspar, corundum, ruby, silicon oxide, mineral, quartz

Enter: The development of industry and the achievements of mechanical engineering are largely related to the creation and use of strong, stable, light (especially in aviation) metallic and non-metallic materials.

The requirements for the material depend on its operating conditions: mechanical loading, temperature, the influence of the external environment, etc. For example, the frictional parts of the tractor must be resistant to abrasive wear (especially in the conditions of Central Asia); cotton picker spindles should be made of material resistant to both abrasive and chemical corrosion; aircraft struts (longer, stringer, etc.) are made of material with static strength and high stiffness; fire resistance-heat resistance (650-850ºC) requirements are imposed on aircraft engine material; the upper layer ("paning") of supersonic aircraft is made of light materials operating at 350-550ºC. It should be said that composite materials (including nanomaterials) are increasingly used in modern machines. Their volume reaches from 5-10% to 70-80%. Composite materials have excellent special properties. High precision; resistance to abrasion; heat and low conductivity; if necessary, it can be superconducting material; chemical stability, good light transmission**.**



a) b) s) d)

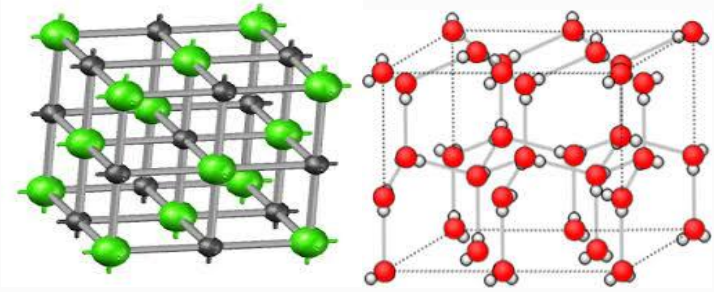
Figure 1. a) ionic bond; b) atomic bonding; c) molecular bond; d) metal bond

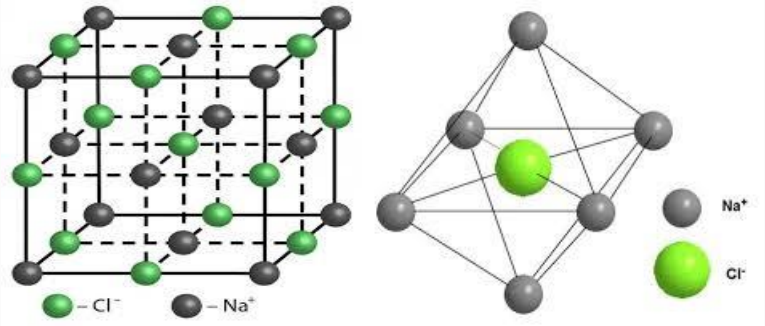
Dependence of properties of substances on the type of crystal lattice. At the nodes of the atomic crystal lattice, there are atoms connected by covalent bonds. Examples of atomic crystal lattice substances are diamond, silicon, germanium, boron. Substances with an atomic crystal lattice are characterized by a high melting point and hardness. There are positive and negative ions in the ionic crystal lattice, and the bond between them is ionic. Salts, alkalis and oxides of metals usually have an ionic crystal lattice. Ionic crystal lattice substances are characterized by high melting points, hardness, density and good electrical conductivity [6].

In the places where the molecular crystal lattice is located, there are molecules that are held together by intermolecular Van Der Waals forces. Examples of substances with a molecular crystal lattice are ice, iodine, naphthalene, and carbon dioxide. Intermolecular bonds are much

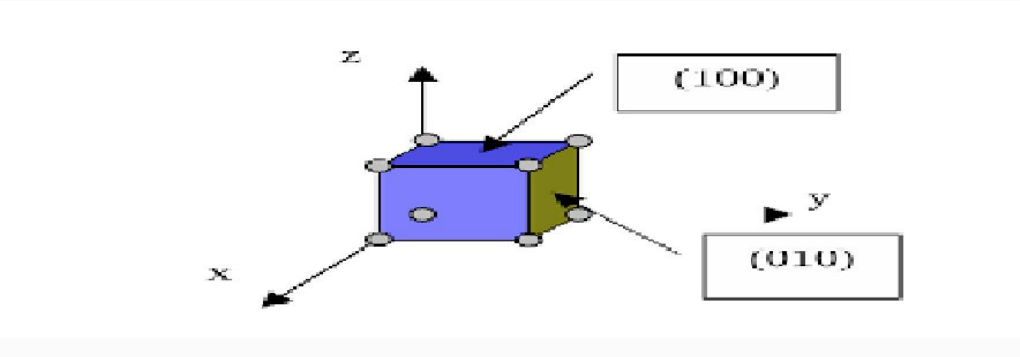
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weaker than covalent and ionic bonds; therefore, substances with a molecular crystal lattice are distinguished by low melting points, low hardness and the possibility of sublimation (transition from a solid state to a gas state, bypassing the liquid state)[1]. Metals are characterized by a metallic crystal lattice, the nodes of which contain positively charged metal ions, and valence electrons (called electron gas) move freely between them. Metal lattice materials are characterized by mechanical strength, solubility, flexibility, good thermal and electrical conductivity, and metallic luster. The properties of crystalline bodies are determined not only by the nature of the connection between particles, but also by their mutual location in relation to each other. In diamond crystals, all carbon atoms are connected by non-polar covalent bonds and are located at the same distance from each other, forming tetrahedra. In graphite crystals, all six carbon atoms are connected by non-polar covalent bonds, and such planar hexagons are connected by weak intermolecular bonds.





2 – picture. Crystal lattice structure



3 – picture. Miller indices

Atomically SiC, SiO2, B, Si, diamond, graphite, black and red phosphorus. In substances with a molecular crystal lattice, the molecules are located at the nodes of the crystal lattice, the strength of this connection is weak. Substances with a molecular crystal lattice are characterized by low melting points, that is, they are soluble and volatile, significantly compressible,

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sometimes odorous, and sublimation or sublimation phenomena, such as iodine and solid carbon **dioxide (Fig. 4)**

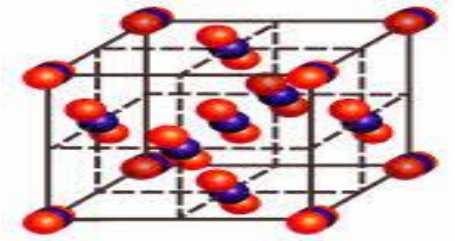
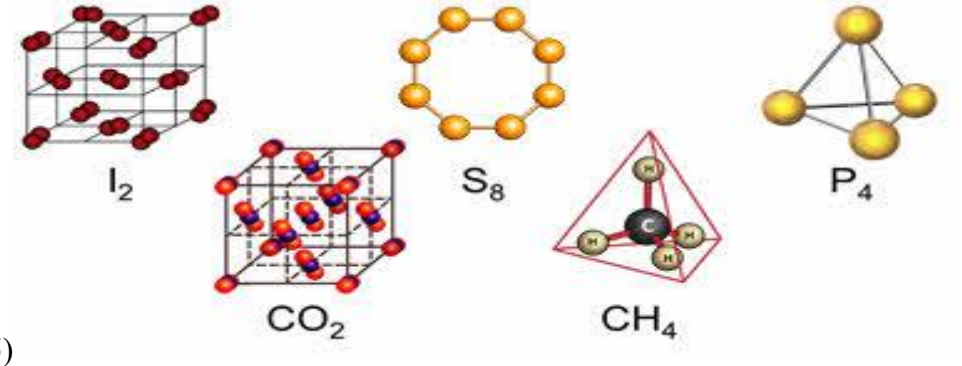


Figure 4 Molecular crystal lattice structure.

Substances with a molecular crystal lattice are characterized by low hardness; most of these substances are easily soluble in water. Gases and liquids in a state of solid aggregation have a molecular crystal lattice. For example, crystalline iodine, sulfur, white phosphorus, carbon dioxide, most organic compounds (Figure



5)

Figure 5. Crystal structure of elements of crystalline iodine, sulfur, white phosphorus, carbon dioxide, methane.

In substances with an atomic crystal lattice, atoms are arranged in nodes. Bonds between atoms in crystal lattices are covalent, very strong. These substances are characterized by high boiling and melting points, that is, they are refractory and non-volatile, very hard, practically insoluble in water and odorless. Diamond and graphite are examples of this type of crystal lattice substances[4].

Diamond Graphite



Figure 6. Crystal structure of diamond and graphite

It is known that diamond hardness is rated as the highest value on the Mohs scale. Due to its high hardness, diamond is used for making drills, grinding tools, and glass cutters. A diamond is a jeweler's stone, they use a polished diamond - a diamond. Graphite is also a substance with an atomic crystal lattice, but nevertheless it is soft because it has a layered structure. In the crystal lattice of graphite, carbon atoms lying in one plane are connected in regular hexagons. The bonds between the layers are weak, so graphite is soft. Graphite, like diamond, is refractory. It is used in the production of electrodes, solid lubricants, pencil rods, and neutron moderators in nuclear reactors. Atomic crystal lattices contain not only simple but also complex substances. For example, all types of aluminum oxide. Such as emerald, corundum, ruby, sapphire (Fig. 7).

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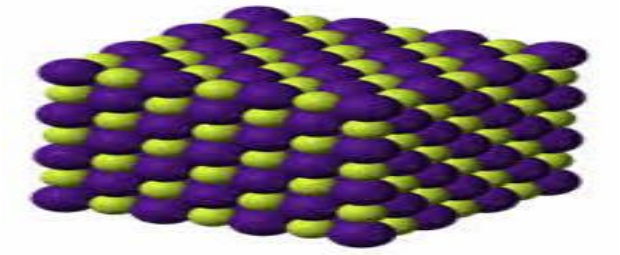
Figure 7. 1) Najdak, 2) corundum, 3) structure of ruby

The most common silicon compound is quaternary silicon oxide, which also has an atomic crystal lattice (Figure 8). Almost pure silicon oxide is the mineral quartz.



Figure 8. The appearance of silicon oxide is the structure of the mineral quartz.

In substances with ionic bonds, ions are located at the nodes of the crystal lattice, the bond between particles is ionic, it is strong (Fig.



9).

Figure 9. Ionic type of bond

For substances with an ionic type of bond, the following properties are characteristic: high melting and boiling temperatures, they are refractory and non-volatile, they are hard, brittle and most of them are soluble in water. Their fragility is that if you try to deform such a crystal lattice, then one of its layers will move relative to the other layer until the ions of equal charge are opposite each other. These ions begin to displace each other and the crystal lattice relaxes. Ionic compounds are poor conductors of electricity and heat. But their solutions and solutions conduct electricity. Substances with ionic compounds are odorless. An ionic compound is a large association of ions that are held together in space due to the balance of attractive and repulsive forces[5]

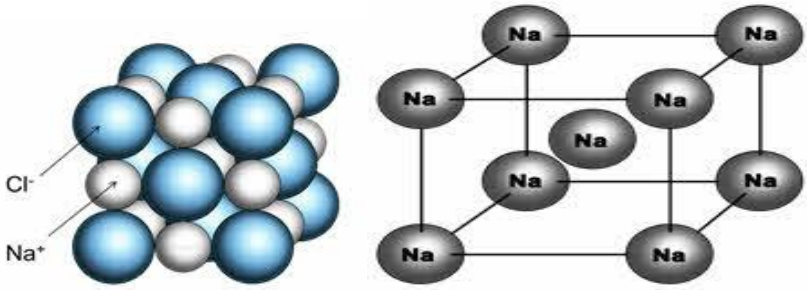


Figure 10. Crystal structure of sodium chloride.

For example, sodium chloride crystals consist of sodium cations and chlorine anions. Each sodium cation is surrounded by six chlorine anions, and each chlorine anion is surrounded

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by six sodium cations. The smallest structural unit of a crystal is the unit cell. The structure of the unit cell depends on the size ratio of the cation and anion. In substances with a metallic type of bond, the atom-ions are located at the nodes of the crystal lattice, and the bond between them is metal. A link can have different strengths. The metal crystal lattice determines the properties of metals: flexibility, electrical and thermal conductivity, metallic luster, the ability to form alloys.

Metals are expressed in the ability to deform under the influence of mechanical stress. This property is based on the forging, rolling, and wire drawing capabilities of metals. Plasticity is explained by the movement of layers under the influence of force without breaking the interconnection (Fig. 11)

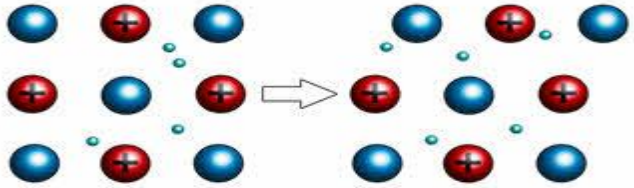


Figure 11. Movement of layers under the influence of plastic force, without breaking the interconnection.

For example, if you put a few drops of water on two formed glass plates, the plates will move freely relative to each other, but it will be very difficult to separate them. Thus, in this experiment, water played the role of free electrons in the metal crystal lattice. The most malleable metals include gold, silver and copper. You can make the thinnest film of gold, three thousandths of a millimeter thick. The high electrical conductivity of metals is caused by the presence of free electrons, which have a directed movement under the influence of electric current (Fig. 12)

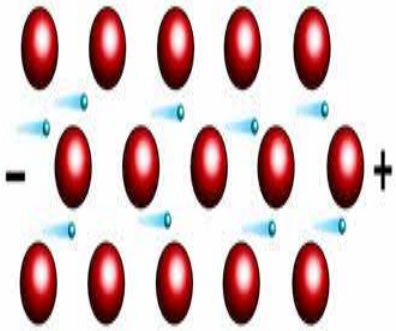


Fig. 12. Observation of thermal conductivity of metals, movement of free electrons.

The best conductors of the electric eye are silver and copper, slightly worse - aluminum. However, in most cases, aluminum is used as electrical wires, not copper. The thermal conductivity of metals is also explained by the movement of free electrons, which collide with atomic ions at the nodes of the crystal lattice and exchange energy with them. Thanks to this feature, metal dishes heat up evenly. Metal-type crystal lattice substances have a metallic luster due to the reflection of light rays[7].

Types of crystal lattices of some metals and their parameters.

Table 1

Metallarning nomi	Panjaraning turi	Panjaralarning parametrlari A^0 hisobida		
		A	B	C
Aluminum	A cube with concentric sides	4.041	-	-

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Vannadium	Volume centered cube	3.034	-	-
Tungsten	Volume centered cube	3.158	-	-
Iridium	A cube with concentric sides	3.832	-	-
Cobalt	Hexagonal	2.5	-	4.07
Cobalt	A cube with concentric sides	3.54	-	-
Silver	A cube with concentric sides	4.078	-	-
Magnesium	Hexagonal	3.203	-	5.2
Copper	A cube with concentric sides	3.607	-	-
Molybdenum	Volume centered cube	3.14	-	-
Nickel	Hexagonal	2.49	-	4.08
Nickel	A cube with concentric sides	3.157	-	-
Niobium	Volume centered cube	3.294	-	-
Gold	A cube with concentric sides	4.07	-	-
Platinum	A cube with concentric sides	3.915	-	-
Zinc	Hexagonal	2.659	-	5.607
Tantalum	Volume centered cube	3.296	-	-

Grid parameters are extremely important. Current methods of scientific investigation - methods of using X-rays allow to accurately measure the parameters of crystal lattices. Both in the face-centered cubic lattice and in the hexagonal lattice, where the atoms (ions) are densely packed, the atoms are denser than those in the other lattices. For example, in each of these two lattices, the atomic volume is 74% of the lattice volume, whereas in a volume-centered cubic lattice, the atomic volume is 68% of the entire lattice volume. Table 2

№	Crystal Syngonia	Sizes (parameters) describing elementary cells
1	Triclin	$a_1 \neq a_2 \neq a_3 \quad \alpha \neq \beta \neq \gamma$
	Monocline	$a_1 \neq a_2 \neq a_3 \quad \alpha = \beta = 90° \neq \gamma$
3	Rhombic	$a_1 \neq a_2 \neq a_3 \quad \alpha = \beta = \gamma = 90°$
4	Tetragonal	$a_1 = a_2 \neq a_3 \quad \alpha = \beta = \gamma = 90°$
5	Cubic	$a_1 = a_2 = a_3 \quad \alpha = \beta = \gamma = 90°$
6	Trigonal	$a_1 = a_2 = a_3 \quad \alpha = \beta = \gamma \neq 90° < 120°$
7	Hexagonal	$a_1 = a_2 \neq a_3 \quad \alpha = \beta = 90° \quad \gamma = 120°$

3- table

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Crystal Syngonia	Definition of point groups		Point group name
	International		
1. Trikilin	$\frac{1}{1}$	Monohedral	Monoedrik Pinakoidal
2. Monocline	2 m 2/m	Pinacoidal	O‘qli diedrik O‘qsiz diedrik Prizmatik
3. Rhombic	222 mm mmm	Axial dihedral	Rom tetraedrik Romb-piramidal Romb dipiramidal
4. Tetragonal	4 442 2/m 2/mm 2/mmm 4 4 2/m	Arrowless dihedral	Tetraognal pyramidal Tetragnal trapesiyoedirik Tetrognal dipiramidal Ditetrognal piramidal Ditetrognal dipiromidal Tetrognal tetraedrik Tetrognal skalenoedrik
5. Triognal	3 32 $\frac{3m}{3}$ 3m	Prismatic	Trigonal pyramidal Trigonal rapesioedrik Ditrigonal pyramidal Romboedrik Ditrigonal ckalenoedrik
6. Hexagonal	6 6m2 6 622 6/m 6/mm 6/mmm	Rome is tetrahedral	Trigonal dipiramidal Ditrigonal dipiramidal Geksognal priamidal Geksognal trapesioedrik Geksognal dipiramidal Digeksognal piramidal Digeksognal dipiramidal
7. Cubic	23 m3 43m 4332 m3m	Rhombus-pyramidal	Tritetraedrik Didodeksaedrik Geksatetraedrik Triontaedrik Geksantoedrik

Each symmetry group is defined by the main generating symmetry operations. In addition to point symmetry, crystals also have translational symmetry. There are 14 possible translational symmetry operations for a crystal lattice. One unit cell can be assigned to each translational symmetry operation. As a result, 14 different elementary grids are created, these elementary grids are called Brave grids. Translational symmetry is when a crystal overlaps itself when we move it along a certain vector. Each syngonia of crystals can only have a specific type of Brave grid[8].

The complete symmetry of the crystal lattice is determined by the spatial symmetry group. In the spatial symmetry group, the operations of point and translational symmetry of the crystal are embodied. There are 230 space groups in total, and any crystal belongs to one of these groups

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according to its structure. If the spatial symmetry group of a crystal is known, it is very easy to derive its crystal structure, so it is important to know the symmetry group of the crystal. Currently, crystal symmetry is determined using X-rays. This branch of science is called crystallography[9].

1. Triclinic syngonia lattices are just simple R-shaped lattices. The number of parameters representing the Brave grid is 6: three edges and three corners.

2. Monoclinic syngonia can have two Brave lattice shapes. One of them has a simple R-shaped cell, and the other has a centralized base, that is, an S-shaped cell. These grids are determined by 6 parameters (a1, a2, a3, a, b, g).

3. Rhombic syngonia can have four different Brave grids; R - simple, S - centered base, volume centered - I and side centered - F type lattices. Grids of this form are determined by four parameters (a1 a2, a3, a).

4. Tetragonal syngonia has two types of grids, i.e. R and I, and is defined by three parameters (a1, a2, a).

5. **Trigonal syngonia** is defined by two parameters (a1, a) in this syngonia there is only R-shaped Brave lattice.

6**. There is one Brave lattice in the hexagonal syngonium**, defined by four parameters. This cell belongs to the S-shape, and in many cases it is represented as a simple cell with three R-shapes.

7. Cubic syngonia can have three types of cells: R-, I-, and F-shaped cells. Cubic syngony can be defined by two parameters (a, a). In general, the use of one or another material for machine parts depends on specific working conditions and, of course, economic competition. Details of machines (mechanisms) work in different conditions: say, to dynamic stresses, at different temperatures (low and high); in different environments (alkaline, acidic, neutral, active gas), etc. These are the materials used. All of these usages come from technological economic requirements[10]

It ensures the structural strength of the material in accordance with the requirements of use. The structural strength of the material refers to its complex characteristics: These are the sum of the criteria of strength, reliability, long-term. Depending on the conditions of use, the strength criterion of the materials is selected. For materials used in mechanical engineering (especially aircraft engineering), the mass efficiency of the material is important. Efficiency is evaluated by comparative (relative) characteristics.[11]

Relative strength:

$$Б_c = Б / pg. \quad (1)$$

where Б-material strength, Б-kg/mm2, -density g/cm3, =9.8 free fall acceleration.

Relative virginity:

$$\gamma_c = E / \rho \cdot g \quad (2)$$

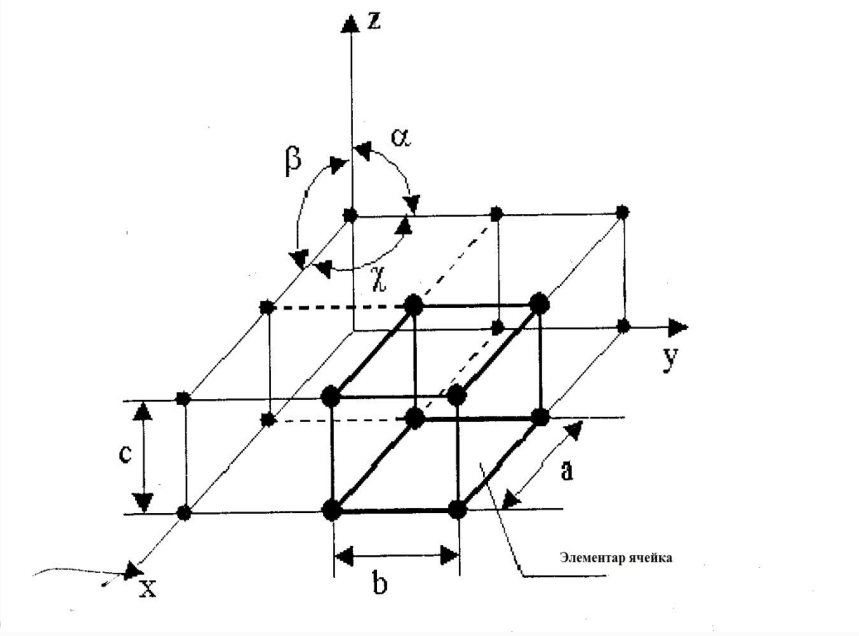
where E is the modulus of elasticity.

Technological requirements (technological quality of the material) are aimed at ensuring the minimum amount of labor in the preparation of details and constructions, of course, providing the necessary properties.

All metals and alloys are crystalline solids; that is, up to a certain temperature (T melting) it remains solid and retains its shape and size. After this temperature, it becomes liquid. Crystalline bodies are represented by the orderly arrangement of their particles (atoms) in space. This is called a crystal lattice. A crystal lattice is an imaginable spatial lattice; particles (atoms,

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ions) are located in its nodes; which in turn forms a solid (Figure



13)

Figure 13. Crystal lattice diagram.

Metals and alloys are crystalline bodies in which positive ions form crystal lattices. In amorphous bodies (glass, wood, porcelain), atoms are arranged irregularly and do not form a crystal lattice.

An elementary (simple) cell is a volume element with the least number of atoms. Repeat this many times to see the crystal in space. The main indicators (parameters) of crystals are as follows:

1. Dimensions of the ribs of the elementary cell, a, v, s-lattice period - the distance between the centers of the nearest atoms. (Fig. 13).
2. Angles between axes (a, b, g).
3. Coordination number (K). This shows the number of atoms in the lattice that are the same minimum distance from the desired atom.
4. Lattice basis - the number of atoms corresponding to the elementary cell of one lattice.

The density of the arrangement of atoms in the crystal lattice is the volume occupied by the atoms when viewed conventionally as a spherical sphere. The volume occupied by these atoms is taken in relation to the cell volume. The volume is 0.68 for a centered cubic lattice, and 0.74 for an edge-centered cubic lattice. Types of crystal lattices were studied and classified by the French scientist O. Brave. Crystal bodies have 14 different lattices: cubic, rhombic, hexagonal, tetragonal, etc. The most common for metals are 3 types.

1. Volume-centered cubic (H.M.K.). (Fig. 14, a) Atoms are located at the vertices of the cube and in its center. This applies to the following metals: V, W, Ti, Fe_{α}.

2. Concentric cube (Yo.M.K.) (Fig. 14 b). Atoms are located at the vertices of the cube and in the center of each of its 6 sides. These metals are**:** (*Ag,Au,Fe*).

3. Hexagonal: it is based on a hexagon (Fig. 14 c). This, in turn, is of 2 types: simple atoms are located at the vertices of the cell and in the center of the base. There are 3 additional atoms in the densely packed middle surface. Metals with a hexagonal lattice: (*Zn,Mg,Cg,Ti*). The average distance between the centers of neighboring atoms is 4-5 A (0.4-0.5 nm).

Amorphous objects are randomly arranged in space: tar, glass paraffin. Amorphous bodies soften when heated, become organized, and then turn into a liquid state. When cooled, the process is reversed. All amorphous bodies are isotropic. This means that atoms have the same

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property in all directions. Crystal lattice objects are all anisotropic, that is, their properties are different in all directions[12].

Some metals have the phenomenon of polymorphism (allotropy), that is, they have different structures under different conditions. With changes in temperature and pressure, it changes from one crystal structure (lattice) to another structure (lattice). These are metals: Fe, Co,Ti,Mn,Ca…

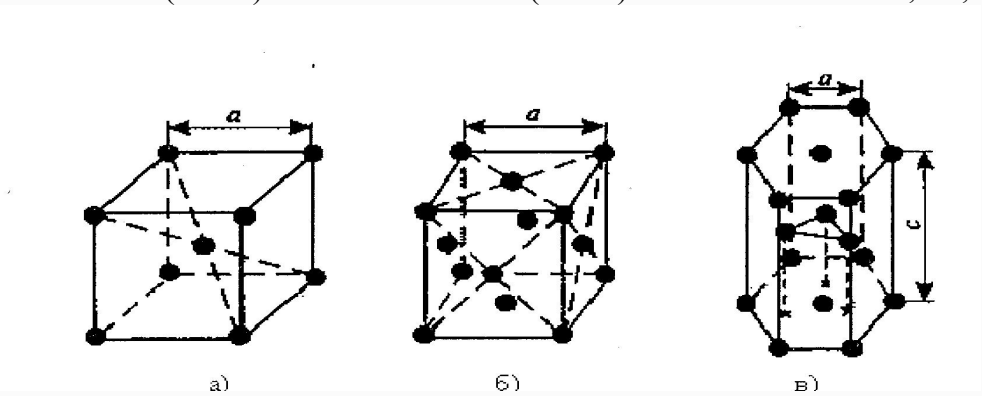


Figure 14. The main types of crystal lattices: a – cubic centered in size; b - cubic with centered sides; v – hexagonal.

During an allotropic change, heat is released or absorbed. The different alpotrolic forms of a metal are denoted by the Greek alphabet. For example, iron:

Fe_α this is the temperature $t\langle 911^0 C$ do X.M.K

$911^0 C < t < 1392^0 C -$ Yo.M.K $- Fe_\gamma$

$1392 < t < 1539^0 C -$ X.M.K $- Fe_\beta$.

Fe_β - it is high temperature.$Fe_{2\,\alpha}$

Now, with a change in pressure, there can be an allotropic change. An example of this is carbon: graphite is formed at low temperature; at high temperature - diamond is formed. Alloys can be refined (strengthened) and softened by heat treatment using the phenomenon of polymorphism.

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