Program courses

Crystal Physics

The purpose and tasks of course "Crystal Physics" is to give the regular description of physical properties of crystals by tensors. Thus the crystal is considered as the single-phase continuous medium in respect to symmetry and anisotropy. The used mathematical apparatus used based on tensor analysis, allows to study features which are the general for various properties of crystals. **The student should know** the specific features of crystals related to symmetry and anisotropy of the crystal medium, the thermodynamic relations describing various physical properties, and also bases of the mathematical apparatus allowed to study these properties from the uniform point of view.

<u>The student should be able</u> to use in practice the received knowledge for research of crystals properties for development of new materials with the set properties, for the new devices and technical devices creation, for development of new technologies, and also for effective work with the scientific literature.

Theme 1 Mathematical basis of crystal physics

Scalars, vectors, the first, second, third and fourth rank tensors. Recording with summation indexes. Transformation of coordinate axes. Transformation of vector components. Transformation of point coordinates. The transformation law of product of coordinates. Transformation of the second rank tensor component. Definition of any rank tensor. The transformation matrix. The difference between transformation of a matrix and a tensor. Symmetric and antisymmetric tensors.

The general equation of the second order surface. A characteristic surface. The main axes of coordinates. Reduction ways of the second rank tensor to the principal view. Construction of the Moor circle

Simplification of the equations at reduction to main axes. The value describing property in the given direction, its definition and analytical expressions in general and special cases. Geometrical properties of a characteristic surface. Length of a radius-vector. Properties of a radius-vector and a normal. Values ellipsoid of the second rank tensor.

Theme 2. Influence of crystals symmetry on their properties.

Basic symmetry elements of crystals. Point group of symmetry, an elementary cell. Syngony. Crystallographic systems. Neumann's principle. Influence of crystal symmetry on the properties described by first and second rank tensors.

Theme 3. The physical properties of crystals described by first rank tensor.

Pyro-electricity, electrocaloric effect. Ferroelectricity. Influence of crystal symmetry on these properties.

Theme 4. <u>Equilibrium physical properties</u>.

Paramagnetic and diamagnetic susceptibilities. The general relations. Energy of crystal magnetization. Forces and the moments of forces. The moment of forces acting on a crystal in a homogeneous magnetic field. The force acting on a crystal in a non-uniform magnetic field. The mechanical moment acting on a crystal in a non-uniform magnetic field. A magnetic susceptibility of a crystal powder.

Electric polarization. Difference between electric polarization and magnetization. An electrostatic field in homogeneous anisotropic dielectric.

Theme 5. Field tensors: stress tensor and deformation tensor

Concept of a stressed state. Homogeneous and non-homogeneous state. The proof that the stresses are described by the second rank tensor. The stress surface. Special forms of stress tensor. Distinction between the stress tensor and second rank tensors describing the crystal equilibrium properties.

Deformation tensor. One-dimensional deformation. Bidimentional deformation. Homogeneous bidimentional deformation. Three-dimensional deformation. Homogeneous three-dimensional deformation. Generalization on a case of non-homogeneous deformation. Deformation and symmetry of crystals. Thermal expansion of crystals. A cone of zero thermal expansion in the calcite crystal.

Theme 6. <u>The 3-rd rank tensors. Piezoelectricity</u>.

Direct piezoelectric effect. Reduction of independent modules number. The matrix method. Inverse piezoelectric effect. Influence of crystal symmetry. Analytical method. Examples for some symmetry classes.

Theme 7. The fourth rank tensors. Elasticity.

Hooke's law. Matrix designations. Energy of the deformed crystal. Reduction of number of independent modules because of restrictions applied by crystal symmetry. A relation between stress and deformations for isotropic materials. Relations between pliability and hardness. Examples for various crystallographic symmetry classes. Numerical values of elastic constants.

Theme 8. The crystal optics.

Effect of double refraction. Optical indicatrix. A refraction index. A wave surface. Influence of crystal symmetry. Uniaxial and biaxial crystals. Determination of double refraction value for a crystal plate of any orientation.

Electrooptical effect. Photoelasticity.

Theme 9. <u>The properties describing transport processes</u>.

Heat conductivity. Coefficient tensors of heat conductivity and thermal resistance. Two special cases of a stationary thermal stream. The general case of a stationary thermal stream. A thermal stream from a dot source in the anisotropic medium.

Thermoelectric effects in crystals.

Condensed state physics

<u>The purpose and problems of a course</u> are to acquaint students with the structure and physical properties of solids; to establish connection between properties of individual atoms and molecules and the properties which are found out at their association crystals. Basing on simple physical models of various solids the aim is to establish interrelation of their real structure with physical properties and laws of the processes occuring in these bodies under various external

conditions. The purpose is to acquaint students with properties of binary compounds and construction of phase diagrams.

The student should know

Two approaches to treatment of properties of solid and the phenomena occuring in them: macroscopical (phenomenological), peculiar to classical physics, when a solid is the continuous environment without a extending in a detail of its internal structure; and microscopic (atomistic) when the description and an explanation of properties of solid state is based on quantum mechanics laws.

Features of a crystals, structural types of solids, the thermal, electric, mechanical and magnetic properties, and theoretical approaches to interpretation and the quantitative description of the phenomena in solids.

The student should be able

Based on physical models of a structure of various solids and, basing on the basic physical laws the student should be able to explain a behavior of solids under various external conditions, practically to apply the received knowledge to the development of new materials with the set properties, to the development of new technologies of modern materials reception, and also to work with the scientific literature.

THE THEMATIC PLAN

Theme 1. The nature of interaction forces between atoms in crystals

Aggregate states of the condensed phases. Structural features of a solid state, types of the structures, the mixed structures (gas- and liquid crystal states), types of bonding in solids. Classification of bonding, general characteristics of types of bonding. Energy of an ionic crystal bonding, Madelung energy. Electronegativity and a degree of bonding ionicity. Ionic radius. The physical nature of covalent bonding. An orientation and a saturation of covalent bonding. Experimental definition of a ionicity degree. Metal bonding and its basic properties. The physical nature of forces of an attraction and repulsing. Molecular bonding. An origin and universality of Van der Vaals forces, an estimation of bonding. Features of new materials structure; conducting polymers, quasicrystals. The solving of tasks.

Theme 2. Crystalography principles.

Geometry of a crystal lattice. Elementary and primitive cells. Crystalographic planes and directions in a lattice. Miller's indexes, their connection with the equation of a plane. Factor of compactness. The solving of tasks.

Theme 3. <u>Solid solutions</u>

Types of solid solutions. The ordered solid solutions. Kurnakov temperature. Temperature dependence of a degree of short range ordering.

Theme 4. Diagrams of state and methods of their construction

Concept of a phase. Equilibrium conditions of multiphase and multicomponent systems. Gibbs phase rule. Thermodynamic interpretation of phase diagrams construction. Phase diagrams for systems with the unlimited and limited solubility and with absence of solubility. The analysis of diagrams. The solving of tasks.

Theme 5. Thermal properties of solids

Oscillations of a linear chain of atoms, the equation of oscillation, the dispersion law, of density of states, a spectrum of normal oscillations. Oscillations of a linear chain of the atoms consisting of two-types atoms. The dispersion law, acoustic and optical branches of oscillations. Classical model of a heat capacity of solids. Average energy of thermal oscillations of harmonic oscillator. Dulong and Petit law. Einstein model of a thermal capacity of solid. Quantization of oscillator energy. Average energy of thermal vibrations of quantum oscillator. Temperature dependence of a thermal capacity in Einstein's model at low temperatures. Einstein's temperature.

Debye model of a thermal capacity of solids. An acoustic spectrum of a crystal in Debye approximation. A thermal capacity of solid. T3 law. Debye temperature.

Thermal expansion as consequence of unharmonicity of atom fluctuations in a solid. Linear expansion factor at average temperatures and its relation with crystal constants. A deviation of thermal expansion from a linear law at low and high temperatures.

Lattice heat conductivity of solid. Heat conductivity of phonon gas within the framework of the molecular-kinetic theory. Influence of lattice defects on heat conductivity. Dimensional effect, a role of umklapp processes.

Theme 6. Electric properties of solids.

The classical electron theory of metals (model of free electrons). The law of the Ohm and Wideman-Franz in classical model of free electrons, the thermal capacity of free electron gas in metals.

Difficulties of the classical theory of free electrons. The quantum theory of free electrons. Quantization of energy of free electrons. Fermi - Dirac distribution. Fermi's energy. Function of density of states.

Paramagnetism and diamagnetism of electronic gas in the quantum theory free electrons.

Mechanisms of electrons dispersion at passing of an electric current. Matissen's rule. Residual resistance. Temperature dependence of specific resistance of metals.

Theme 7. <u>Semiconductors</u>

Self-conductivity of semiconductors. The holes concept. Concentration and mobility of carriers of electrical current and temperature dependence of conductivity.

Impurity conductivity of semiconductors. Thermal ionization of impurity center. Donor and acceptor levels. Mobility of carriers of a current at impurity atoms presence.

Photoconductivity, Photoelectric threshold. Dependence of photoconductivity on intensity of light. A role of traps.

Exitons. Frenkel's model of tightly coupled exiton. Model of slightly coupled exiton, Exiton waves concept.

Theme 8. Magnetic properties of solids

Classification of solids by magnetic properties. Elementary carriers of magnetism. The nature of diamagnetism and value of a magnetic susceptibility. Lanzheven expression.

The nature of paramagnetism. The magnetic moment of atom. Orientation paramagnetism of the localized magnetic moments. Curie law.

Magnetic properties of ferromagnets. Weiss phenomenological theory. The nature of ferromagnetism. An intramolecular field and exchange interaction. Heisenberg model. Spin waves concept, magnon concept. Antiferromagnetism. Ferrimagnetism.

Literature

1. Киттель Ч. Введение в физику твердого те л а. М.: Наука, 1963,1978. Элементарная Ч. 1965 2. Киттель физика твердого тела. M.: Наука, 3. Уэрт Ч.. Томсон Р 1969. Физика твердого тела. M.: Мир, 4. Епифанов Г.И. Физика тела Л/Т.: Высш. 1965. твердого школа, Каганов 5. М.И., ЛифшицИ.М. Квазичастицы. M.: Наука, 1976. Каганов 6. М.И. Электроны, фононы, магноны. M.: Наука, 1981. 7. Боровик Е.С., Мильнер А.С. Лекции по ферромагнетизму. Харьков: Изд. ХГУ, 1960. 8. Уманский Я.Е.. Скаков Ю.Л. Физика металлов. M.: Атомизлат. 1978. 9. Шульце Г. Металлофизика.

INTERACTION OF THE IRRADIATION WITH MATTER

The various mechanisms of damage of different solids (crystals, insulators, metals) during irradiation with fast heavy ions or atoms depending on their velocity are discussed.

APPLICATION OF COMPUTERS IN SCIENTIFIC RESEARCHES AND IN EDUCATION

Problems of experimental data visualization, methods of data compressing, fundamentals of the modern cryptography are considered.

MECHANISMS AND KINETICS OF CRYSTAL GROWTH

Crystal nucleation and growth theory principles, methods of crystallization process analysis, the main principles and methods of crystal growth are setted out.

DIFFUSION IN CRYSTALS

Atomic theory of diffusion, kinetics of diffusion, the problem of diffusion in crystals with defects of crystal lattice are setted out.