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DEFECTS IN CRYSTALS AND THEIR PROPERTIES

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Annotation

This article provides information about crystals, defects in the structure of crystals and concepts about their types. The article also contains information about the importance of defects in the structure and properties of matter.

Key words

crystals, defects, defect types, line and point defects, Schottky defects, Frenkel defects.

Defects in crystals (from Latin defectus - lack, flaw), violations of the periodicity of the crystal structure in real single crystals. In idealized crystal structures, atoms occupy strictly defined positions, forming regular three-dimensional lattices (crystal lattices). In real crystals (natural and artificially grown), various deviations from the correct arrangement of atoms or ions (or their groups) are usually observed. Such defects can be either atomic scale or macroscopic in size, visible even to the naked eye (see Defects in metals). In addition to static defects, there are deviations from the ideal lattice of another kind, associated with thermal vibrations of the particles that make up the lattice (dynamic defects, see Vibrations of the crystal lattice).

Defcts in crystals are formed during their growth (see Crystallization), under the influence of thermal, mechanical and electrical influences, as well as during irradiation with neutrons, electrons, X-rays, ultraviolet radiation (radiation defects), etc. There are point defects (zero-dimensional), linear (one-dimensional), defects that form surfaces in the crystal (two-dimensional), and volumetric defects (three-dimensional). A one-dimensional defect in one direction has a size significantly larger than the distance between neighboring atoms of the same name (lattice parameter), and in the other two directions it is of the same order. A two-dimensional defect in two directions has dimensions greater than the distance between nearest atoms [1]

Point defects. Some atoms or ions may be absent from places corresponding to the ideal lattice pattern. Such defective places are called vacancies. Foreign (impurity) atoms or ions may be present in crystals, replacing the main particles that form the crystal, or intercalating between them. Point dynamism in a crystal also includes its own atoms or ions that have been displaced from normal positions (interstitial atoms and ions), as well as color centers—combinations of vacancies with conduction electrons (F-centers) and with impurity atoms and conduction electrons (Z-centers) or with holes (V-centers). Color centers may be caused by irradiation of the crystals.

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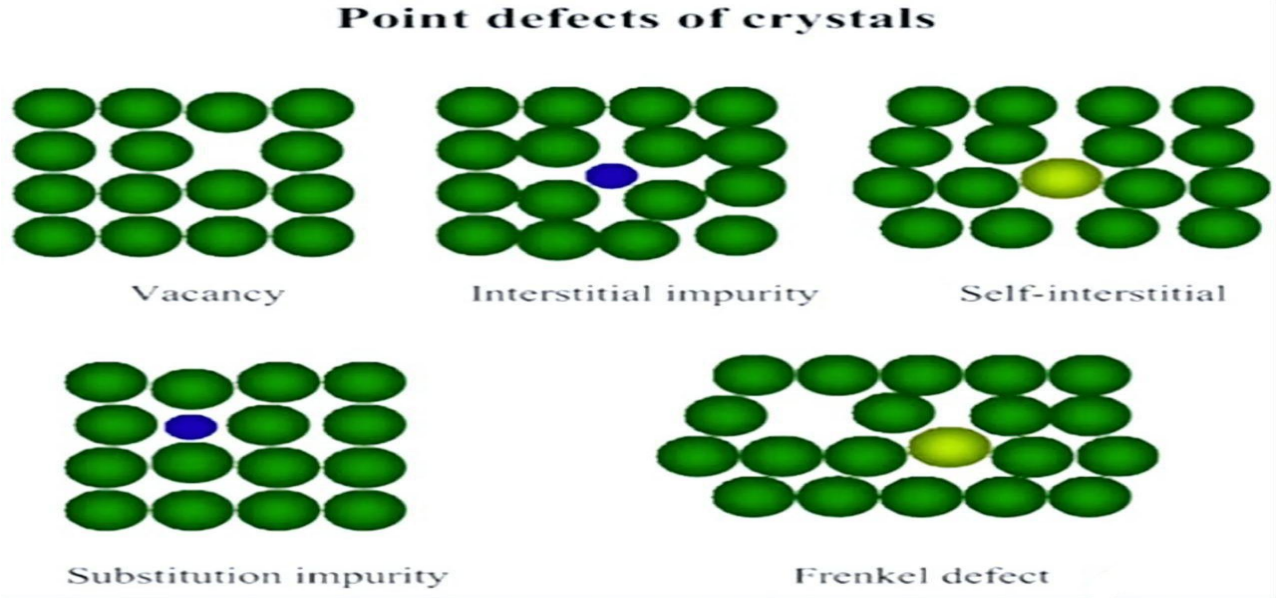

In ionic crystals formed by particles of two types (positive and negative), point defects appear in pairs. Two vacancies of opposite sign form a Schottky defect. A pair consisting of an interstitial ion and a vacancy left by it is called a Frenkel defect. Atoms in crystals are located at equal distances from each other in rows stretched along certain crystallographic directions. If one atom is displaced from its position by the impact of an incident particle caused by irradiation, it can, in turn, displace a neighboring atom, and so on. In this way, a whole row of atoms will be displaced, and on some segment of the row of atoms one atom will be superfluous. Such a violation in the arrangement of atoms or ions along certain directions with the appearance of an extra atom or ion in a separate section of the row is called crowdion. Irradiation removes atoms or ions from the equilibrium position and in other directions, and the movement is transmitted along the relay to increasingly distant atoms. As one moves away from the site of collision of the incident particle with a crystal atom, the momentum transfer becomes localized (focused) along the most densely packed directions. Such a relay transfer of the momentum of the incident particle to the ions or atoms of the crystal with constant focusing of the momentum along densely packed atomic rows is called a focuson [2].

Linear defects. In real crystals, some atomic planes may break off. The edges of such dangling (extra) planes form edge dislocations. There are also screw dislocations, which involve the twisting of atomic planes in the form of a spiral staircase, as well as more complex types of dislocations. Sometimes linear dislocations in crystals are formed from an accumulation of point defects arranged in chains (see Dislocations).

Two-dimensional defects. Such dichotomies in crystals are the boundaries between sections of the crystal rotated at different (small) angles relative to each other; twin boundaries (see twinning), stacking faults (monatomic twin layers), boundaries of electric and magnetic domains, antiphase boundaries in alloys, boundaries of inclusions of another phase (for example, martensitic), boundaries of grains (crystallites) in crystal aggregates. Many of the surface defects are rows and networks of dislocations, and the collection of such networks forms grain boundaries in polycrystals; impurity atoms and foreign particles collect at these boundaries [3].

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Volumetric defects. These include clusters of vacancies that form pores and channels; particles deposited on various defects (decorating), for example gas bubbles, mother liquor bubbles; accumulations of impurities in the form of sectors (hourglasses) and growth zones. In crystals, defects cause elastic distortions of the structure, which, in turn, cause the appearance of internal mechanical stresses (see Mechanical stress). For example, point defects, interacting with dislocations, strengthen or soften crystals. D. in crystals affect absorption spectra, luminescence spectra, light scattering in a crystal, etc., change electrical conductivity, thermal conductivity, ferroelectric properties (see Ferroelectrics), magnetic properties, etc. The mobility of dislocations determines the plasticity of crystals; accumulations of dislocations cause the appearance of internal stresses and destruction of crystals. Dislocations are places where impurities accumulate. Dislocations interfere with the processes of magnetization and electrical polarization due to interaction with domain boundaries. Volume defects reduce ductility, affect the strength, and the electrical, optical and magnetic properties of the crystal in the same way as dislocations[13].

Zero-dimensional (or point) defects in a crystal include all defects that are associated with the displacement or replacement of a small group of atoms (intrinsic point defects), as well as with impurities. They arise during heating, doping, during crystal growth and as a result of radiation exposure. They can also be introduced as a result of implantation. The properties of such defects and the mechanisms of their formation have been best studied, including motion, interaction, annihilation, and evaporation.

• A vacancy is a free, unoccupied atom, site of a crystal lattice.

• Intrinsic interstitial atom is an atom of the main element located in the interstitial position of the unit cell.

• Impurity atom substitution is the replacement of an atom of one type with an atom of another type at a site in the crystal lattice. Substitution positions may contain atoms that differ relatively little in size and electronic properties from the base atoms[11-12].

• Interstitial impurity atom - the impurity atom is located in the interstices of the crystal lattice. In metals, interstitial impurities are usually hydrogen, carbon, nitrogen and oxygen. In semiconductors - are impurities that create deep energy levels in the bandgap, such as copper and gold in silicon.

Complexes consisting of several point defects are also often observed in crystals, for example: a Frenkel defect (vacancy + own interstitial atom), bivacancy (vacancy + vacancy), A-center (vacancy + oxygen atom in silicon and germanium), etc [4]

Point defects increase the energy of the crystal, since a certain amount of energy was spent on the formation of each defect. Elastic deformation causes a very small fraction of the energy of vacancy formation, since ion displacements do not exceed 1% and the corresponding deformation energy is tenths of an eV. During the formation of an interstitial atom, displacements of neighboring ions can reach 20% of the interatomic distance, and the corresponding energy of elastic deformation of the lattice can reach several eV. The main share of energy spent on the formation of a point defect is associated with a violation of the periodicity of the atomic structure and the bonding forces between atoms. A point defect in a metal interacts with the entire electron gas. Removing a positive ion from a site is equivalent to introducing a point negative charge; conduction electrons are repelled from this charge, which causes an increase in their energy. Theoretical calculations show that the

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energy of formation of a vacancy in the fcc lattice of copper is about 1 eV, and that of an interstitial atom is from 2.5 to 3.5 eV. Despite the increase in crystal energy during the formation of its own point defects, they can be in thermodynamic equilibrium in the lattice, since their formation leads to an increase in entropy. At elevated temperatures, the increase in the entropy term TS of the free energy due to the formation of point defects compensates for the increase in the total crystal energy U, and the free energy turns out to be minimal.

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Atoms undergoing vibrational motion continuously exchange energy. Due to the randomness of thermal motion, energy is unevenly distributed between different atoms. At some point, an atom can receive such an excess of energy from its neighbors that it will occupy a neighboring position in the lattice. This is how the migration (movement) of point defects occurs in the bulk of the crystals[9-10].

If one of the atoms surrounding a vacancy moves to a vacant site, then the vacancy will correspondingly move to its place. Consecutive elementary acts of moving a certain vacancy are carried out by different atoms. The figure shows that in a layer of close-packed balls (atoms), in order to move one of the balls to a vacant place, it must move balls 1 and 2 apart. Consequently, to move from a position in a node where the energy of an atom is minimal to an adjacent vacant node, the atom must pass through a state with increased potential energy, overcome the energy barrier. For this, the atom needs to receive excess energy from its neighbors, which it loses while “squeezing” into a new position. The height of the energy barrier Em is called the activation energy of vacancy migration [6].

The main source and sink of point defects are linear and surface defects - see below. In large perfect single crystals, the decomposition of a supersaturated solid solution of its own point defects is possible with the formation of the so-called. microdefects.

Complexes of point defects The simplest complex of point defects is a bivacancy (divacancy): two vacancies located at adjacent lattice sites. Another well-known complex is the so-called Frenkel pair - an atom in an interstitial site and its nearby vacancy. Complexes consisting of two or more impurity atoms, as well as impurity atoms and their own point defects, play a major role in metals and semiconductors. In particular, such complexes can significantly affect the strength, electrical and optical properties of solids [7].

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One-dimensional (linear) defects are crystal defects, the size of which in one direction is much larger than the lattice parameter, and in the other two - comparable to it. Linear defects include dislocations and disclinations. General definition: dislocation is the boundary of an area of incomplete shear in a crystal. Dislocations are characterized by a shear vector (Burgers vector) and an angle φ between it and the dislocation line. When φ=0 the dislocation is called a screw; at φ=90° - edge; at other angles it is mixed and can then be decomposed into helical and edge components. Dislocations arise during crystal growth; during its plastic deformation and in many other cases. Their distribution and behavior under external influences determine the most important mechanical properties, in particular such as strength, plasticity, as well as electrical conductivity, etc. Disclination is the boundary of the region of incomplete rotation in the crystal. Characterized by a rotation vector [8].

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