Crystal-Chemical Interpretation of Amphoteric Influence of Bismuth Impurity in Tin Telluride

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Tin telluride is the special material of IV-VI compounds over a wide enough range of homogeneity, which lies completely on the side of chalcogen; it is characterized by only *p*-type of conductivity and high concentration of holes, which increases with the content of tellurium [1]. Optimization of parameters of SnTe is associated with the need to reduce the concentration of current carriers by influence on the defect subsystem. This can be achieved by doping with various impurities, among which elements of V group of the Periodic Table (in particular, bismuth) are important [2].

In this paper within the crystal-quasichemical formalism defect subsystem of tin telluride crystals doped by bismuth has been analyzed. In SnTe:Bi the dopant is distributed between the cationic and anionic sublattices. Thus, dopant, replacing tin in its sublattice, is ionized from the state $Bi^0(s^2p^3)$ into the state $Bi^{3+}(s^2p^0)+3e^-$ (where it is a donor) and relatively to Sn^{2+} sublattice it is Bi_{Sn}^{1+}. In tellurium sublattice dopant is ionized $Bi^0(s^2p^3)\rightarrow Bi^{3-}(s^2p^6)+3h^+$ (where it is an acceptor) and relatively to Te^{2-} sublattice it is Bi_{Te}^{1-}. This leads to the experimentally observed amphoteric effect of dopant.

The character of change of disproportionation of dopant charge state (Bi^{3+}, Bi^{3-}) and its effect on the electrical properties of the material have been determined. In particular, it has been found that in the initial stages of doping (up to 1.5 at.% of Bi) there is a predominance of impurity ions in the cation sublattice Bi_{Sn}^{1+}. With increasing impurity concentration (> 1.5 at.%) processes of self-compensation are amplified, indicating the increasing the share of bismuth ions in tellurium positions Bi_{Te}^{1-}, which leads to the increase of the concentration of holes, and consequently increase of the electrical conductivity.

On the basis of the proposed crystal-quasichemical formulae the analytical expressions for the concentration of point defects and Hall concentration of current carriers in SnTe:Bi crystals have been derived, and their dependences on the dopant content have been calculated. It has been shown that the dominant point defects are bismuth ions in lattice sites of tin telluride Bi_{Sn}^{1+}, Bi_{Te}^{1-}, doubly charged tellurium V_{Te}^{2+} and tin V_{Sn}^{2-} vacancies; the ratio between them is determined by the concentration of dopant Bi.

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2. Shperun V.M., Freik D.M., Prokopiv V.V. Teluryd olova. Fizyko-khimichni vlastyvosti. – Ivano-Frankivsk: Plai, 2002. – 250 p.