New Areas of Optimization of Thermoelectric Parameters of Lead Telluride and Germanium Telluride Based Solid Solutions

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IV-VI semiconductor compounds and their solid solutions are basic materials for thermoelectric energy converters that operate in the medium temperature area [1-2]. Point defects and their complexes largely responsible for the physical and chemical properties of the material. At present there is no consensus about the nature of these defects and their charge states. Lead telluride hasn-type conductivity in metal excess presence relative to stehiometry and p-type conductivity in chalcogen excess presence and germanium telluride has only hole conductivity [1].

The basis of the method of crystalquasichemical analysis is superposition of doping cluster formed on the basis of lead telluride antistructure, and the crystal formula of stoichiometric compound. Crystalquasichemical model of nonstoichiometric PbTe with a complex range of Frenkel defects (V_{Pb}^{2-}, V_{Pb}^{-}, V_{Te}^{2+}, Pb_i^{2+}, Te_i^{0}), and *p*-GeTe (V_{Ge}^{2-},V_{Ge}^{4-}), and based on them ternary systems have been offered. Dependences of concentration of point defects, electrons and holes, and the Hall concentration of current carriers on the size and nature of deviation from stoichiometry of *n*- and *p*-PbTe and solid solution composition have been calculated on the basis of the first developed crystalquasichemical formulas and equations of full electroneutrality. Thus hole conduction of lead telluride relates to a vacancy in cation sublattices V_{Pb}^{2-}, V_{Pb}^{-}, and electronic – in anion sublattices V_{Te}^{2+}, of lead telluride crystal structure.

The influence of chemical composition and the deviation from stoichiometry on the side of tellurium on the ratio between two- (V_M^{2-}) and fourfold charged (V_M^{4-}) cationic vacancies (dominant defects in this case) and thermoelectric properties of PbTe-SnTe solid solution have been specified.

A similar analysis has been done for germanium telluride and germanium telluride based solid solutions. Thus that the main areas of optimization of thermoelectric parameters of PbTe, GeTe based materials are decrease of the thermal conductivity (PbTe-SnTe, PbTe-Sb_2Te_3), and increase of electric conduction and activity of point defects (PbTe-SnTe, PbTe-GeTe), and the incorporation of noncentral dopant ions in solid solutions (Pb-Te-Se-S).

1. Abrykosov N.Kh., Shelimova L.E.: Semiconductors Materials on the basis of combinations of AIVBVI, M. Science, 1975, 196 p.
2. Ioffe A.F.: Semiconductor thermoelements. M.-H. Publishing House of USSR Academy of Sciences, 1960, 346 p.