Defective Subsystem and Modification of Crystals' Properties of Compounds A^2B^6

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Metal chalcogenides of the second subgroup of the periodic table are perspective materials in electronic engineering for making detectors for γ - and x-rays, photo receiving and radiating structures of visible and infrared light spectrum. These materials are characterized by high quantum yield of photo-luminescence and cathode excitement. However, the largest quantum yield can be obtained only in homo-n-p-transition, which requires the ability to grow material of hole and electron conductivity type.

It is known that the basic electrical and photovoltaic properties of semiconductors are determined by their own defects and impurities, which are almost always present in the crystal. The concentrations of different types of defects depend on each other, and therefore, the development of the model of point defects that would enable, on one hand, to identify the relationships that exist between the concentrations of defects and on the other - to establish qualitative and quantitative dependency of the physical crystals' properties of compounds A^2B^6 on the concentration of defects.

In this work, the crystalquasichemical formulas of non-stoichiometric metal chalcogenides of the second subgroup of n- and p-type conductivity have been proposed provided the existence of the complex defect subsystem after the scheme of Schottky-Frenkel. On their basis, the concentration dependencies of the prevailing defects have been calculated, as well as major current carriers and Hall concentration which would depend on the degree of deviation from the stoichiometric disproportion of the charge state of point defects.

By using the obtained crystalquasichemical formulas one can determine not only the prevailing types of point defects, but also their concentration depending on chemical composition, in particular, the magnitude of deviation from stoichiometry (α, β) and content of alloying elements (M, X) respectively. Based on quasi-chemical equations of the formation of point defects, the annealing processes of double temperature treatment of MX crystals have been described and the dominant defects have been determined. Crystalquasichemical formulas of the non-stoichiometric n- and p-MX (M – Zn, Cd; X – Te, Se, S) have been proposed provided the realization of the complex spectrum of point defects. Besides, the analysis of the principal models of point defects in ZnX crystals with the concomitant process of self alloying by p-MX and chacolgenide – n-MX has been performed when interacting with oxygen, and also the mechanisms of defect formation in solid solution on the basis of metal chalcogenides.

This research is sponsored by NATO's Public Diplomacy Division in the framework of "Science for Peace" (NATO SPS 984536)).