Physico-Chemical nanomaterials science

Thermodynamics of defects in ZnTe crystals

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Zinc telluride is a direct band gap semiconductor which can be successfully used for quantum-sized structures, semiconductor lasers, solar energy converters and modern electronics [1]. Point defects of such crystal lattice are affected on almost all range of semiconductor materials properties. Therefore, the definition of dominant point defects in the structure of zinc telluride is still relevant task. One method for establishing the dominant type of defects in crystals is a simulation of defect subsystem relying on the experimental data of Hall measurements and using quasi-chemical formalism [2].

The defect subsystem of ZnTe crystal has been investigated under the process of two-temperature annealing in a pair of components using the thermodynamic potentials method. The concentrations of point defects and free charge carriers as functions of the annealing temperature T and partial vapor pressure of components $P_{Zn,Te}$ have been calculated. It has been established that under annealing in zinc vapor (P_{Zn} = 13300 Pa) at temperatures T = (1000-1200) K the dominant defects are doubly ionized zinc vacancies, and under annealing in tellurium vapor (P_{Te} = 13300 Pa) in the same temperature range the dominant defects are once ionized zinc vacancies.

A close agreement between the formation energy of neutral zinc vacancy that has been calculated in our work and theoretically known values, and a satisfactory correlation of our concentration values of free charge carriers with experimental data indicates the adequacy of the presented defect subsystem model and improves the conclusions that have been made on their basis.

1. *Horichok I.V., Nykyruy L.I., Parashchuk T.O., Bardashevska S.D. and Pylyponuk M.P.*. Thermodynamics of defect subsystem in zinc telluride crystals / Modern Phys. Let. B, – 2016, **N 1650172**, P. 1-10.
2. *Horichok I.V., Fochuk P.M., Verzhak Ye.V., Parashchuk T.O., Freik D.M., Panchuk O.E., Bolotnikov A.E., James R.B.*. Compensation mechanism of bromine dopants in cadmium telluride single crystals // Journ. of Cryst. Growth, Elsevier. - 2015. - **415**. - P. 146–151.