Quasi-Chemical Analysis of Point Defects in Cadmium Telluride Crystals Doped by Bromine

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Cadmium telluride is a promising material for creating highly efficient optoelectronics devices and detectors of ionizing radiation. To improve and stabilize the characteristics of the material can be achieved by doping with various impurities, in particular bromine. For the development of science-based technologies CdTe: Br needed reliable information about its defective condition.

In this paper, using quasichemistry reaction modeled the formation of point defects in crystals of cadmium telluride doped with bromine and based on this calculated concentration dependence of the point defects and free carriers from technological factors of the two-temperature annealing.

It is shown that alloying effect of bromine impurity in CdTe crystals deal with replacing defects Br_{Te}^{+} and with them complexes of own point defects $\left(2Br_{Te}^{+}V_{Cd}^{2-}\right)^{0}$, which is dominant throughout the all studied range of annealing process parameters and determine the concentration of free charge carriers in the material.

Calculated Isothermal and Isobaric concentration dependence of the free charge carriers (electrons *n* and holes *p*) and its dominant own and impurity point defects: doubly ionized cadmium vacancies $\left[V_{Te}^{2+}\right]$ and tellurium $\left[V_{Cd}^{2-}\right]$; interstitial atoms of cadmium $\left[Cd_{i}^{2+}\right]$ and tellurium $\left[Te_{i}^{2-}\right]$; singly ionized atoms of bromine in the node tellurium $\left[Br_{Te}^{+}\right]$ and complexes $\left(2Br_{Te}^{+}V_{Cd}^{2-}\right)^{0}$ in bromine doped cadmium telluride crystals under conditions of two-temperature annealing in a couple of cadmium.

Determined equilibrium constant of complex formation of impurity replacement defects with own point defects $\left(2Br_{Te}^{+}V_{Cd}^{2-}\right)^{0}$.

The calculation showed that the concentration of electrons *n* does not depend from the annealing temperature T and at the same time linearly depends from the vapor pressure of cadmium P_{Cd}, which well agrees with experiment. This confirms the adequacy of the chosen model of creating defects in the crystals of cadmium telluride doped by bromine in which dominant defects are singly ionized impurity atoms in the node tellurium Br_{Te}^{+} and complexes $\left(2Br_{Te}^{+}V_{Cd}^{2-}\right)^{0}$.