Quasichemical Models of Point Defects in CdTe:Br

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The influence of dopant and annealing conditions on electrical properties of cadmium telluride monocrystals doped with bromine, grown by Bridgman technique and annealed in an atmosphere of cadmium at temperatures T = (800-1100) K and pressure of cadmium vapour P_{Cd} = (10^3-10^5) Pa have been studied and analyzed. To explain the electrical properties of CdTe:Br two models of quasichemical reactions of defect formation have been considered. In these models, addition to own point defects V_{Cd}^{-}, V_{Cd}^{2-}, Te_i^{-}, V_{Te}^{2+}, Cd_i^{2+}, it has been taken into account that all introduced impurity in the studied range of technological parameters is completely dissolved as singly ionized defects Br_{Te}^{+}, and its donor effect can be compensated by: 1) own acceptor point defects, in particular Te_i^{-}, V_{Cd}^{2-}, V_{Cd}^{-}; 2) complexes of impurity defects of substitution with own point defects $(Br_{Te}^{+}V_{Cd}^{2-})^{-}$.

Based on the model of defect subsystem of the material without associative centres experimental isothermal and isobaric dependences of the concentration of current carriers couldn't be explained satisfactorily by compensation of donor action of bromine dopant by only own point defects. In the case of the model of compensation of bromine dopant by complexes of impurity defects of substitution with own point defects $(Br_{Te}^{+}V_{Cd}^{2-})^{-}$, calculated dependences of concentration of current carriers on the annealing process conditions consistent with experimental data both quantitatively and qualitatively.

The nature of the curves of the concentration of current carriers is explained by dependences of concentration of point defects in the material. Dominant defects in CdTe:Br are singly ionized impurity bromine atoms in the tellurium sublattice Br_{Te}^{+} and acceptor complexes $(Br_{Te}^{+}V_{Cd}^{2-})^{-}$.

With the increase of the partial pressure of cadmium vapour concentration of associative centres $(Br_{Te}^{+}V_{Cd}^{2-})^{-}$ decreases. This leads to the almost linear increase of the concentration of current carriers that satisfactory agreement with experiment. Changing the annealing temperature in the range of (800-1100) K at constant pressure of cadmium vapour practically does not change the ratio between the concentrations of Br_{Te}^{+} and $(Br_{Te}^{+}V_{Cd}^{2-})^{-}$, which leads to keeping of the electron concentrations at the same level.

In quasichemical model of defect subsystem of CdTe:Br crystals equilibrium constant and enthalpy of quasichemical reaction that describes the formation of acceptor complexes of impurity defects of substitution with own point defects $(Br_{Te}^{+}V_{Cd}^{2-})^{-}$ have been taken equal to: $K = 1 \cdot 10^{-22} \exp(1.15 / kT)$.