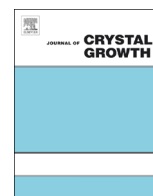




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Compensation mechanism of bromine dopants in cadmium telluride single crystals

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ABSTRACT

Cadmium telluride single crystals, doped by Bromine, were grown by Bridgman method and annealed under cadmium overpressure ($P_{Cd} = 10^2 - 10^5$ Pa) at 800–1100 K. Their electrical properties at high- and low-temperature have been investigated. The influence of impurities on the crystal electrical properties has been analyzed by using the defective subsystem model, which includes the possibility of formation of point intrinsic (V_{Cd}^{2-} , Cd_i^{2+} , V_{Te}^{2+} , Te_i^{2-}) and replacement defects (Br_{Te}^+ , Br_{Te}^+), and also point defects complexes ($Br_{Te}^+ V_{Cd}^{2-}$), $(2Br_{Te}^+ V_{Cd}^{2-})^0$. It was established that the concentration dependence between free charge carriers and annealing process parameters ($n(T)$, $n(P_{Cd})$) are determined by two dominant defects – Br_{Te}^+ and $(2Br_{Te}^+ V_{Cd}^{2-})^0$. Their content varies with the annealing temperature and the vapor pressure of the component; the concentration of other defects is much smaller and almost does not influence the electron density.

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1. Introduction

Among the elements of the VII group of the periodic table that are used for doping CdTe, most attention has been given to chlorine due to the possibility of obtaining high ohmic crystals and the prospects of using it for manufacturing of uncooled highly sensitive detectors of X- and gamma-ray radiation [1]. The impact of other elements of the same group on the physical properties of cadmium telluride is less well studied, although they also exhibit self-compensation of impurities, but to a lesser extent than chlorine [2–3]. These findings suggested the possibility of obtaining a material with a controlled concentration of free charge carriers, which is essential for some electronics applications. However, for assuring the targeted growth of CdTe:Br single crystals with predetermined physical properties, it was necessary for us to first carry out additional studies of its defect subsystem due to (1) the critical influence of the type and charge state of the dominant point defects, and, (2) the lack of a unified point of view on self-compensation processes in CdTe:Br [2–8].

According to Refs. [1–8], during the doping of cadmium telluride by halogens, the impurity atoms replace tellurium in the anion sublattice, and create a shallow donor level in the crystal's bandgap. The

electrical effects of ionized impurity atoms in cadmium telluride are compensated by the crystal's acceptor defects, or by complex associates, which include stoichiometric, impurity and dopant related defects [1–8]. The formation of complexes is due to a decrease in the system's free energy compared to the energy of the system with only single point defects. The main considered complexes were the acceptor complex $\{(A_{Te}^+ V_{Cd}^{2-})^-\}$ and the neutral complex $(2A_{Te}^+ V_{Cd}^{2-})^0$, (where $A = Cl, Br, I$), the existence of which has been confirmed experimentally [8]. Moreover, several researchers [9–11] analyzed the possibility of the formation of neutral complexes and DX centers. Their formation is associated with a change in the lattice symmetry in the neighborhood of the substitution defect that deforms the atomic bonds and, consequently, the possibility of binding to or yielding free electrons, so, by this process, affecting the crystal's electrical properties. In contrast to complexes containing cadmium vacancies, there are no reliable data about the existence of large numbers of free vacancies.

In [12–13] a theoretical calculation of the concentration of free charge carriers in CdTe:Cl was carried out using a model of a crystal defect subsystem that takes into account the possibility of compensating for impurity defects in CdTe by cadmium vacancies with the formation of complexes of the $(A_{Te}^+ V_{Cd}^{2-})^-$ type. Satisfactory agreement with the experimental data was obtained. This highlights the adequacy of this model. Given the expected similarity of the

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electronic structure of chlorine and bromine atoms, it also gives a reason to use a similar model to explain the influence of bromine impurities on the electrical properties of cadmium telluride.

2. Experimental

Single crystals were grown by the Bridgman method. Cadmium telluride was synthesized in quartz ampoules using cadmium and tellurium (6 N purity), additionally purified by zone melting. The concentration of background impurities in the source component did not exceed 10^{-5} wt%. The melt was maintained at 1393 K for 24 h and then directionally solidified at a speed of 3 mm/h. The material was doped by adding CdBr_2 to the starting charge. The concentration of bromine in the melt was $\sim 10^{19}$ at/cm³.

The as-grown single crystals were cut by wire into 3 mm thick wafers. From their base we prepared rectangular shaped samples. High-temperature Hall effect measurements were carried out under two-temperature annealing conditions on samples placed in an evacuated ampoule in two-zone furnace, where the first zone governed the temperature of the sample, and the second controlled the temperature and pressure of the Cd vapor [14–15].

3. Experimental results: analysis of, and thermodynamic model for the crystal's defect subsystem

The samples we investigated demonstrated n-type conductivity over the whole range of investigated temperatures, 200–900 °C. However, the values of the electron mobility were smaller than those observed in undoped CdTe (Fig. 1), especially at lower temperatures. For example, the mobility is about a factor of 3 smaller at room

temperature. The reason is the high concentration of bromine in the samples. During the initial heating, we held the crystal at 300, 400, 500, and 600 °C for 2–6 h (Fig. 2) with the aim of observing the changes in electrical properties as mentioned before [2]. Indeed, a rapid increase in the conductivity and electron density happened at ~ 500 °C after 30 min of holding the material at this temperature (Fig. 2). However, the rise was not very steep, which can be explained by the high bromine content.

The peculiarity of the perceived experimental dependences between electron density and technological parameters of annealing (Fig. 3) is that the value of n does not depend on the annealing temperature, T , but at the same time, it depends on the vapor pressure of cadmium P_{Cd} . Because the rate of change of carrier concentration with the change of vapor pressure for CdTe:Br differs from the magnitude of the rate change for pure crystals suggests that their defects are not dominant in the doped material. We explain the lack of dependence of $n(T)$ by the fact that all impurities in the crystal are dissolved ones, and the carrier concentration is determined by ionized impurity atoms, the concentration of which does not change with temperature. Otherwise, if some of the impurities present in the sample are not dissolved, the temperature change would alter the amount of dissolved bromine and, therefore, the concentration of electrons too; however, we did not observe this. Also it is unlikely that the amount of dissolved impurities depends on the components of vapor pressure or on the temperature.

Thus, we assume that the defect subsystem model can be implemented for CdTe:Br crystals. According to this model all introduced impurities at the studied range of technological parameters are completely dissolved and exist in the form of defects Br_{Te} (neutral and singly ionized), and their donor effects are compensated by acceptor defects in such a way that $n=f(P_{\text{Cd}})$ and $n \neq f(T)$. The highest probability is that the compensating defects are doubly

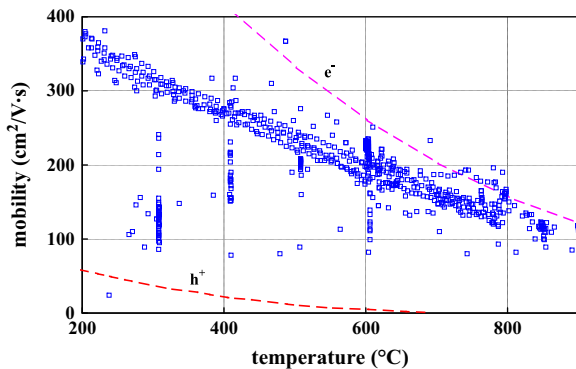


Fig. 1. The temperature dependence of the electron mobility in the CdTe:Br sample.

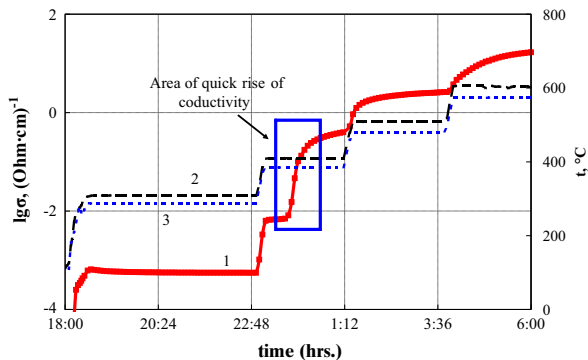


Fig. 2. Time dependence of the charge-carrier conductivity (thick solid red line 1), temperature of the CdTe:Br sample (dashed black line 2), and the Cd zone (dotted blue line 3). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

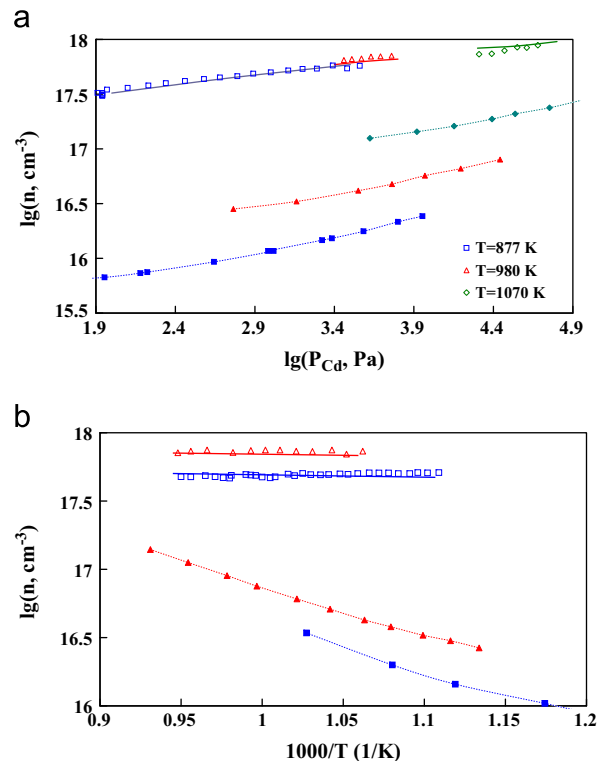


Fig. 3. Experimental and theoretically calculated isothermal dependences (above; \square – 870 K, Δ – 970 K, \diamond – 1070 K) and isobaric (below; \square – 1000 Pa, Δ – 10000 Pa) of the electron density in undoped- (closed symbols) and bromine-doped (open symbols) cadmium telluride crystal under conditions of both temperature annealing and cadmium overpressure.

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