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DEGRADATION UNDER INFLUENCE OF RADIATION DEFECTS OF DETECTOR PROPERTIES OF $Cd_{0.9}Zn_{0.1}Te$ IRRADIATED BY NEUTRONS

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This work is devoted to the study by computer simulation of the mechanisms of the influence of radiation defects, arising under the influence of neutron irradiation, on the changes in electrical properties: resistivity ρ, electron mobility μ_n, lifetime of nonequilibrium electrons τ_n and holes τ_p in $Cd_{0.9}Zn_{0.1}Te$ and charge collection efficiency η of uncooled ionizing radiation detectors based on this material. Radiation defects, which are corresponded by deep energy levels in the band gap, act as trapping centers of nonequilibrium charge carriers, noticeably affect the degree of compensation by changing ρ of the detector material, the recombination processes, decreasing τ_n and τ_p, and also the scattering of conduction electrons, decreasing μ_n, that ultimately can cause degradation of the charges collection efficiency η. The specific reasons for the deterioration of the electrophysical and detector properties of this semiconductor under the influence of neutron irradiation were identified, and the main factors affecting the increase in the resistivity of $Cd_{0.9}Zn_{0.1}Te$ during its bombardment by low-energy and high-energy neutrons, leading to complete degradation of the recording ability of detectors based on this materials, were found. The recombination of nonequilibrium charge carriers is noticeably stronger than the decrease in μ_n affects the degradation of detector properties, therefore, the effect of recombination processes at deep levels of radiation defects on the degradation of τ_n, τ_p, and η of detectors based on $Cd_{0.9}Zn_{0.1}Te$ was studied. A comparative analysis of the properties of $Cd_{0.9}Zn_{0.1}Te$ with the previously studied CdTe:Cl was made. An attempt was made to explain the higher radiation resistance of $Cd_{0.9}Zn_{0.1}Te$ compared to CdTe:Cl under neutron irradiation by the influence of the radiation self-compensation mechanism with participation of deep donor energy levels: interstitial tellurium and tellurium at the site of cadmium. In addition, the rate of recombination at defect levels in $Cd_{0.9}Zn_{0.1}Te$ is, ceteris paribus, lower than in CdTe:Cl due to the smaller difference between the Fermi level and the levels of radiation defects in cadmium telluride. The relationship between the band gaps of $Cd_{0.9}Zn_{0.1}Te$ and CdTe:Cl, the concentration of radiation defects, the Fermi level drift during irradiation, and the radiation resistance of the detectors were also noted. The important role of purity and dopant shallow donor concentration in initial state of the detector material is indicated.
KEY WORDS: detector properties, simulation, CdTe, CdZnTe, neutron irradiation, radiation defects

The $Cd_{0.9}Zn_{0.1}Te$ compound is considered to be a promising semiconductor material for room temperature detectors, which are intended for recording x-ray and gamma radiation and can be used in astronomy, dosimetric environmental monitoring and nuclear medicine imaging. $Cd_{0.9}Zn_{0.1}Te$ is the material of good electrophysical properties [1–4]: high resistivity $\rho = 10^9$–10^{11} Ω·cm, high electronic mobility $\mu_n = 1100$–1200 cm^2/(V·sec), acceptable values of the lifetimes of nonequilibrium electrons $\tau_n \sim 10^{-6}$ sec and nonequilibrium holes $\tau_p \sim 10^{-6}$ sec. Along with $Cd_{0.9}Zn_{0.1}Te$, CdTe is often considered as a detector material. During operation, the detectors are exposed to ionizing radiation, the effect of which on the crystals is the subject of research, for example, irradiation with protons [5], electrons [6], gamma rays [7], and neutrons [8] which have increased penetrating power. As a result of neutron bombardment, the radiation defects arise in a semiconductor crystal, which correspond to energy levels in the band gap, acting as centers of capture and recombination of nonequilibrium charge carriers generated by the detected radiation. These defects noticeably affect upon the degree of compensation, changing ρ of the detector material, and upon the recombination processes, decreasing τ_n and τ_p, and also on the scattering of conduction electrons, decreasing μ_n. Ultimately, the radiation defects are capable to cause complete degradation of the charges collection efficiency η of detector, the specific reasons for which are not fully understood. To increase the radiation resistance and improve the detector quality of $Cd_{0.9}Zn_{0.1}Te$, it is necessary to study and try to understand the mechanisms of the influence of radiation defects, which arise in a crystal under the neutron irradiation, on the electrophysical and detector properties of this material. However, due to the high resistivity of $Cd_{0.9}Zn_{0.1}Te$, such a task is practically impossible to resolve only by experimental methods [8-10], therefore, it is very important to apply additionally the numerical simulation basing on known experimental results using as initial data.

The aim of the work was to study by modeling method the mechanisms of the influence of radiation defects arising in $Cd_{0.9}Zn_{0.1}Te$ under the influence of neutron irradiation on the change in resistivity ρ, electron mobility μ_n, lifetimes of nonequilibrium electrons τ_n, nonequilibrium holes τ_p, and charge collection efficiency η in radiation detectors based on this material, as well as a comparative analysis of the properties of $Cd_{0.9}Zn_{0.1}Te$ and cadmium telluride which was previously studied in [11].

PHYSICAL MODELS AND MATERIAL COMPOSITION

The applied models and their testing are described in detail in [12], and the spectral characteristics of the initial and irradiated CdTe:Cl and $Cd_{0.9}Zn_{0.1}Te$ are taken from paper [10]. First the electroneutrality equation was compiled with including of all impurities and defects experimentally recorded in [10]. This equation was numerically solved with respect

to the Fermi level F, then the concentrations of free electrons ***n*** and holes ***p*** were determined in the approximation of parabolic zones. The electron mobility μ_n was calculated using an approximation of the pulse relaxation time (tau approximation) with taking into account scattering mechanisms at ionized and neutral centers, acoustic phonons, piezoelectric phonons, optical phonons, as well as scattering on clusters of point defects and doping inhomogeneities. The hole mobility μ_p was assumed to be unchanged and equal to 70 $cm^2/(V \cdot s)$. The specific conductivity was calculated by the formula: $e \cdot n \cdot \mu_n + e \cdot p \cdot \mu_p$. The resistivity was calculated as the reciprocal of the conductivity, consisting of electronic and hole components. The lifetime of nonequilibrium charge carriers was calculated according to the Shockley - Read - Hall recombination model, and the detector charges collection efficiency was determined by the Hecht equation [13, p. 489]. The distance between the detector electrodes was assumed to be equal 5 mm, and the electric field strength - 1000 V/cm.

The changes in F, ρ, μ_n, τ_n, τ_p, and η have been simulated depending on the content of radiation defects and doping shallow donor, for which the aluminum, indium, bismuth and lead can be used in $Cd_{0.9}Zn_{0.1}Te$. The simulation was carried out using the following characteristics of the i-ths impurities and defects levels as the initial data, experimentally measured and published in the technical literature: concentration N_i, position in the bandgap E_i, and capture cross section for nonequilibrium charge carriers σ_i.

The initial compositions of background impurities and defects were determined which ensured that the calculated value $\rho = 1 \cdot 10^{11}$ Ω·cm for $Cd_{0.9}Zn_{0.1}Te$ coincides with the value experimentally measured in [10] before neutron exposure. A typical initial composition of the $Cd_{0.9}Zn_{0.1}Te$ detector material is presented in Table. Similar composition was described, for example, in [7, 10, 14, 15]. The specific composition of the material is taken from [10]. The Table also show the capture cross sections for the levels σ_i, the order of magnitude of which was determined in [16], where the contributions of all levels to the currents of charge carriers emitted into the corresponding zones were taken into account. The charge state of defects is indicated by a plus sign for donors whose energy is measured relative to the conduction-band bottom E_C, and a minus sign - for acceptor levels with energy relative to the valence band top E_V.

The notation and probable nature of some levels are taken from [7, 10, 15]. Doping impurity of shallow donor, introduced into the matrix of the materials under study, are intended to compensate for shallow acceptors (A, A1, C, X) and to achieve a high-resistance state necessary for the operation of the detectors. The levels of A, A1, C, X, according to opinion of most researchers, are complexes of cadmium vacancies with various background impurities. The cadmium vacancy appears to correspond to DX or J.

Table

Composition of $Cd_{0.9}Zn_{0.1}Te$ before irradiation with a specific resistance of $1 \cdot 10^{11}$ Ω·cm [10].

Defect	A^-	$A1^-$	C^-	X^-	DX^{2-}	J^-	Z^+	Y^-	W^-	Te_{Cd}^+	V_{Te}^+
E_i, eV	0.14	0.16	0.25	0.29	0.41	0.45	0.52	0.67	0.70	0.74	1.1
σ_i, cm^2	10^{-19}	$2 \cdot 10^{-19}$	$3 \cdot 10^{-19}$	10^{-18}	10^{-16}	10^{-16}	10^{-17}	10^{-17}	10^{-17}	10^{-18}	10^{-16}
N_i,cm^{-3}	$5 \cdot 10^{15}$	$5 \cdot 10^{14}$	$5 \cdot 10^{14}$	$5 \cdot 10^{14}$	$3 \cdot 10^{15}$	$3 \cdot 10^{15}$	$1 \cdot 10^{15}$	$3 \cdot 10^{15}$	$3 \cdot 10^{15}$	$1.45 \cdot 10^{16}$	$1 \cdot 10^{16}$

The calculated electrophysical properties of unirradiated material corresponded to well-known values: $\mu_n = 1200$ $cm^2/(V \cdot sec)$, lifetimes τ_n, $\tau_p \sim 10^{-6}$ sec. The changes in ρ, μ_n, τ_n, τ_p, the position of the Fermi level **F** in the band gap of $Cd_{0.9}Zn_{0.1}Te$, and variation in the charges collection efficiency η of detector based on this material have been simulated depending on the content of radiation defects and the doping shallow donor at T = 20˚C – operating temperature of the detector. It should be noted that since in paper [10] all the results, and conclusions are of a qualitative nature, the model dependences and modeling results obtained in this paper can also be only of qualitative those.

RESULTS AND DISCUSSION

In paper [10], the studied material $Cd_{0.9}Zn_{0.1}Te$ was irradiated by the fluxes of low-energy neutrons (~ 10 eV) with fluences from 10^{10} to 10^{14} N/cm^2 and high-energy neutrons (~ 0.5 – 1 MeV) with fluences from 10^{11} to 10^{13} N/cm^2. The radiation donor level Z in cadmium telluride occurs already after the first stage of irradiation and it is present in the crystal at all subsequent stages, and at the moment of complete degradation of the detector recording properties, this defect reaches the maximum amplitude in spectrum. According to the authors of [10], tellurium interstitial Te(I) can be considered as a defect Z which causes complete degradation of the detector properties. In $Cd_{0.9}Zn_{0.1}Te$, the same Z level with an energy of E_C – 0.52 eV was also present, but it was often suppressed in the spectra by the peak of the acceptor level J, the content of which noticeably correlated with the degree of radiation damage of the irradiated sample. In addition, during irradiation of the studied materials, the amplitudes of the peaks and the concentration of defects Te_{Cd}, V_{Te}, and also the complex V_{Cd}–Im (cadmium vacancy–impurity) increase significantly. It was of interest to simulate the dynamic of change in the resistivity of $Cd_{0.9}Zn_{0.1}Te$ with an increase in the concentration of radiation defect Z which causes an abrupt decrease in the charge collection efficiency and complete degradation of detector properties, while the content of radiation defects J, Te_{Cd}, V_{Te} is increasing. The result of simulation is shown in Fig. 1. The concentration of the radiation defect J monotonically increases from $3 \cdot 10^{15}$ to $2.1 \cdot 10^{16}$ cm^{-3}, and the concentration of the Te_{Cd} defect does from $1.45 \cdot 10^{16}$ to $3.2 \cdot 10^{16}$ cm^{-3}. It can be seen from Figure 1, that as the concentration of defect Z increases during irradiation, the resistivity of material increases monotonically, which was observed experimentally in [10]. However, after higher doses of irradiation by high-energy neutrons with a fluence of 10^{13} N/cm^2 and radiation damage which can

be associated with a concentration of N(Z) = $2 \cdot 10^{16}$ cm^{-3}, the resistance of $Cd_{0.9}Zn_{0.1}Te$ reaches almost the maximum value $\rho = 2.12 \cdot 10^{11}$ Ω·cm, which corresponds to the qualitative results of paper [10]. When comparing with similar model dependences for CdTe:Cl from [11] (Fig. 1), we can see that in $Cd_{0.9}Zn_{0.1}Te$ there is no sharp jump in the resistivity Δρ at N (Z) = $2 \cdot 10^{16}$ cm^{-3}, as in CdTe.

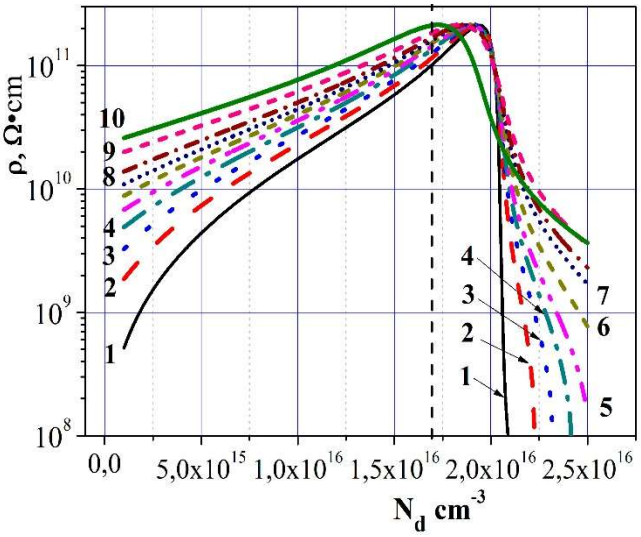


Figure 1. Specific resistance of $Cd_{0.9}Zn_{0.1}Te$ depending on the content of doping shallow donors at various concentrations of defect Z. Z content, cm^{-3}: 1 – $1 \cdot 10^{15}$, 2 – $2 \cdot 10^{15}$, 3 – $3 \cdot 10^{15}$, 4 – $4 \cdot 10^{15}$, 5 – $5 \cdot 10^{15}$, 6 – $7 \cdot 10^{15}$, 7 – $1 \cdot 10^{16}$, 8 – $1.4 \cdot 10^{16}$, 9 – $1.6 \cdot 10^{16}$, 10 - $2 \cdot 10^{16}$. The vertical dashed line corresponds to the studied sample.

On the contrary, a monotonic increase in the $Cd_{0.9}Zn_{0.1}Te$ resistivity is observed, which occurs due to the gradual drift of the Fermi level to the middle of the band gap towards the radiation level Z with increasing its concentration. This increasing of ρ is also confirmed experimentally. In this case, a displacement of the F level closer to the conduction band, observed in [11] for CdTe, does not occur due to the action of the radiative self-compensation mechanism, which appears in an increase of the concentration of radiation defects J (E_V + 0.45 eV) and Te_{Cd} (E_C - 0.74 eV), that together with the defect Z (E_C - 0.52 eV) hold F near the middle of the band gap. In addition, a pivotal role also here is that $Cd_{0.9}Zn_{0.1}Te$ has a larger band gap in comparison with E_G of CdTe:Cl; therefore, in order for Fermi level to reach the middle of E_G in $Cd_{0.9}Zn_{0.1}Te$, a higher content of the radiation defect Z is required than in CdTe:Cl. Fig. 2 shows the behavior of Fermi level in $Cd_{0.9}Zn_{0.1}Te$.

Figure 2 demonstrates that in $Cd_{0.9}Zn_{0.1}Te$ there is an insignificant difference in the F position between the initial state with N(Z) = $1 \cdot 10^{15}$ cm^{-3} and after irradiation with the concentration of defect Z N(Z) = $2 \cdot 10^{16}$ cm^{-3}, while for CdTe:Cl in [11] this difference in position of Fermi level is significant. In other words, during irradiation, the electrophysical properties of $Cd_{0.9}Zn_{0.1}Te$ change noticeably less than the properties of cadmium telluride. This simulation result is confirmed by the well-known fact, experimentally confirmed also in [10], of the higher radiation resistance of $Cd_{0.9}Zn_{0.1}Te$ in comparison with CdTe:Cl.

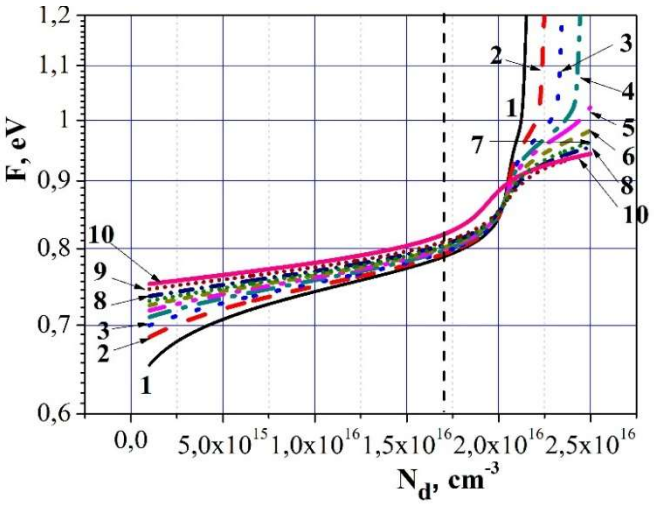
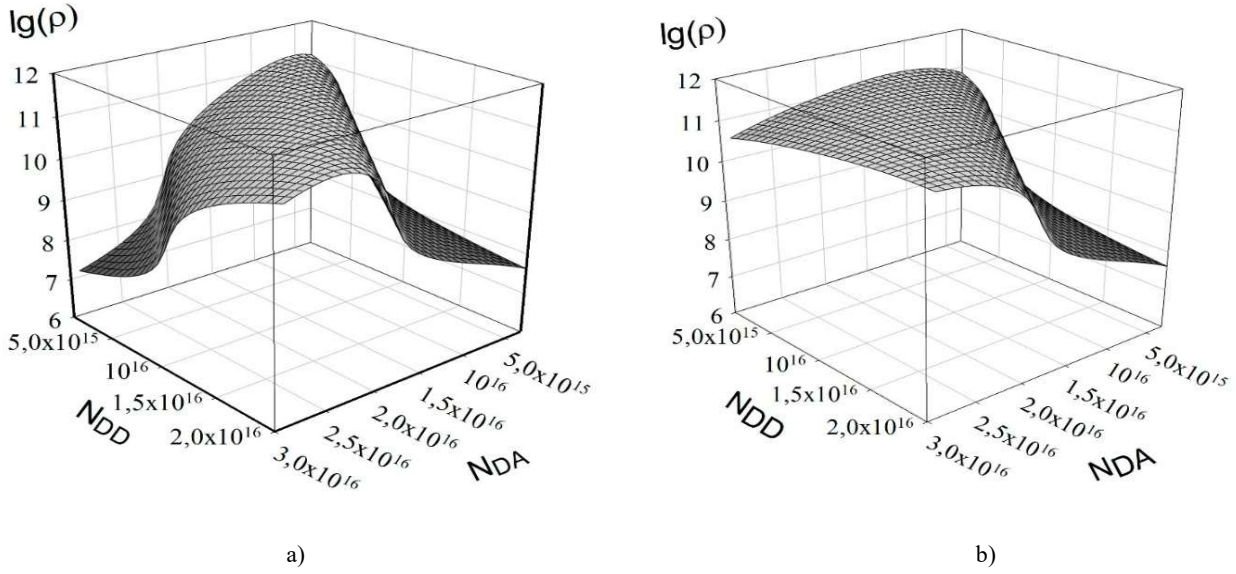


Figure 2. The positions of the Fermi level in $Cd_{0.9}Zn_{0.1}Te$, measured from the top of valence band, depending on the content of shallow donor at different concentrations of the radiation donor defect Z (cm^{-3}). Z concentrations in $Cd_{0.9}Zn_{0.1}Te$ are the same as for the numbered dependences in Fig. 1. The vertical dashed line corresponds to the studied sample.

Neutron irradiation of $Cd_{0.9}Zn_{0.1}Te$ also leads to the expansion of the region of the high-resistance state, which makes it possible to maintain the working capacity of the detector during irradiation. Figure 3 shows the behavior of the resistivity $Cd_{0.9}Zn_{0.1}Te$ at the concentration $N(Te_{Cd}) = 1.45 \cdot 10^{16}$ cm^{-3} (a) and after irradiation with high-energy neutrons at the concentration $N(Te_{Cd}) = 3.2 \cdot 10^{16}$ cm^{-3} (b) depending on concentrations of radiation defects: acceptor J (N_{DA}) and donor Z (N_{DD}). We see that the expansion of the high-resistance region occurs due to an increase in the concentration of the Te_{Cd} anti-structural defect during neutron irradiation.



a) b)

Figure 3. Dependences of the decimal logarithm of the $Cd_{0.9}Zn_{0.1}Te$ resistivity on the concentration N_{DA} of the acceptor defect J and the concentration N_{DD} of the donor defect Z: a) the content of Te_{Cd} is $1.45 \cdot 10^{16}$ cm^{-3}; b) the content of Te_{Cd} is $3.2 \cdot 10^{16}$ cm^{-3}.

The initially measured fluences of neutron irradiation of investigated sample were 10^{11} N/cm^2 for high-energy neutrons and 10^{10} N/cm^2 for low-energy neutrons. In the process of further irradiation, the material gradually lost its detector properties until complete degradation after bombardment by low-energy neutrons with the fluence of 10^{14} N/cm^2. The integrated flux of high-energy neutrons, after which the detector properties $Cd_{0.9}Zn_{0.1}Te$ were completely degraded, was 10^{13} N/cm^2. Since the specific resistance of material increases after neutron irradiation, degradation of the detector properties can occur due to a decrease in the electron mobility μ_n and to a decrease in the lifetimes of nonequilibrium charge carriers τ_n, τ_p. In earlier paper [12, Fig. 3] it was shown that a decrease of μ_n in $Cd_{0.9}Zn_{0.1}Te$ can be caused by the scattering of conduction electrons by clusters of point defects, but no more than two to three times, and it is not capable to lead to complete degradation of detector properties. Thus, a complete loss of recording properties should occur due to a significant decrease in the lifetime of nonequilibrium charge carriers. Approximate quantitative estimates based on the experimental results of paper [17] showed that the rate of band-to-band recombination of nonequilibrium charge carriers is about by ten orders of magnitude lower than the rate of recombination at deep levels of defects in wide-gap semiconductors such as CdTe and $Cd_{0.9}Zn_{0.1}Te$. Figure 4 shows the donor content dependence of the charges collection efficiency **η** in detectors based on $Cd_{0.9}Zn_{0.1}Te$, calculated according to the Hecht equation for which the lifetimes of nonequilibrium electrons and holes were calculated according to the Shockley-Read statistics describing recombination of charge carriers at the energy levels of impurities and structural defects. Basing on a comparison of the graphs of Fig. 4 and the results of paper [10], it follows that the concentration of the radiation defect Z in the studied materials $N(Z) = (1–2) \cdot 10^{16}$ cm^{-3} approximately corresponds to the content of this radiation defect after the high-energy neutrons fluence of 10^{13} N/cm^2.

The concentration of radiation defects Z, equaled to $N(Z)=(1–3) \cdot 10^{15}$ cm^{-3}, approximately corresponds to its content in $Cd_{0.9}Zn_{0.1}Te$ after irradiation by low-energy neutrons with fluences $10^{12}–10^{13}$ N/cm^2. Figure 4 also shows that when the content of the radiation defect Z: $N(Z) = (1–3) \cdot 10^{15}$ cm^{-3}, the registering properties of the detectors based on $Cd_{0.9}Zn_{0.1}Te$ are partially lost, which qualitatively corresponds to the experiment of paper [10].

Quantitative studies have shown that the degradation of $Cd_{0.9}Zn_{0.1}Te$ detector charge collection η occurs due to capture and recombination of nonequilibrium charge carriers at the radiation level of a deep donor with an energy $E = E_C – 0.52$ eV, presumably Te (I), as well as at the deep level of Te_{Cd} defect with energy $E_C – 0.74$ eV. It was established also that in $Cd_{0.9}Zn_{0.1}Te$ the radiation defect of the tellurium vacancy V_{Te}, which is dominant in the spectra in peak amplitude [10], does not participate in compensation and does not capture nonequilibrium charge carriers due to the large difference between the V_{Te} energy level and the Fermi level in the semi-insulating state at room temperature.

The simulation established also that the degradation of the detector properties of the material under study occurs mainly due to a noticeable decrease in the lifetime of nonequilibrium electrons by several tens of times. Capture and

recombination of nonequilibrium holes at radiation levels have little effect on the degradation of charge collection in $Cd_{0.9}Zn_{0.1}Te$ detectors during its irradiation. It can be seen from Fig. 5, where the behavior of the lifetime of nonequilibrium electrons τ_n (a) and holes τ_p (b) was shown.

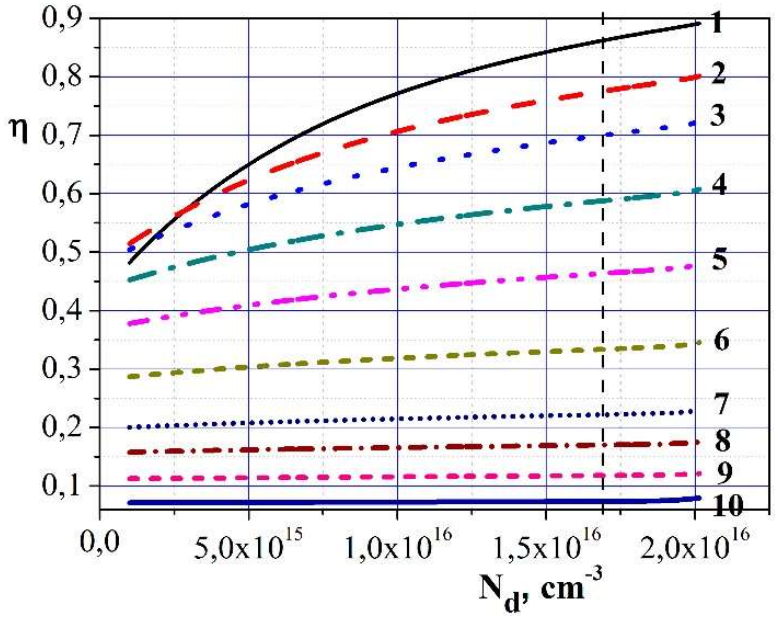
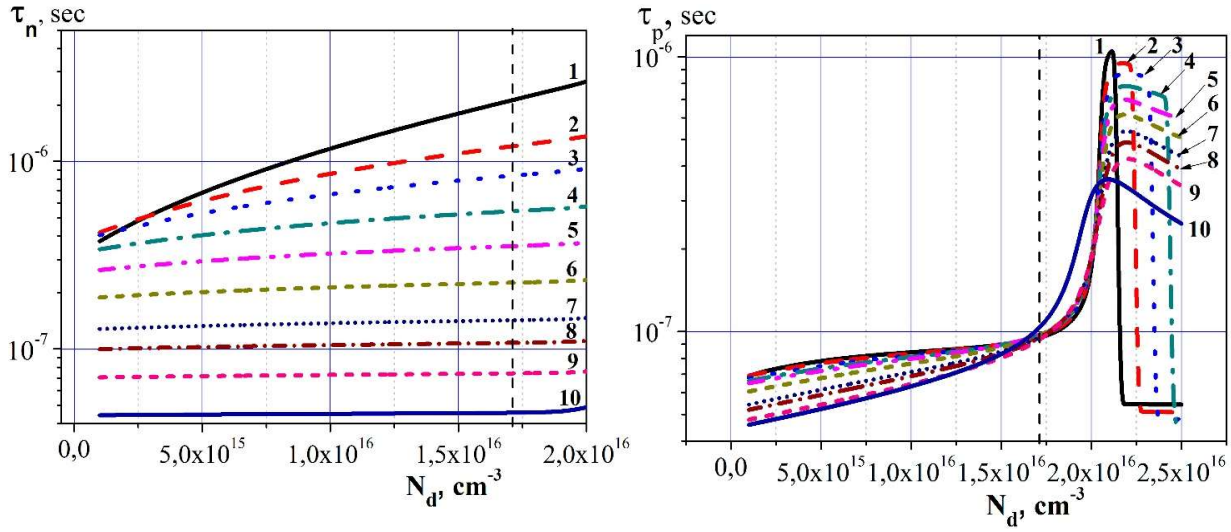


Figure 4. Charge collection efficiency of detectors based on $Cd_{0.9}Zn_{0.1}Te$ depending on the content of doping shallow donors for different concentrations of radiation defect Z, which are equaled to concentrations for numbered curves in Fig. 1,2. The vertical dashed line corresponds to the studied sample.



a) b)

Figure 5. Dependences of the lifetimes of nonequilibrium electrons (a) and holes (b) in $Cd_{0.9}Zn_{0.1}Te$ on the concentration of doping shallow donors for different concentrations of the radiation defect Z, which are the same as in the numbered curves in Fig. 1, 2, 4. The vertical dashed lines correspond to the studied sample.

Figure 5 demonstrates that the lifetime of nonequilibrium electrons τ_n in the studied $Cd_{0.9}Zn_{0.1}Te$ decreases quite significantly compared to the lifetime of nonequilibrium holes τ_p as the concentration of radiation defects, arising under neutron irradiation, increases. The jump in τ_p by an order of magnitude (Fig. 5b) in the concentration range $N_d = 2 \cdot 10^{16}$-$2.5 \cdot 10^{16}$ cm^{-3} is explained by the fact that within this interval the Fermi level passes far from the energy levels of defects, capture and recombination centers (see Table and Fig. 2), therefore, the rate of recombination of nonequilibrium charge carriers decreases significantly.

The results obtained in this and earlier studies can be compared with the data of [18], where, using the SRIM program, the Monte Carlo method was used to simulate the effect of neutron radiation with an energy of 1–2 MeV on the formation of radiation damage in $Cd_{0.9}Zn_{0.1}Te$ crystals. The type and number of originating radiation defects was investigated. The calculated data were compared with the experimental results of the study of the operation of $Cd_{0.9}Zn_{0.1}Te$ detector, both

the initial one and the material irradiated with a ^{252}Cf source of fast neutrons. The defect concentration was measured using thermally stimulated current spectroscopy (TSC), and the detector spectra were recorded for ^{241}Am gamma radiation source (59.5 keV). It was shown that the concentration of vacancies, anti-structural defects of cadmium substitution at the site of tellurium, interstitial atoms, and related defects increases during neutron irradiation, which, according to the authors of [18], caused a deterioration in the detector characteristics of $Cd_{0.9}Zn_{0.1}Te$. Besides, the complete degradation of the detector occurred already after an irradiation dose of $5 \cdot 10^{10}$ N/cm^2, while in the experiment of paper [10], the detector degraded only after an irradiation dose of 10^{13} N/cm^2 by fast neutrons. The position of the Fermi level in the band gap, measured in [18], relative to the bottom of the conduction band E_C in the initial sample was equal to 0.707 eV, and in the sample irradiated with a dose of $5 \cdot 10^{10}$ N/cm^2 it became E_C–0.513 eV with a decrease in resistivity from $3.49 \cdot 10^9$ to $6.12 \cdot 10^8$ Ohm·cm.

We carried out a comparative analysis of the simulation results based on the experimental data of [10] with the experimental results of paper [18]. As a result, it was found that the very low radiation resistance of the detector in [18] can be explained by the fact that the as-grown $Cd_{0.9}Zn_{0.1}Te$ crystal there turned out to be a material of lower detector quality. Namely, in the initial state, they produced a semiconductor with a high content of interstitial Cd^{++} (Cd_I) and substitutional defect of cadmium in site of tellurium (Cd^{+}_{Te}), which are defects of the donor type. Under the influence of these electrically active deep donors, the Fermi level already in the as-grown material was above the middle of the band gap, which determined the electronic conductivity registered in [18] using Hall measurements. The bombardment of such a material by fast neutrons led to a further increase in the concentration of Cd_I and Cd_{Te} defects with a shift of the Fermi level even closer to the conduction band and, as a result, a noticeable drop in resistivity, a sharp increase in the leakage current and complete detector degradation, which required a relatively small irradiation dose - $5 \cdot 10^{10}$ N/cm^2. There can be two main reasons for such a low radiation resistance of the detector described in [18]. First, the as-grown material could be doped with an excessively large amount of indium, which immediately led to electronic conductivity, while hole conductivity is required for the detector to operate. Therefore, a relatively small dose of radiation was required in order to increase the concentration of deep donors and thus shift the Fermi level even closer to the conduction band, lowering the specific resistance ρ. Secondly, there was a weak effect of the radiative self-compensation process of the irradiated detector material due to a possible insufficient removal of background impurities from the as-grown crystal. Namely, cadmium vacancies formed under the influence of neutron irradiation interacted with background impurities and In dopant and formed A centers – neutral or with a charge increased by one with respect to initial state of double charged cadmium vacancy (V_{Cd}^{2-}), which, in turn, prevented the stabilization of the Fermi level and led to its drift to the conduction band decreasing resistivity ρ. Moreover, some of these complexes have such shallow energy levels that their registration could not be possible at a starting temperature of 80 K in the TSC technique. And neutral complexes are not electrically active; therefore, they are not recordable at all. The decrease in ρ led to an increase in noise which finally completely suppressed the main peak of the spectrum. The much more radiation-resistant detector in paper [10] demonstrated a much different behavior, namely it was the material which only increased the resistivity under the influence of high-energy neutron irradiation, since there the Fermi level in the initial state located below the middle of the band gap. And degradation of this detector material occurred for another reason: due to a decrease in the charge collection efficiency owing to capture and recombination of nonequilibrium carriers at deep levels of radiation defects.

CONCLUSIONS

The experimentally registered gradual increase in the $Cd_{0.9}Zn_{0.1}Te$ resistivity during bombardment by neutrons is caused by a gradual increase in the concentration of interstitial tellurium Te(I) with an energy level of 0.52 eV, measured relative to the bottom of the conduction band E_C. An increase in the content of Te(I) shifts the Fermi level to the middle of the band gap. The resistivity of $Cd_{0.9}Zn_{0.1}Te$ increases monotonically due also to an increase in the content of the anti-structural donor defect Te_{Cd}, which increases the size of the region of the high-resistance state in the ranges of concentration of radiation defects and also shifts Fermi level to the middle of band gap. The absence of degradation of resistivity occurred due to the action of the radiation self-compensation mechanism with the formation of a sufficient number of individual acceptor cadmium vacancies not creating the complexes with impurities.

The degradation of the charge collection efficiency of $Cd_{0.9}Zn_{0.1}Te$ under neutron irradiation occurs due to capture and recombination of nonequilibrium electrons at the radiation level of a deep donor with energy $E = E_C - 0.52$ eV, presumably Te (I), as well as at deep level of Te_{Cd} defect with energy $E_C - 0.74$ eV.

The well-known fact of higher radiation resistance of $Cd_{0.9}Zn_{0.1}Te$ compared to CdTe:Cl under neutron irradiation can be explained by the fact that in $Cd_{0.9}Zn_{0.1}Te$ there is a stronger mechanism of radiation self-compensation with the participation of deep donor levels (Te (I) and Te_{Cd}) than in CdTe:Cl. Perhaps this is why in the $Cd_{0.9}Zn_{0.1}Te$ material, unlike CdTe:Cl, there is no rearrangement of the crystal structure after neutron irradiation with ultimate fluence 10^{13} N/cm^2 of high-energy neutrons ($E \sim 10^5$ eV). In addition, due to the higher difference between the Fermi level and the deep levels of radiation defects in $Cd_{0.9}Zn_{0.1}Te$, the rate of recombination at the levels of radiation defects, ceteris paribus, is lower in it than in CdTe:Cl. It can also be noted that, due to the larger band gap of the E_G in $Cd_{0.9}Zn_{0.1}Te$, the Fermi level drifts in this material to a larger depth than in CdTe and therefore a higher concentration of the corresponding radiation defects is required to reach a middle of E_G and maximum of ρ, and therefore higher radiation doses are needed.

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ДЕГРАДАЦІЯ ПІД ВПЛИВОМ РАДІАЦІЙНИХ ДЕФЕКТІВ ДЕТЕКТОРНИХ ВЛАСТИВОСТЕЙ $Cd_{0.9}Zn_{0.1}Te$, ОПРОМІНЕНОГО НЕЙТРОНАМИ

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Представлена робота присвячена дослідженню методом комп'ютерного моделювання механізмів впливу радіаційних дефектів, що виникають під дією нейтронного опромінення, на зміну електрофізичних властивостей - питомого опору ρ, електронної рухливості μ_n, часу життя нерівноважних електронів τ_n та дірок τ_p, в $Cd_{0.9}Zn_{0.1}Te$ і ефективності збору зарядів неохолоджуваного детектору іонізуючих випромінювань η на основі цього матеріалу. Радіаційні дефекти, яким в забороненій зоні відповідають глибокі рівні енергії, діють як центри захоплення нерівноважних носіїв заряду, помітно впливають на ступінь компенсації, змінюючи ρ детекторного матеріалу, на процеси рекомбінації, знижуючи τ_n і τ_p, а також на розсіювання електронів провідності, зменшуючи μ_n, що зрештою здатне викликати деградацію ефективності збору зарядів η. Були з'ясовані конкретні причини погіршення електрофізичних та детекторних властивостей під дією нейтронного опромінення та встановлені основні фактори, які впливають на підвищення питомого опору $Cd_{0.9}Zn_{0.1}Te$ при бомбардуванні тепловими та високоенергетичними нейтронами, що призводять до повної деградації реєструвальної здатності детекторів на основі цього матеріалу. Рекомбінація нерівноважних носіїв заряду помітно сильніше ніж зниження μ_n впливає на деградацію детекторних властивостей, тому був досліджений вплив процесів рекомбінації через глибокі рівні радіаційних дефектів на деградацію τ_n, τ_p, η детектору на основі $Cd_{0.9}Zn_{0.1}Te$. Проведено порівняльний аналіз властивостей $Cd_{0.9}Zn_{0.1}Te$ і раніш дослідженого CdTe:Cl. Зроблена спроба пояснення більш високої радіаційної стійкості $Cd_{0.9}Zn_{0.1}Te$ у порівнянні з CdTe:Cl при нейтронному опроміненні впливом механізму радіаційної самокомпенсації за участю більш глибоких донорних рівнів енергії: міжвузлового телуру, телуру на місці кадмію. Крім того, внаслідок меншої різниці між рівнем Фермі і рівнями радіаційних дефектів в телуриді кадмію темп рекомбінації через рівні дефектів в $Cd_{0.9}Zn_{0.1}Te$ при інших рівних умовах нижчий, ніж в CdTe:Cl. Також був відзначений зв'язок між шириною забороненої зони $Cd_{0.9}Zn_{0.1}Te$ і CdZn:Cl, концентрацією радіаційних дефектів, дрейфом рівня Фермі в процесі опромінення та радіаційною стійкістю детекторів. Вказано на важливу роль чистоти і концентрації легуючого мілкого донора в початковому стані детекторного матеріалу.

КЛЮЧОВІ СЛОВА: детекторні властивості, моделювання, CdZnTe, CdTe, опромінення нейтронами, радіаційні дефекти

ДЕГРАДАЦИЯ ПОД ВЛИЯНИЕМ РАДИАЦИОННЫХ ДЕФЕКТОВ ДЕТЕКТОРНЫХ СВОЙСТВ $Cd_{0.9}Zn_{0.1}Te$, ОБЛУЧЁННОГО НЕЙТРОНАМИ

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Данная работа посвящена исследованию методом компьютерного моделирования механизмов влияния радиационных дефектов, возникающих под действием нейтронного облучения на изменение электрофизических свойств - удельного сопротивления ρ, электронной подвижности μ_n, времени жизни неравновесных электронов τ_n и дырок τ_p, в $Cd_{0.9}Zn_{0.1}Te$ и эффективности сбора зарядов неохлаждаемых детекторов ионизирующих излучений η на основе этого материала. Радиационные дефекты, которым в запрещённой зоне соответствуют глубокие уровни энергии, действуют как центры захвата неравновесных носителей заряда, заметно влияют на степень компенсации, изменяя ρ детекторного материала, на процессы рекомбинации, снижая τ_n и τ_p, а также на рассеяние электронов проводимости, уменьшая μ_n, что в конечном итоге приводит к деградации эффективности сбора зарядов η. Были выяснены конкретные причины ухудшения электрофизических и детекторных свойств под действием нейтронного облучения и установлены основные факторы, влияющие на повышение удельного сопротивления $Cd_{0.9}Zn_{0.1}Te$ при бомбардировке тепловыми и высокоэнергетическими нейтронами, приводящих к полной деградации регистрирующей способности детекторов на основе этого материала. Рекомбинация неравновесных носителей заряда заметно сильнее чем снижение μ_n влияет на деградацию детекторных свойств, поэтому было исследовано влияние процессов рекомбинации через глубокие уровни радиационных дефектов на деградацию τ_n, τ_p, η детектора на основе $Cd_{0.9}Zn_{0.1}Te$. Проведён сравнительный анализ свойств $Cd_{0.9}Zn_{0.1}Te$ и ранее исследованного CdTe:Cl. Сделана попытка объяснения более высокой радиационной стойкости $Cd_{0.9}Zn_{0.1}Te$ по сравнению с CdTe:Cl при нейтронном облучении влиянием механизмом радиационной самокомпенсации с участием более глубоких донорных уровней энергии: межузельного теллура, теллура на месте кадмия. Кроме того, вследствие меньшей разницы между уровнем Ферми и уровнями радиационных дефектов в теллуриде кадмия темп рекомбинации через уровни дефектов в $Cd_{0.9}Zn_{0.1}Te$ при прочих равных условиях ниже, чем в CdTe:Cl. Также был отмечена связь между шириной запрещённой зоны $Cd_{0.9}Zn_{0.1}Te$ и CdZn:Cl, концентрацией радиационных дефектов, дрейфом уровня Ферми в процессе облучения и радиационной стойкостью детекторов. Указано на важную роль чистоты и концентрации легирующего мелкого донора в исходном состоянии детекторного материала.

КЛЮЧЕВЫЕ СЛОВА: детекторные свойства, моделирование, CdZnTe, CdTe, облучение нейтронами, радиационные дефекты