

## MECHANISMS OF DEGRADATION OF THE DETECTING PROPERTIES OF CdTe AND CdZnTe UNDER GAMMA RADIATION EXPOSURE<sup>†</sup>

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This work is devoted to the study of the mechanisms of the influence of radiation defects, arising under the influence of gamma irradiation, on the change in resistivity  $\rho$ , lifetime of nonequilibrium electrons  $\tau_n$  and holes  $\tau_p$ , in CdTe:Cl and Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te as well as the collection efficiency  $\eta$  of uncooled radiation detectors based on these materials, by computer simulation method. Radiation defects, that 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  $\rho$  of the detector material, the recombination processes by decreasing  $\tau_n$  and  $\tau_p$ , what ultimately can cause degradation of the charges collection efficiency  $\eta$ . The specific reasons for the deterioration of the detector properties of CdTe:Cl and Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te under the influence of gamma irradiation were identified, and the main factors leading to complete degradation of the recording ability of detectors based on these semiconductors during their bombardment by <sup>60</sup>Co gamma quanta were determined. The gradual degradation of the spectroscopic performance of CdTe:Cl-based detectors during gamma irradiation occurs due to the continuous formation of cadmium vacancies  $V_{Cd}$  and acceptor complexes  $V_{Cd} - Cl$ , which continuously shift Fermi level towards valence band and decrease  $\rho$ . The complete performance degradation of CdTe detectors takes place mainly due to the capture of nonequilibrium electrons at energy level of interstitial tellurium Te(I). The invariable spectroscopic properties of CdZnTe-based sensors under gamma irradiation up to 25 kGy occur due to the mechanism of radiative self-compensation by formation of substitutional defect Te<sub>Zn</sub>. At the final stage of irradiation, a sharp deterioration in the detector properties of CdZnTe occurs, mainly due to the capture and recombination of nonequilibrium charge carriers at the level of the Te(I) defect. The different radiation resistances of CdZnTe and CdTe:Cl can be explained by different behavior of Fermi level  $E_F$  in these semiconductors under gamma irradiation.  $E_F$  in CdZnTe under radiation exposure remains near the middle of band gap, and in CdTe it drifts to the valence band. The rate of capture and recombination through Te(I) donor level in CdTe:Cl is lower than in CdZnTe due to the larger difference between the Fermi level and the radiation defect Te(I) level in cadmium telluride. Thereby, the complete degradation of the CdTe:Cl detector occurs at a higher concentration of radiation defect Te(I), and hence after a higher irradiation dose of 50 kGy compared with a dose of 30 kGy required for degradation of CdZnTe detector properties.

**Keywords:** detector properties, simulation, CdTe, CdZnTe, gamma irradiation, radiation defects

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CdTe is considered as a promising material for semiconductor uncooled gamma-ray sensors used in radiation control and monitoring systems of radiation materials, in nuclear power, in imaging systems, as well as in nuclear medicine and solar power engineering [1-4]. A certain disadvantage of CdTe detectors is appeared in the polarization effect that appears in the matrix after long term operation. Currently, cadmium telluride is usually doped with zinc up to 10 – 15 wt% in order to increase the bandgap  $E_G$  and resistivity  $\rho$ , what allows increasing the bias voltage to prevent the polarization effects [5]. At present, Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te (CZT), which has the band gap of about 1.57 eV at 300 K and the resistivity  $\rho$  higher by 1–2 orders of magnitude as compared to that of CdTe, is very common semiconductor material for  $\gamma$ -ray sensors operating at room temperature [6, 7]. The application of up-to-date CZT-based detectors, for example, with orthogonal coplanar strip electrodes, allows to achieve the photo-peak resolution in pulse amplitude spectra of about 1% at 662 keV [8, 9].

In the process of achieving the detecting quality in CdTe and CZT, some intrinsic defects appear in their matrix with the corresponded energy levels in the band gap, which change the degree of compensation, decreasing  $\rho$ , and act as traps of nonequilibrium charge carriers generated by the registered gamma radiation. To electrically compensate the charged states of the trap levels and increase the crystal resistivity, CdTe is often doped with chlorine, and CZT is doped with aluminum, indium, or yttrium. Al, In, Y act as substitutional impurities instead of cadmium, and Cl - instead of tellurium [10]. These compensating donor dopants are introduced to CdTe and CZT materials in the amount of 1-2 ppm or  $\sim 10^{16}$  cm<sup>-3</sup> [11, 12].

When CdTe and CZT detectors are used in an aggressive radiation environment, they are exposed to irradiation with gamma quanta, which can cause radiation damage in the crystal structure and, therefore, significantly affect their spectroscopic performance. Elucidation of the mechanisms of this effect is of great importance for detectors application in various fields, as well as for the improvement of radiation monitoring methods. Previous studies of <sup>60</sup>Co gamma irradiation [13–15] have shown that CdTe materials are insensitive to radiation damage up to an absorbed dose of several thousand gray. When the dose exceeds this value, the resistivity begins to decrease gradually. The spectroscopic performance continuously deteriorates, although the detectors can still operate in spectroscopic mode under irradiation of

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25 kGy. Irradiation doses over 30 kGy cause the actual degradation of the electrophysical and detector properties [14, 15]. Low-dose gamma-irradiation of CZT causes an increase in resistivity with its subsequent decrease at larger doses [16, 17]. High doses of gamma irradiation of CZT induce radiation defects that accumulate negative space charges, which significantly distorts the distribution of the electric field and reduces the mobility of electrons due to increase of the effect of scattering on clusters of ionized impurities [18]. This experimental fact is in agreement with the numerical simulations results obtained in [19], where it was shown that a decrease in the electron mobility  $\mu_n$  in  $\text{Cd}_{0.9}\text{Zn}_{0.1}\text{Te}$  by approximately two to three times could be caused by the scattering of conductivity electrons on clusters of charged point defects. Earlier experimental studies of radiation damage caused by gamma-quanta bombardment in CdTe and CZT detectors were mainly devoted to the effect of radiation dose on device performance [1, 3, 13–17]. Detector materials CdTe and CZT have a high resistivity of  $10^9$ – $10^{11}$   $\Omega\cdot\text{cm}$ , what greatly complicates investigating at a microscopic scale the mechanisms of change and degradation of their electrophysical and detector properties under the influence of radiation defects, basing only on experimental techniques. In this regard, it is very important to use mathematical and computer simulation as an additional research tool based on known experimental results and proven physical models.

The object of the work was a model study of the effect of radiation defects arising under the influence of gamma irradiation on the degradation mechanisms of the electrophysical and detector properties of CdTe:Cl and  $\text{Cd}_{0.9}\text{Zn}_{0.1}\text{Te}$ . Calculations of the electron mobility  $\mu_n$ , resistivity  $\rho$ , lifetime of nonequilibrium electrons  $\tau_n$  and holes  $\tau_p$ , and charge collection efficiency  $\eta$ , depending on the concentration of doping shallow donors for different impurity and defect compositions of the samples, before and after gamma irradiation, have been carried out.

### MATERIALS AND MODELS

The main parameters of the  $i$ -th deep levels of defects that determine the detector properties of CdTe, CdZnTe are the concentration  $N_i$ , capture cross section  $\sigma_i$ , and position in the band gap (activation energy)  $E_i$  [17, 20, 21]. Measurements of  $N_i$ ,  $\sigma_i$ ,  $E_i$  are carried out using techniques based on the forced filling of energy levels with electrons and holes, followed by their emission into the corresponding bands. The measurements at certain instants of the currents of charge carriers emitted from the levels in a wide temperature range make it possible to obtain spectra with pronounced peaks at certain temperatures corresponding to the certain positions of the energy levels  $E_i$ . The height of the peaks and their width are determined, respectively, by the concentration of levels  $N_i$  and the capture cross section  $\sigma_i$  of nonequilibrium charge carriers. Overlapping these peaks can significantly distort the true values of  $N_i$ ,  $E_i$ , and  $\sigma_i$ . In this regard, in published works, as a rule, there are disagreements in measuring the positions of energy levels in the band gap and even the lack of reproducibility of these values in different papers of the same authors. Nevertheless, in [14–16, 20], as well as in some other papers of these authors, there is an acceptable repeatability of  $E_i$  measurements, based on a well-developed technology of CdTe and CZT detectors production, what allows using the results, obtained by these authors, for correct identification of levels of radiation-induced and technological defects, as well as for studies of their evolution under radiation exposure. To get more accurate values of the capture cross sections  $\sigma_i$ , one can use the results of paper [22], where the contribution of all levels to the currents emitted into the corresponding bands was simultaneously taken into account.

The applied models and their testing are described in detail in [19], and the spectral characteristics of the initial and irradiated CdTe:Cl and  $\text{Cd}_{0.9}\text{Zn}_{0.1}\text{Te}$  are taken from [14, 15]. First, an equation of electroneutrality was compiled with all impurities and defects, which were experimentally recorded in [14], taken into account. This equation was solved numerically with respect to the Fermi level  $E_F$ , then the concentrations of free electrons  $n$  and holes  $p$  were determined in the parabolic band approximation. The electron mobility  $\mu_n$  was calculated in the momentum relaxation time approximation (tau-approximation) taking into account the mechanisms of scattering by ionized and neutral centers, acoustic and piezoelectric phonons, optical phonons, as well as scattering by clusters of point defects. The hole mobility  $\mu_p$  was assumed to be invariable and equal to 70  $\text{cm}^2/(\text{V}\cdot\text{s})$ . Specific conductivity was calculated using the formula:  $e\cdot n\cdot\mu_n + e\cdot p\cdot\mu_p$ . Resistivity was calculated as the reciprocal of conductivity. Basing on the experimentally measured band-to-band recombination coefficients [23], it was found that the rate of band-to-band recombination in the materials under study at room temperature was approximately ten orders of magnitude lower than the rate of recombination through deep levels of impurities and defects, described by the Shockley-Reed-Hall statistics which was therefore assumed to be the basis for calculating the lifetimes of nonequilibrium charge carriers  $\tau_n$ ,  $\tau_p$ . The charge collection efficiency  $\eta$  of the detector was determined by the Hecht equation [24, p. 489]. As in [14, 15], the distance between the electrodes was assumed to be 1 mm, and the electric field strength was 500 V/cm for CdTe:Cl and 3000 V/cm for CZT.

The specific composition of the materials was taken from [14, 15], then the concentrations of background impurities and defects were determined, which ensured the coincidence of the calculated values  $\rho = 2\cdot 10^9$  and  $\rho = 1\cdot 10^{11}$   $\Omega\cdot\text{cm}$  respectively for CdTe and CZT with the values experimentally measured by the authors of paper [15] before irradiation. A typical initial composition of the CdTe detector material is presented in Table 1, and  $\text{Cd}_{0.9}\text{Zn}_{0.1}\text{Te}$ -based material – in Table 2. In addition to [14, 15], a similar composition is described, for example, in [12, 17, 25, 26]. The table also lists the capture cross sections for the levels  $\sigma_i$ , whose order of magnitude was determined in [22]. The charge state of defects is indicated as plus (+) for the donors, whose energies are measured relative to the bottom of the conduction band  $E_C$ , and by minus (–) for the acceptor levels with energy relative to the top of the valence band  $E_V$ .

Indications and the probable nature of some levels are described in [12, 17, 25]. The alloying impurities of the shallow donor levels ( $\text{Cl}_{\text{Te}}$ ,  $\text{In}_{\text{Cd}}$ ) introduced into the matrix of the studied materials are designed to compensate for

acceptors (AX, A0, A, A1, K, X) and achieve a high-resistance state required for detectors operation. The defects AX, A0, A, A1, K, X, according to the authors [14, 15, 16, 20], as well as to the most of the researchers, are complexes of cadmium vacancies with various alloying and background impurities. Similarly, the vacancy of cadmium may correspond to D or J defect [17, 27]. Donor levels I<sup>+</sup> and H1<sup>+</sup> represent, respectively, a tellurium vacancy V<sub>Te</sub> and substitutional defect Te<sub>Zn</sub> or Te<sub>Cd</sub> [28-30]. At the final stage of gamma irradiation, the donor defect Z appears in the PICTS spectra, which apparently corresponds to the interstitial tellurium Te(I). At the final stage of gamma irradiation, a donor level Z appears in the PICTS spectra, the nature of this defect is not unambiguous: it can be either interstitial cadmium Cd(I) or interstitial tellurium Te(I) [27, 28]. The author of this paper assume that the defect Z is interstitial tellurium.

**Table 1.** Composition of the initial CdTe with a resistivity of 2·10<sup>9</sup> Ω·cm

Defect	Cl <sub>Te</sub> <sup>+</sup>	AX <sup>-</sup>	A0 <sup>-</sup>	A <sup>-</sup>	A1 <sup>-</sup>	X <sup>-</sup>	D <sup>2-</sup>	G <sup>-</sup>	H <sup>-</sup>	H1 <sup>+</sup>	I <sup>+</sup>
E <sub>i</sub> , eV	0.014	0.11	0.12	0.14	0.16	0.28	0.35	0.64	0.77	0.82	1.01
σ <sub>i</sub> , cm <sup>2</sup>	1·10 <sup>-21</sup>	3·10 <sup>-20</sup>	4·10 <sup>-20</sup>	10 <sup>-19</sup>	2·10 <sup>-19</sup>	4·10 <sup>-19</sup>	7·10 <sup>-17</sup>	3·10 <sup>-17</sup>	1.3·10 <sup>-17</sup>	4·10 <sup>-17</sup>	10 <sup>-18</sup>
N <sub>i</sub> , cm <sup>-3</sup>	1.7·10 <sup>16</sup>	3.3·10 <sup>14</sup>	7·10 <sup>15</sup>	2·10 <sup>15</sup>	2·10 <sup>15</sup>	2·10 <sup>15</sup>	2·10 <sup>15</sup>	8·10 <sup>15</sup>	9·10 <sup>15</sup>	7·10 <sup>15</sup>	8.5·10 <sup>15</sup>

**Table 2.** Composition of the initial CdZnTe with a resistivity of 1·10<sup>11</sup> Ω·cm

Defect	In <sub>Cd</sub> <sup>+</sup>	A <sup>-</sup>	A1 <sup>-</sup>	K <sup>-</sup>	X <sup>-</sup>	D <sup>2-</sup>	J <sup>-</sup>	Y <sup>-</sup>	W <sup>-</sup>	H1 <sup>+</sup>	I <sup>+</sup>
E <sub>i</sub> , eV	0.019	0.14	0.16	0.25	0.29	0.35	0.53	0.67	0.70	0.86	1.1
σ <sub>i</sub> , cm <sup>2</sup>	1·10 <sup>21</sup>	2·10 <sup>-19</sup>	2·10 <sup>-19</sup>	6·10 <sup>-19</sup>	4·10 <sup>-19</sup>	7·10 <sup>-17</sup>	5·10 <sup>-17</sup>	10 <sup>-17</sup>	10 <sup>-17</sup>	10 <sup>-18</sup>	10 <sup>-18</sup>
N <sub>i</sub> , cm <sup>-3</sup>	1.9·10 <sup>16</sup>	2·10 <sup>15</sup>	2·10 <sup>15</sup>	2.5·10 <sup>15</sup>	2.5·10 <sup>15</sup>	2·10 <sup>15</sup>	5·10 <sup>14</sup>	3·10 <sup>15</sup>	3·10 <sup>15</sup>	5·10 <sup>15</sup>	4.5·10 <sup>15</sup>

The calculated electrophysical properties of the unirradiated materials corresponded to known values: μ<sub>n</sub>~1200 cm<sup>2</sup>/(V·sec), the lifetimes of electrons τ<sub>n</sub> and the holes τ<sub>p</sub> were about 10<sup>-6</sup> seconds for both materials. The changes in ρ, μ<sub>n</sub>, τ<sub>n</sub>, τ<sub>p</sub>, the positions of the Fermi level E<sub>F</sub> in the band gap of CdTe:Cl and CZT, as well as the change in the charge collection efficiency η of the detector based on these materials were simulated depending on the content of radiation defects and the concentration of alloying donors N<sub>D</sub> at T = 20°C – operating temperature of the detectors.

## RESULTS AND DISCUSSION

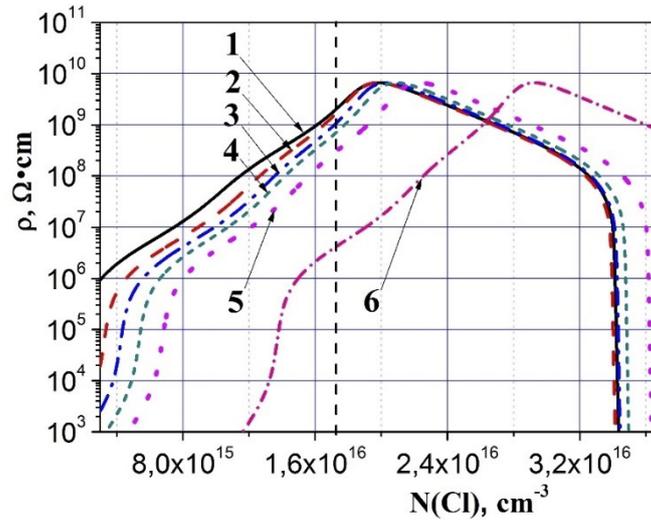
The effect of radiation damage caused by the <sup>60</sup>Co gamma irradiation of two sets of detectors based on CdTe:Cl and Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te, on the changes of their resistivity and spectroscopic properties, was experimentally investigated in [14, 15]. The initial dose of γ-irradiation of both sets of sensors in a <sup>60</sup>Co gamma cell was 10 kGy. The total doses up to 50 and 30 kGy were delivered in steps of 5 kGy each to CdTe:Cl and Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te detectors, respectively. The resistivity and the energy resolution of the main photopeak of the <sup>57</sup>Co spectrum recorded using the detectors under study were determined before and after gamma irradiation. The energy levels in the band gap were determined by photoinduced current transient spectroscopy - PICTS. The measurement results obtained in [14, 15] served as the source data in present work to simulate the change and degradation of electrophysical and detector properties of CdTe:Cl and CZT under the influence of gamma irradiation.

### CdTe:Cl-based detectors

CdTe:Cl-based detectors were exposed to 122 keV <sup>60</sup>Co gamma irradiation by the dose of 10 to 50 kGy. With an increase in the radiation dose, there was a gradual degradation of <sup>57</sup>Co and <sup>122</sup>Am spectra and a shift of the main photopeaks toward lower energies and their gradual broadening by 7-8%, what indicated a decrease in charge collection. In the process of exposure, a gradual decrease in the specific resistance of Δρ for CdTe:Cl was recorded, and Δρ reached 60% at the moment of complete degradation of detector properties after the radiation dose of 50 kGy. The PICTS technique, used to study the behavior of radiation defects, registered an increase in the concentrations of A-centers (AX, A0, A, A1 levels) and a decrease in the relative content of defects G, H, H1, I at an increase in the radiation dose. The peak of defect Z in PICTS spectra appears only in a completely degraded detector. The results obtained in [14, 15] were used in the present work to simulate changes in the electrophysical and detector properties of CdTe:Cl in the process of gamma irradiation.

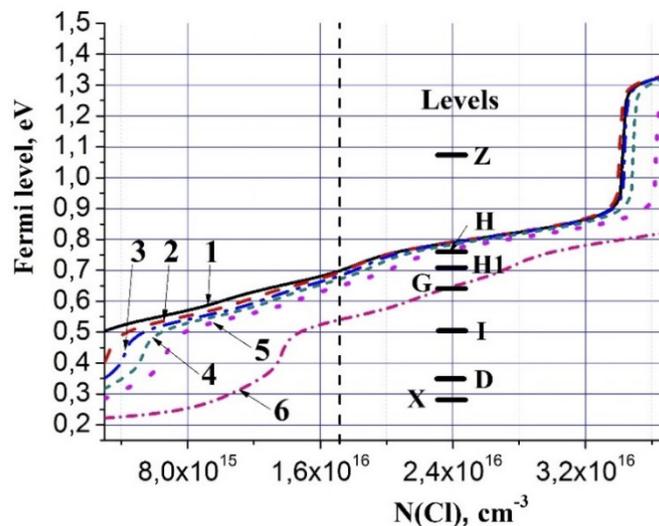
Fig. 1 shows the changes in the specific resistance of CdTe:Cl subject to the concentration of alloying chlorine impurity after different doses of gamma irradiation. The concentrations of irradiation-induced A-centers are gradually increasing and after the dose of 50 kGy reach the following values, cm<sup>-3</sup>: N(AX)=2.5·10<sup>15</sup>, N(A0)=2,1·10<sup>16</sup>, N(A)= 2·10<sup>15</sup>; N(A1)=2.5·10<sup>15</sup>. The concentrations of deep levels are gradually decreasing and at the moment of complete degradation reach the following values, cm<sup>-3</sup>: N(G)=6·10<sup>15</sup>, N(H)=8·10<sup>15</sup>, N(H1)=6.5·10<sup>15</sup>, N(I)=7.5·10<sup>15</sup>. These concentrations are estimated values that gradually changed during irradiation. The variation range of N(Cl) in the figure is presented so that the curves of the specific resistance ρ would pass through the maxima. The vertical dashed line indicates the chlorine concentration at which the hole conductivity and the specific resistance ρ=2·10<sup>9</sup> Ω·cm, measured in [15], is observed in the initial CdTe:Cl, therefore it can indicate the material under study. In Fig. 1 we see a confirmed experimentally gradual decrease in the resistivity with an increase in the radiation dose due to the shift of the curves ρ(N(Cl)) towards greater

chlorine concentrations. This shift is caused by a gradual increase in the content of electrically active acceptor A-centers (AX, A0, A, A1), whose compensation requires increased concentrations of the shallow chlorine donor. We see that after the dose of 50 kGy, the resistance decreases markedly, which leads to an increase in leakage currents and complete degradation of the detector properties. A significant decrease in  $\rho$  occurred due to the shift of the Fermi level towards the A centers levels and valence band.



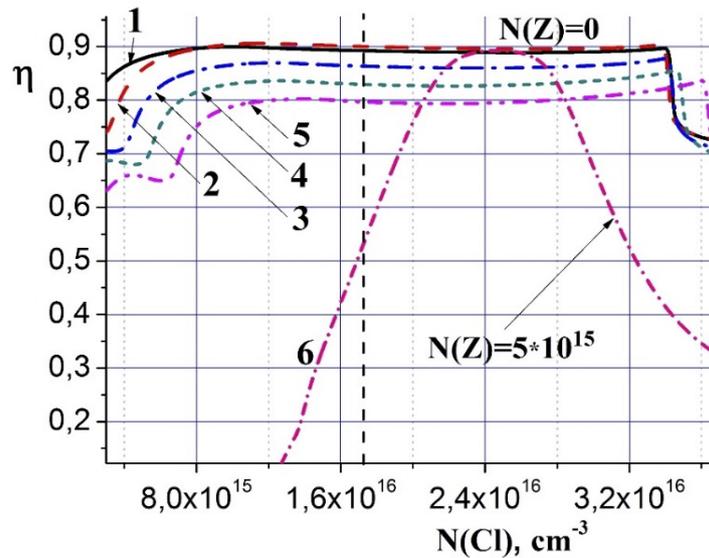
**Figure 1.** Dependences of the of CdTe:Cl resistivity on the Cl concentration after different doses of gamma irradiation, kGy: 1 – initial, whose composition is shown in Table 1; 2 - 10; 3 - 15; 4 - 20; 5 - 25; 6 - 50. The vertical dashed line indicates the concentration of doping chlorine ( $1.7 \cdot 10^{16} \text{ cm}^{-3}$ ) for the test sample

Fig. 2 shows the dependences of the Fermi level on the concentration of the substitutional impurity  $\text{Cl}_{\text{Te}}$  after different doses of gamma irradiation. For the sample under study, a shift in the Fermi level, which is accompanied by an increase in the hole conductivity and a decrease in  $\rho$ , is clearly visible. With an increase in the concentration of shallow levels of A-centers, the content of deep levels G, H, H1 slightly decreases and, for this reason, the Fermi level does not stabilize in the vicinity of these deep levels and, correspondingly, the electrophysical properties vary, what leads to a gradual degradation of the recording ability of the CdTe:Cl-based detector. This agrees with the experiment, described in [14, 15], where it has been demonstrated by the example of a number of PICTS spectra (Fig. 2, [15]), from which it can be concluded that the detector spectroscopic performance gradually deteriorates with simultaneous increase in the radiation dose and the content of radiation A-centers. The decrease in resistivity is accompanied by an increase in leakage currents and noise in the pulse amplitude spectra. Degradation of spectroscopic performance and decrease in charge collection may also occur due to the capture of nonequilibrium electrons by the level of the defect Z, as well as by the partially ionized levels H, H1, and G, through which the Fermi level passes during irradiation.



**Figure 2.** The Fermi level, measured from the valence band, subject to the concentration of the doping chlorine after different doses of gamma irradiation. The parameters of curves 1–6 correspond to the numbered curves in Fig. 1. The vertical dashed line indicates the test sample.

The change in the charge collection efficiency  $\eta$  was calculated subject to the content of radiation defects, which is shown in Fig. 3. It can be seen from the graphs that the radiation defect Z which presumably corresponds to the interstitial tellurium Te(I) exerts the decisive influence on the degradation of the detector spectroscopic properties. The authors of [14, 15] experimentally confirm that the peak of the Z defect in the PICTS spectrum appears only in a completely degraded detector. The simulation has also shown that the charge collection efficiency  $\eta$  of detector, whose initial composition is shown in Table 1, clearly correlates with the value of resistivity  $\rho$ : the higher is  $\rho$ , the higher is  $\eta$ , and, on the contrary, in the low-resistance state the collection of charges drops sharply. In this case, in order to realize the experimentally known fact of spectrometric performance degradation of CdTe due to the appearance of the defect Z, the capture cross section  $\sigma$  of nonequilibrium charge carriers for Z must be about  $10^{-15}$  cm<sup>2</sup>.



**Figure 3.** Dependences of the charge collection efficiency on the concentration of doping chlorine after different doses of gamma irradiation. The parameters of curves 1–6 correspond to the numbered curves in Fig. 1, and for 1–5  $N(Z) = 0$ , for curve 6 –  $N(Z) = 5 \cdot 10^{15}$  cm<sup>-3</sup>; The vertical dashed line indicates the test sample

An increase in the concentration of the radiation donor defect Z partly compensates the increase in the concentration of the acceptor A centers, and narrows the concentration range of the doping Cl<sub>Te</sub>, in which high values of  $\eta$  take place (see Fig. 3, curve 6). The narrowing of the region of high  $\eta$  is caused by the capture of nonequilibrium electrons at the level of the defect Z. It should be noted that the necessary condition for the large capture cross section  $\sigma \sim 10^{-15}$  cm<sup>2</sup> for complete degradation of the detector properties under the influence of the defect Z is explained by the large difference between level  $E_Z = E_C - 0.47$  or  $E_Z = E_V + 1.05$  eV and Fermi level  $E_F$ .

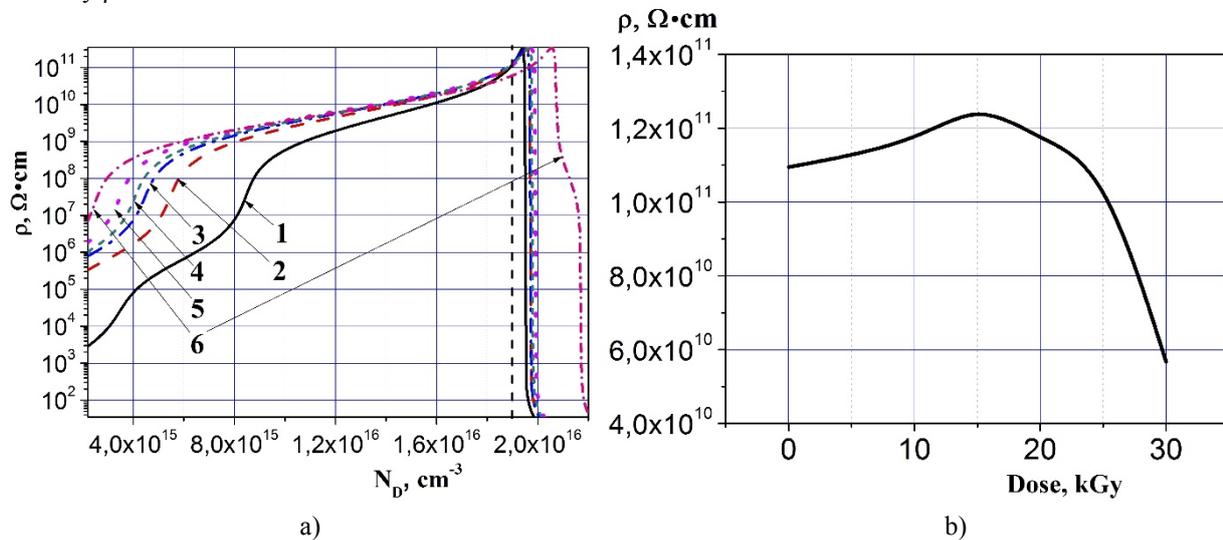
### CdZnTe-based detectors

Let's consider the simulation results of changes in the electrophysical and detector properties of CZT under the influence of gamma irradiation, described in [14, 15], where a batch of Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te detectors were irradiated with doses from 10 kGy to complete degradation of their detector properties after 30 kGy. The detectors did not change their performance during irradiation, and then, at the final stage, they suddenly lost their spectroscopic properties (see Fig. 8 [15]). It follows from the PICTS spectra shown in Fig. 5 in [14] and Fig. 11 of paper [15] that the content of radiation defects, presented by shallow levels A, K, X, D, slightly increases in the process of gamma quanta bombardment. However, the concentrations of defects corresponded to Y and W deep levels and, in particular, of the donor level H1 ( $E_C - 0.82$  eV) located near the middle of the band gap, increase noticeably. Thus, the phenomenon of radiation self-compensation is realized by increasing the content of deep levels. A noticeable peak of the defect Z appears in the PICTS spectrum at the final stage of exposure after the dose of 30 kGy, when the spectroscopic properties are completely degraded. The calculations of the changes in  $\rho$ ,  $\eta$ , and  $E_F$  in the process of gamma irradiation were performed with these features taken into account.

Fig. 4 shows the behavior of the Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te resistivity after different irradiation doses; a)  $\rho$  as a function of the concentration of the doping shallow donor  $N_D$ , b) the dependence of  $\rho$  on the irradiation dose. The matrix composition of the initial, unirradiated detector is shown in Table 2. In the process of gamma irradiation, the concentration of radiation defects K, X, Y, W, H1 in the material gradually increases, and the relative content of the defect I decreases. After the irradiation dose of 25 kGy, these defects were assigned the following concentrations, cm<sup>-3</sup>:  $N(K)=2,7 \cdot 10^{15}$ ,  $N(X)=2,7 \cdot 10^{15}$ ,  $N(Y)=3,2 \cdot 10^{15}$ ,  $N(W)=3,2 \cdot 10^{15}$ ,  $N(H1)=1 \cdot 10^{16}$ ,  $N(I)=4 \cdot 10^{15}$ .

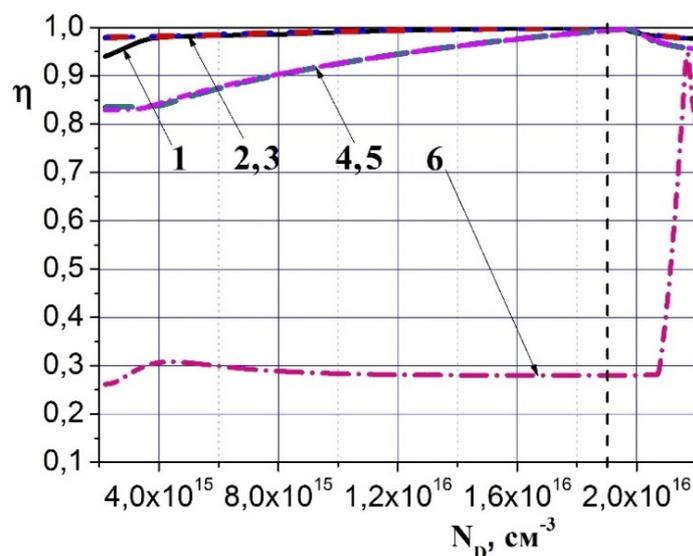
The donor defect Z which appears in the spectrum at the final stage of gamma irradiation was assigned a concentration of  $1 \cdot 10^{15}$  cm<sup>-3</sup>, and the defects, presented by deep levels, were assigned the following concentrations, cm<sup>-3</sup>:  $N(Y)=4 \cdot 10^{15}$ ,  $N(W)=4,2 \cdot 10^{15}$ ,  $N(I)=2 \cdot 10^{15}$ . Fig. 4b shows that at the initial stage of gamma irradiation the resistivity

increases and then decreases, that was confirmed experimentally in [14, 15, 17]. The simulation has shown that the effect of an increase in  $\rho$  is explained by an increase in the content of a deep donor H1 which can act as the  $\text{Te}_{\text{Zn}}$  antisite defect. An increase in the concentration of the radiation level H1 shifts the Fermi level  $E_F$  closer to the middle of the band gap, increasing  $\rho$ . In the course of further irradiation, the resistivity decreases, although it remains quite high even after a dose of 25 kGy  $\rho = 1.1 \cdot 10^{11} \Omega \cdot \text{cm}$ .



**Figure 4.** Dependences of the resistivity of  $\text{Cd}_{0.9}\text{Zn}_{0.1}\text{Te}$  on the concentration of the dopant donor impurity after different irradiation doses. a) 1 – initial, unirradiated; 2 – 10 kGy; 3 – 15 kGy; 4 – 20 kGy; 5 – 25 kGy; 6 – 30 kGy. The vertical dashed line indicates the test sample. b) Dependence of  $\rho$  on the irradiation dose.

For this reason the spectroscopic properties of the detector remain at a high level, what is confirmed experimentally (see [15] Fig. 5). At the final stage after a dose of 30 kGy, when the spectroscopic properties are completely degraded, the resistivity decreases to a value of  $\rho = 5.9 \cdot 10^{10} \Omega \cdot \text{cm}$ . The simulation has shown that the main reason for the complete degradation of the detector is the capture of nonequilibrium electrons at the radiation defect Z, which can be represented by interstitial tellurium  $\text{Te}(\text{I})$ , that appears after the dose of 30 kGy with a noticeable decrease in the charge collection efficiency  $\eta$  to 0.3, as shown in Fig. 5. The charge collection is reduced due to the decrease in the lifetime of nonequilibrium electrons to the value of  $9.3 \cdot 10^{-9}$  sec. The resistivity has little effect on the performance degradation, since it decreases slightly, remaining high in value  $\sim 10^{10} \Omega \cdot \text{cm}$ . Indeed, the simulation of the dependences  $\rho(N_D)$  and  $\eta(N_D)$  with the assumed concentrations of defects in the degraded detector shows that only introduction of the defect Z with a capture cross section of  $7 \times 10^{-15} \text{ cm}^2$  and a concentration of  $1 \times 10^{15} \text{ cm}^{-3}$  leads to obtaining a sharp decrease in the spectroscopic properties.



**Figure 5.** Dependences of the charge collection efficiency on the concentration of the dopant donor impurity after different gamma irradiation doses. Curves 1–6 correspond to the numbered curves in Fig. 4. The vertical dashed line indicates the test sample.

The simulation performed in this work is in qualitative agreement with the experimental results of [14, 15], according to which the resistivity in the degraded CZT-based detector remains higher than even in the initial  $\text{CdTe:Cl}$ , which

demonstrated an acceptable spectroscopic performance. Thus, a decrease in  $\rho$  of the CZT-based detector has less effect on the degradation of its recording properties compared to the effect of capture of nonequilibrium carriers at the level of the radiation donor defect Z (Te(I)).

### CONCLUSIONS

Degradation of the spectroscopic performance of detectors based on high-purity CdTe:Cl occurs gradually during gamma irradiation due to the continuous formation of cadmium vacancies  $V_{Cd}$  and acceptor complexes  $V_{Cd}-Cl$  when their concentration increase. As a result, the content of the donor impurity Cl and the compensation of acceptors somewhat decrease. The hole concentration and hole conductivity increase, and  $\rho$  decreases. Due to the relatively low initial resistivity of CdTe, its further decrease causes an increase in the leakage currents and increment of noise in amplitude spectrum. Along with the formation of  $V_{Cd}$ , tellurium atoms are knocked out into the interstice (defect Z), thereby increasing the content of donor defects - tellurium vacancies  $V_{Te}$  which, remaining neutral, do not affect the electrical compensation and capture processes due to the large difference between the  $V_{Te}$  level and the Fermi level. The continuously increasing concentration of the Te(I) at the final stage of gamma irradiation provides appearance of Z peak in the PICTS spectrum at the moment of complete degradation of the spectroscopic performance.

The spectroscopic properties of CZT during gamma irradiation remain unchanged up to 25 kGy due to the strong mechanism of radiative self-compensation in this semiconductor, and sharp degradation occurs only at the final stage of radiation exposure after a dose of 30 kGy with the appearance of a donor defect Z ( $E_C - 0.52$  eV). The mechanism of radiative self-compensation is realized by increasing the relative content of the deep donor center H1 which is the  $Te_{Zn}$  antisite defect. In other words, tellurium in the irradiated CZT occupies mainly the sites of zinc vacancies  $V_{Zn}$ , and in a small amount – sites of  $V_{Cd}$ , since zinc atoms are almost two times lighter than those of cadmium, and a greater amount of Zn than that of Cd is knocked out from the lattice sites by gamma quanta. The deep donor  $Te_{Zn}$  fixes the position of the Fermi level near the middle of the band gap of CdZnTe, and at the same time stabilizes its electrophysical and detector properties. An increase in the content of the Te(I) (defect Z), at its certain concentration, leads to a complete degradation of the spectroscopic properties of a CZT-based detector due to the capture of nonequilibrium electrons at the Z level. This degradation occurs despite self-compensation by the H1 level and maintaining a fairly high resistivity of the detector material.

The noticeable difference in the radiation resistance of CdTe:Cl (50 kGy) and  $Cd_{0.9}Zn_{0.1}Te$  (30 kGy) can be explained by different behavior of Fermi level  $E_F$  in these semiconductors during irradiation. In the case of CdTe:Cl, the Fermi level gradually shifts towards the valence band during irradiation and increase in Z concentration, and moves slightly away from the level Z ( $E_C - 0.47$ ), thereby reducing the rate of capture of nonequilibrium charge carriers on it. However, at a certain Z concentration after the dose of 50 kGy, a complete degradation of properties occurs. For the case of CdZnTe, the Fermi level is approximately in the middle of the band gap due to self-compensation, and, therefore, it is closer to the donor level Z. For this reason, the rate of capture and recombination at this level in CdZnTe is higher than that in CdTe:Cl. Thus, the complete degradation of the CdZnTe-based detector properties occurs at a lower concentration of radiation defect Z or Te(I) and hence after the lower irradiation dose of 30 kGy.

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### МЕХАНІЗМИ ДЕГРАДАЦІЇ ДЕТЕКТОРНИХ ВЛАСТИВОСТЕЙ CdTe ТА CdZnTe ПІД ВПЛИВОМ ГАММА-ОПРОМІНЕННЯ

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Представлена робота присвячена вивченню методом комп'ютерного моделювання механізмів впливу радіаційних дефектів, що виникають під дією гамма-випромінювання, на зміну питомого опору  $\rho$ , часу життя нерівноважних електронів  $\tau_n$  і дірок  $\tau_p$  в CdTe:Cl і Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te, а також ефективності збору зарядів  $\eta$  неохолоджуваних детекторів випромінювання на основі цих матеріалів. Радіаційні дефекти, яким відповідають глибокі енергетичні рівні в забороненій зоні, діють як центри захоплення нерівноважних носіїв заряду, помітно впливають на ступінь компенсації, змінюючи  $\rho$  матеріалу детектора, процеси рекомбінації, зменшуючи  $\tau_n$  і  $\tau_p$ , що в кінцевому підсумку може викликати зниження ефективності збору зарядів  $\eta$ . Виявлені конкретні причини погіршення детекторних властивостей CdTe:Cl і Cd<sub>0.9</sub>Zn<sub>0.1</sub>Te під дією гамма-випромінювання від <sup>60</sup>Co, а також основні чинники, що призводять до повної деградації реєструвальної здатності детекторів на основі цих напівпровідників в процесі їх експлуатації. Поступове погіршення спектроскопічних характеристик детекторів на основі CdTe:Cl при гамма-опроміненні відбувається через безперервне утворення вакансій кадмію V<sub>Cd</sub> і акцепторних комплексів V<sub>Cd</sub>-Cl, які безперервно зміщують рівень Фермі в бік валентної зони і зменшують  $\rho$ . Повна деградація характеристик детекторів з CdTe відбувається в основному через захоплення нерівноважних електронів на рівні енергії міжвузельного телуру Te(I). Незмінні спектроскопічні властивості сенсорів на основі CdZnTe при гамма-опроміненні до 25 кГр обумовлені механізмом радіаційної самокомпенсації за рахунок утворення дефектів заміщення Te<sub>Zn</sub>. На завершальній стадії опромінення відбувається різке погіршення детекторних властивостей CdZnTe через захоплення і рекомбінації нерівноважних носіїв заряду на енергетичному рівні дефекту Te(I). Різну радіаційну стійкість CdZnTe і CdTe:Cl можна пояснити різним поведінкою рівня Фермі E<sub>F</sub> в цих напівпровідниках при гамма-опроміненні. E<sub>F</sub> у CdZnTe при радіаційному впливі знаходиться поблизу середини забороненої зони, а в телуриді кадмію дрейфує в бік валентної зони. Швидкість захоплення і рекомбінації через донорний рівень Te(I) в CdTe:Cl менша, ніж в CdZnTe через більшу різницю між рівнем Фермі і рівнем радіаційного дефекту Te(I) в телуриді кадмію. Таким чином, повна деградація детектора CdTe:Cl відбувається при більш високій концентрації радіаційного дефекту Te(I) і, отже, після більш високої дози опромінення 50 кГр у порівнянні з дозою 30 кГр, необхідною для деградації детекторних властивостей CdZnTe.

**Ключові слова:** детекторні властивості, моделювання, CdTe, CdZnTe, гамма-опромінення, радіаційні дефекти