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THE COMPOSITION OF IMPURITIES AND DEFECTS IN $Cd_{1-X}Mg_XTe$:In, NECESSARY TO ENSURE STABLE DETECTOR PROPERTIES

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A model study of the promising new material $Cd_{0.92}Mg_{0.08}Te$:In, intended for X-ray and gamma radiation detectors operating at room temperature, was carried out. The paper highlights the results of quantitative studies of the influence of the content of impurities and structural defects on the electrophysical and detector properties of $Cd_{0.92}Mg_{0.08}Te$:In. An analysis of the calculated values of resistivity ρ and concentrations of free charge carriers, life time of non-equilibrium electrons τ_n, and holes τ_p, charge collection efficiency η with different composition of impurities and defects in this material at temperature T = 298 K was carried out. The optimal ranges of energy and concentration of alloying deep donor, which ensure a stable high-resistive state and acceptable values of η, are established. Compensation of cadmium vacancies with indium admixture was studied. Assumption was made regarding possibility of increasing the operating time of the detector having semi-insulating properties and great charge collection efficiency. A direction for further research has been formulated in order to clarify the nature of a suitable doping deep donor that ensures stable properties of the detector.

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INTRODUCTION

Room temperature solid-state ionizing radiation detectors are currently used in many fields, for example, in medicine, environmental protection, radiation monitoring, atomic energy, and astrophysical research [1, 2]. To produce them it is reasonable using semiconductor compounds that meet certain requirements, among which the following are required: high resistivity $\rho = 10^{10}…10^{11}$ Ω·cm; the product of the mobility μ by the lifetime τ of non-equilibrium charge carriers $\mu\cdot\tau \geq 10^{-3}$ cm^2/V. Nowadays, the room temperature X-ray and gamma radiation detectors based on CdTe and CdZnTe are most common used. Despite their undoubted advantages, they have some drawbacks, so new alternative materials are also currently being developed, in particular CdMnTe and CdMgTe. We have already studied in previous papers [3, 4] the most optimal detector performances and electrophysical properties of CdMnTe of detector quality. Cadmium magnesium telluride (CdMgTe) is concerned as a new promising compound semiconductor that practically meets various requirements to room temperature radiation sensors [5–9], so let's consider this detector material.

CdMgTe (CMT) possess perfect crystallinity due to close lattice parameters of CdTe (6.48 Å) and MgTe (6.42 Å). In addition, the optimal band gap in it can be achieved by using less magnesium compared to the Zn and Mn in CdZnTe and CdMnTe respectively, so matrix in homogeneities due to doping effects in CdMgTe can be minimized. The segregation coefficient of Mg in CdTe is 1.0 [10] compared to 1.35 for Zn, that is an important advantage of CMT over CdZnTe in ensuring a uniform distribution of magnesium throughout the ingot. In order to achieve high values of specific resistance, necessary for producing a detector-quality crystal, the indium shallow donor is usually added to the CdMgTe matrix [11, 12]. Such doping is primarily required to compensate an action of cadmium vacancies always present in grown crystals.

Any semiconductor material of detector quality, as well as CdMgTe, must have a high resistivity $\rho \geq 10^{10}$ Ω·cm. It significantly complicates the experimental study of the influence of the i-th energy levels E_i in the band gap, the capture cross sections of non-equilibrium charge carriers σ_i and concentrations of defects N_i on the lifetime of non-equilibrium electrons τ_n and holes τ_p, the electron mobility μ_n, as well as the charge collection efficiency η of the detector and its resistivity ρ. Model studies of ρ, μ_n τ_n τ_p, η using experimentally determined values E_i, σ_i, N_i make it possible to understand the mechanisms of changes in the electrophysical and detector properties of CdMgTe depending on the content and parameters of impurities and defects.

The purpose of the work was to determine by computer modeling the optimal content of impurities and structural defects as well as the nature of their influence on the electrophysical and detector properties of CMT using the example of $Cd_{0.92}Mg_{0.08}Te$:In experimentally studied in [12]. The calculations of ρ, τ_n, τ_p, μ_n, η depending on the content and parameters of various impurities and defects in the material were performed during the model research.

MATERIALS AND MODELS

To study the maximum possible values of ρ, τ_n, τ_p, μ_n, η for the investigating material $Cd_{0.92}Mg_{0.08}Te$:In, it is necessary to know the composition of its defects and impurities, which was determined in [12] experimentally and presented there in the form of DLTS (Deep Level Transient Spectroscopy) spectra. Since the authors do not provide data about the quantitative content, it was decided to take as a basis the content of impurities and defects at the quantity of $10^{15}…10^{16}$ cm^{-3}, achieved in modern laboratories, and to establish the ratio between their concentrations, basing on the relative heights of the peaks in the presented DLTS spectrum. The order of magnitudes of the capture cross-sections of non-equilibrium charge carriers by energy levels were adopted according to the results of the TSC (thermally stimulated current) experimental technique. Such results were published, for example, in [13]. The data obtained by this technique for direct bandgap semiconductors are in good agreement with the known Shockley–Reed recombination model when calculating the lifetime of non-equilibrium electrons τ_n and holes τ_p. After the analysis of the results [12], the initial composition given in the Table was adopted.

With the exception of the E7 levels, presented in the Table, the energy levels of the donors are measured relative to the bottom of the conduction band E_C, and the acceptor levels do from the top of valence band E_V. The designation E7 refers to the energy levels of a number of deep donors which in the model study were specially introduced into the $Cd_{0.92}Mg_{0.08}Te$ matrix in order to determine the corresponding changes in the resistivity ρ and the charge collection efficiency η.

Defects and impurities in $Cd_{0.92}Mg_{0.08}Te$ [12]

Label	Concentration N_i, см$^{-3}$	Energy level E_i, eV	Capture crosssection σ, cm^2	Possible defects [12]
N_D (In)	$3\cdot10^{15}…5\cdot10^{16}$	E_C – 0.01	$1.6\cdot10^{-22}$	In_{Cd}
E1	$5.3\cdot10^{15}$	E_V + 0.046	$1.2\cdot10^{-21}$	In_{Cd}^+ shallow acceptor
E2	$3.9\cdot10^{15}$	E_V + 0.21	$7.2\cdot10^{-19}$	A-center
E3	$2.6\cdot10^{15}$	E_C - 0.36	$1.6\cdot10^{-18}$	Te-antisite
E4 (V_{Cd})	$1\cdot10^{16}$	E_V + 0.32	$9.9\cdot10^{-18}$	Cadmium vacancy
E5	$2.1\cdot10^{15}$	E_C – 0.76	$6.3\cdot10^{-18}$	$(Te_{Cd}+V_{Cd})^{2-/-}$ [13]
E6	$4\cdot10^{15}$	E_C – 1.0	$3\cdot10^{-18}$	Te_{Cd}
E7	–	E_V + 0.4 – E_V + 1.2	–	Deep donor

The used models and their testing are described in detail in [14]. The electroneutrality equation was formulated up with taking into account all impurities and defects experimentally registered in [12]. This equation was numerically solved with respect to the Fermi level *F*, and then the concentrations of free electrons (*n*) and holes (*p*) were determined under the parabolic band approximation. Electron mobility μ_n was calculated under the momentum relaxation time approximation (tau approximation) with taking into account scattering by ionized and neutral centers, acoustic, piezoelectric and optical phonons. The holes mobility μ_p was considered constant and equaled to 100 cm^2/(V·s). The conductivity was calculated using the formula $e\cdot n\cdot\mu_n + e\cdot p\cdot\mu_p$ (*e* is the electron charge), and the resistivity was evaluated as its reciprocal. The charge collection efficiency of the detector η was determined by Hecht's equation [15, p. 489]. The interelectrode gap of the detector was assumed to be 5 mm, and the electric field strength did 1000 V/cm.

RESULTS AND DISCUSSION

Effective registration of ionizing radiation can be assured at low leakage currents and small background noise in the detector, which becomes possible for specific resistance ρ not lower than 10^{10} **Ω**·cm. Doping with shallow donors, served to compensate for the action of shallow acceptors and cadmium vacancies, is used in CMT manufacturing technologies to achieve this value of ρ. However, such alloying does not always manage to achieve high values of ρ, or the obtained high specific resistance of the CMT detector material turns out to be unstable and, for example, annealing processes after growth can significantly change it [7, 12]. It is necessary to find out the conditions for such a change in ρ and to determine methods of its stabilization.

Fig. 1 shows the behavior of resistivity depending on the content of cadmium vacancies $N_{DA}(V_{Cd})$ and alloying indium N_D(In) for the initial composition of $Cd_{0.92}Mg_{0.08}Te$:In studied in [12]. Hence the reason for the unstable behavior of ρ becomes clear: with a small change in the content of impurities and structural defects, the resistivity of the detector material can noticeably decrease. Therefore, it is necessary to expand the range of concentrations of defects and impurities within that the value $\rho \geq 10^{10}$ Ω·cm is reached.

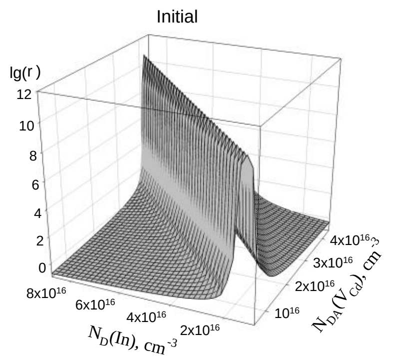
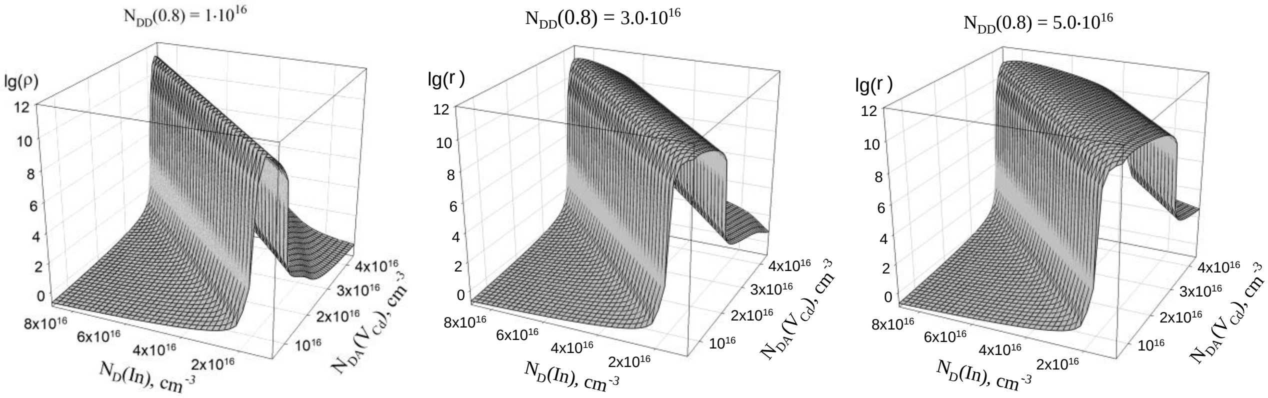


Fig. 1. The decimal logarithm of the $Cd_{0.92}Mg_{0.08}Te$:In resistivity depending on the concentrations of cadmium vacancies (V_{Cd}) and alloying indium

Earlier, in paper [14], it was established that the concentration range of high ρ in CdTe and CdZnTe can be expanded by introducing a deep donor with the energy level close to the middle of the band gap: E_V+0.8 eV. We decided, using this result, to investigate the behavior of ρ with the same change in V_{Cd} and In concentrations as in Fig. 1, but with a different content of a deep donor having the energy of E_V+0.8 eV. Fig. 2 shows the dependences of the resistivity on the content of cadmium vacancies and doping indium at the concentrations of the deep donor N_{DD}= (1…5)·10^{16} cm^{-3}.



a *b* *c*

Fig. 2. The behavior of the decimal logarithm ρ at the concentrations of the deep donor N_{DD} with $E_{DD}=E_V+0.8$ eV, cm^{-3}: a – $1\cdot10^{16}$, b – $3\cdot10^{16}$, c – $5\cdot10^{16}$

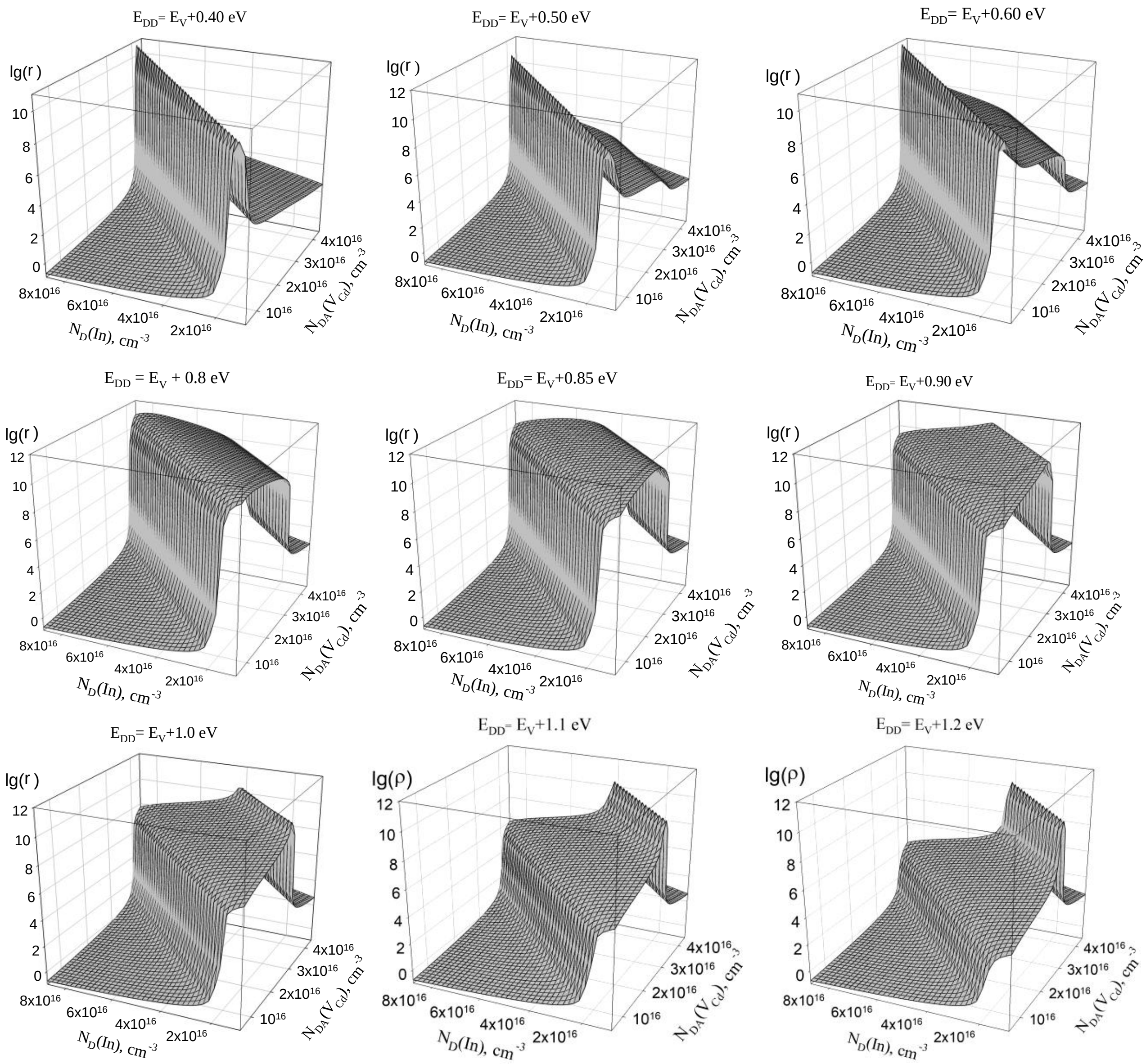


Fig. 3. Decimal logarithm of the resistivity depending on the concentrations of cadmium vacancies and indium after doping with donors having the energy varying from 0.4 to 1.2 eV relative to the top of valence band. For all graphs, the concentration of corresponding deep donors N_{DD} is equaled to $5\cdot10^{16}$ cm^{-3}

We see from Fig. 2 that a gradual increase in the N_{DD} concentration results in a gradual expansion of the high-resistance region with $\rho \geq 10^{10}$ Ω·cm, and at $N_{DD} = 5\cdot10^{16}$ cm^{-3} we get a material quite suitable for detector. The simulations established that a further increase in the concentration of the deep donor causes a decrease in the charge collection efficiency of the detector due to the capture and recombination of non-equilibrium electrons at this deep donor center.

Taking the concentration $N_{DD} = 5\cdot10^{16}$ cm^{-3} as a basis, a model study of the behavior of lg(ρ) was carried out for various donor impurities having the energy which varies from 0.4 to 1.2 eV relative to the top of valence band. The results of the simulation are shown in Fig. 3. The energy levels of the deep donors are indicated directly on the graphs.

We can see from Fig. 3 that, considering the height and width of the high-resistance region, the best materials are those doped with donors having the energy levels of 0.85…0.90 eV relative to valence band. The material, doped by the donor with the energy $E_{DD} \le E_V$+0.95 eV, is acceptable also, but it is not shown in Fig. 3.

It remains to investigate the charge collection efficiency in detectors made of better materials containing donors with the energy levels of 0.85, 0.90, and 0.95 eV relative to E_V. The E_V+0.8 eV level is located too close to the middle of the band gap, so a very high rate of recombination of non-equilibrium charge carriers takes place at it. Fig. 4 shows the dependences of the charge collection efficiency η on the concentration of indium in the corresponding detectors based on the specified materials. The simulation showed that for all concentrations of deep donor levels N_{DD} with the energies 0.85 and 0.90 eV (see Fig. 4), the detector material with the content of indium $1.5\cdot10^{16}$ cm^{-3} possess the highest resistivity ($\rho \ge 10^{10}$ Ω·cm). In addition, for a crystal with a deep donor having energy $E_{DD}=E_V$+0.95 eV the resistivity $\rho > 3\cdot10^9$ Ω·cm at $N_D(In)=1\cdot10^{16}$ cm^{-3}.

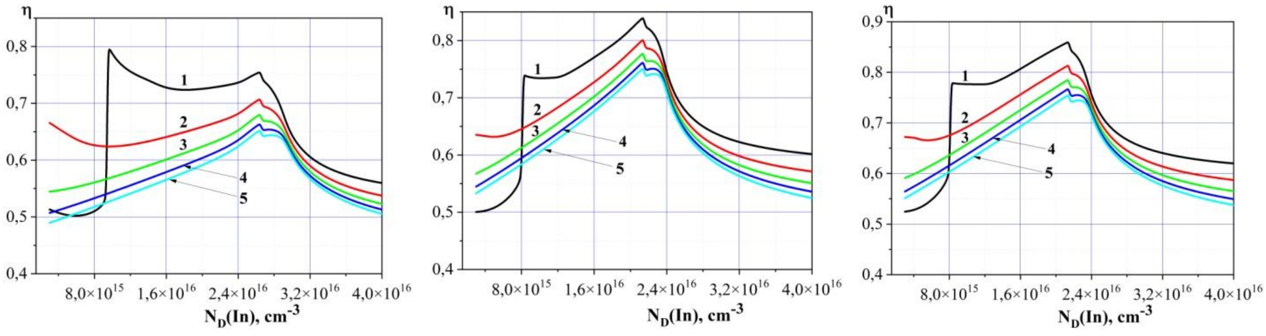


Fig. 4. The charge collection efficiency of $Cd_{0.92}Mg_{0.08}Te$-based detectors doped with deep donors having energies of 0.85 (a); 0.90 (b), and 0.95 eV (c) relative to valence band for the following their concentrations, cm^{-3}: 1 – $1\cdot10^{16}$; 2 – $2\cdot10^{16}$; 3 – $3\cdot10^{16}$; 4 – $4\cdot10^{16}$; 5 – $5\cdot10^{16}$

Fig. 4 shows that with an increase in the content of the deep donor, the expected decrease in charge collection occurs, but the value of η is slightly higher in the detector with the deep donor having energy $E_{DD} = E_V$+0.95 eV. This is explained by the fact that a higher rate of capture and recombination of non-equilibrium charge carriers is always observed at levels located closer to the middle of the band gap $E_G/2$ (~ E_V+0.8 eV) and vice versa. It should be noted that the model, used to calculate the charge collection, only qualitatively display the trend of the studied phenomenon and does not pretend to be quantitatively accurate. The specific value of η in the initial detector may be greater under the condition of producing a cleaner source material with a lower content of cadmium vacancies. Modeling showed that a smaller number of deep donors should be introduced in a cleaner and structurally perfect CMT crystal to expand the high-resistance region as well as compensate for V_{Cd} and shallow background acceptors. That in turn contributes to the increase in charge collection efficiency.

Non-equilibrium electrons make a main contribution to the signal in detector, so the hole conductivity of the detector material is needed to increase the signal/noise ratio. Fig. 5 shows the change in the content of free holes within the V_{Cd} and In concentration range under investigation.

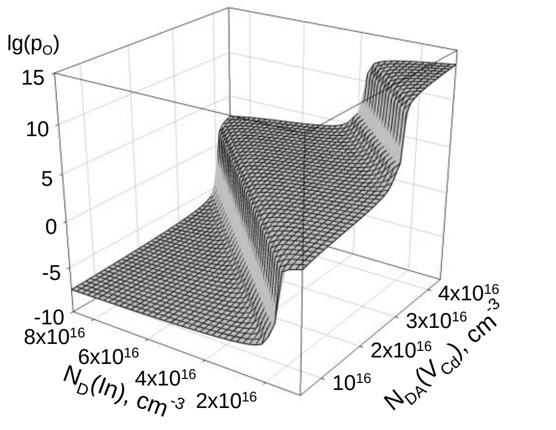


Fig. 5. Dependence of the decimal logarithm of the concentration of free holes p_0 on the content of cadmium vacancies and indium

The surface shown in Fig. 5 does not differ visually for materials doping by the donors having the energies E_{DD}=0.85, 0.90, and 0.95 eV relative to E_V. The simulation showed that there is hole conduction at the area of the highest resistivity, located on the wide plateau in Fig. 5, where a concentration of holes at least an order of magnitude greater than the concentration of electrons. In addition, the calculated lifetime of non-equilibrium electrons τ_n in the high-resistance region was ~ $1\cdot10^{-6}$ s and holes ~$5\cdot10^{-7}$ s. The electron mobility

$\mu_n\cdot$ was ~ 1000 $cm^2/(V\cdot s)$, i.e. $\mu_n\cdot\tau_n \sim 10^{-3}$ cm^2/V, which is quite acceptable for detector quality material.

It should be noted that operating conditions affect the electrophysical and detector properties of CdMgTe and other CdTe-based materials. During the long time of detector operation, it is exposed to radiation with gamma and X-ray quanta, which leads to the formation of radiation defects, primarily cadmium vacancies. As their concentration increases, they gradually change the degree of compensation of electrically active centers and deteriorate the detector properties, in particular, reduce the specific resistance and charge collection. To increase the operating time, the detector material, having semi-insulating properties and great charge collection efficiency within a wide range of the concentration of defects and impurities, should be obtained. One of the ways to increase the stability of detector quality can be doping with deep donors, the specific nature requires further experimental research.

CONCLUSIONS

Thus, it can be expected that a CdMgTe-based detector containing small additive of magnesium (≤ 0.1 at.%), or made of other detector materials based on CdTe, will be more stable during operation if a certain amount of deep donor is alloyed into its matrix. The energy level of the donor should be located above the middle of the bandgap by approximately 0.1…0.15 eV at operating room temperature of the detector. The optimal concentration of such a donor depends on the initial content of background impurities and defects in the matrix of the detector material.

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СКЛАД ДОМІШОК І ДЕФЕКТІВ У $Cd_{1-x}Mg_xTe$:In, НЕОБХІДНИЙ ДЛЯ ЗАБЕЗПЕЧЕННЯ СТАБІЛЬНИХ ДЕТЕКТОРНИХ ВЛАСТИВОСТЕЙ

О.І. Кондрик, Д.О. Солопіхін

Проведено модельне дослідження нового перспективного матеріалу $Cd_{0,92}Mg_{0,08}Te$:In, призначеного для детекторів рентгенівського та гамма-випромінювань, що працюють при кімнатній температурі. У статті висвітлено результати кількісних досліджень впливу вмісту домішок і структурних дефектів на електрофізичні та детекторні властивості $Cd_{0,92}Mg_{0,08}Te$:In. Проведено аналіз розрахункових значень питомого опору ρ і концентрації вільних носіїв заряду, часу життя нерівноважних електронів τ_n і дірок τ_p, ефективності збору заряду η при різному складі домішок і дефектів у цьому матеріалі за температури T = 298 K. Встановлено оптимальні діапазони енергії та концентрації легуючого глибокого донора, які забезпечують стабільний високоомний стан і допустимі значення η. Досліджено компенсацію вакансій кадмію домішкою індію. Було зроблено припущення щодо можливості збільшення часу експлуатації детектора, що має високоомні властивості та високу ефективність збирання заряду. Сформульовано напрямок подальших досліджень з метою з'ясування природи прийнятного легуючого глибокого донора, який забезпечує стабільні властивості детектора.