INFLUENCE OF TRANSPORT PROPERTIES ON ENERGY RESOLUTION OF PLANAR TlBr AND CdZnTe GAMMA-RAY DETECTORS: MONTE-CARLO INVESTIGATION

A.I. Skrypnyk, M.A. Khazhmuradov
National Science Center "Kharkov Institute of Physics and Technology", Kharkov, Ukraine
E-mail: belkas@kipt.kharkov.ua

The response of TlBr- and CdZnTe-detectors to gamma-rays from ^{57}Co and ^{137}Cs was simulated by Monte-Carlo method via Geant4 package. We studied the influence of transport parameters of electrons and holes on energy resolution of detectors. The modification of photopeaks with a changing the ratio of the electron and hole mobility-lifetime products was investigated. All results obtained for TlBr detectors were compared with the results for CdZnTe-detectors. The efficiency for detecting gamma-quanta in the range of energies from 10 keV to 3 MeV by both kinds of detector was researched.

PACS: 29.40.Wk, 85.30De, 07.85.-m

INTRODUCTION

For many years, investigation of wide band-gap semiconductors (CdZnTe, TlBr, HgI_2 and other) is directed to the development of gamma-ray detectors working at room temperatures without additional cooling. However, some features of these semiconductor materials create problems in determining a detector's main operating characteristics. Considerable non-uniformity of electrophysical characteristics of single-crystals is one of the most important factors restraining progress in achieving this goal. The most unstable characteristics include specific resistance of detector and product of mobility μ and mean drift time τ for electrons and holes – $(\mu\tau)_{e,h}$ (transport parameters of charge carriers). Planar gamma-ray detectors based on wide band-gap semiconductors have considerable spread of $(\mu\tau)_{e,h}$ values even if they are produced from one ingot [1]. At the same bias voltage, U_b, the characteristics of such detectors with the same sizes such as sensitivity to the registered radiation δ and charge collection efficiency (*CCE*) will be different. Experiments conducted by Suzuki et al. [1] showed that, for example, in CdZnTe single-crystals, the ratio of charge transport parameters for electrons and holes within the same ingot may vary profoundly from 10 to 100. Furthermore, modification of the ingot's $(\mu\tau)_{e,h}$ product can be due to technological processing of the material during manufacturing into a detector, or may result from the accumulation of defects during growth or operation [2].

For a study of features of room-temperature semiconductor devices which are manufactured for detecting nuclear radiation and measuring the characteristics of the radiation fields Monte-Carlo simulation can be used. A computer experiment helps to overcome the difficulties that are present as at the study of features of semiconductors as at the development of detectors based on them. In the present work, we studied the influence of the $(\mu\tau)_{e,h}$ products and $(\mu\tau)_e/(\mu\tau)_h$ ratio on the spectroscopic characteristics of CdZnTe- and TlBr-detectors using Geant4 simulation package. The detailed Monte-Carlo investigation allowed us to model the response function of planar spectrometers in the gamma-ray energy range to 3 MeV. The dynamics of response function of TlBr-detectors for gamma-ray energies of 122, 136 (^{57}Co source) and 661.7 keV (^{137}Cs source) was explored and compared with the dynamics of response function of CdZnTe-detectors for the same gamma-ray energies. We presented how change of $(\mu\tau)_e/(\mu\tau)_h$ ratio influences on the characteristics of all simulated photopeaks. Also, we investigated the dynamics of theoretical energy resolutions of TlBr- and CdZnTe-detectors.

1. DESCRIPTION OF THE MODEL

We simulated the passage of gamma-quanta through the detector by Monte-Carlo method via the user program code described detail in [3], embedded in Geant4 package – universal toolkit for the simulating the passage of charged particles, neutrons and gamma-quanta through matter. The simulation procedure is divided into 2 parts. Initially, the program calculates the value of the ionization energy, E_i, transferred to the detector by the absorbed gamma-quantum with the initial energy of E_γ. Then we calculate the value of charge induced on the detector's contacts for every interacted photon. The computer model of the detector is approximated as much as possible to a real spectrometric device. It takes into account the statistical effects of pair generation within the detector's volume and the modification in the amplitude of the output pulse under the influence of the electronic noise and charge-carrier capture [3].

To verify the described model we applied experimental data from 6×6×3 mm planar $Cd_{0.9}Zn_{0.1}Te$-detectors, equipped with ohmic contacts. The bias voltage, U_b, was 300 V. The electron mobility-lifetime product $(\mu\tau)_e$ was selected as $3\cdot10^{-3}$ cm^2/V. We specified the total level of noise in the CdZnTe spectrometry systems (Equivalent Noise Charge – *ENC*) at about 300 e^- (electron charge units). The detector's dark current was taken as 3 nA. CdZnTe-detector was irradiated by ^{137}Cs. Fig. 1 presents examples of calculated and experimental response functions of investigated CdZnTe-detectors from ^{137}Cs source. Overall, it is evident that used model is in good agreement with the experimental measurements.

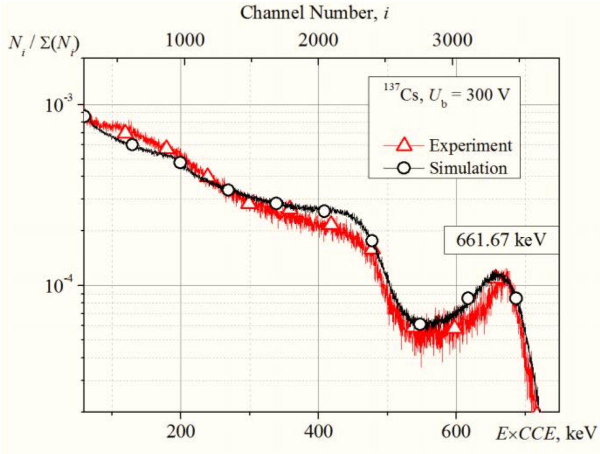

Fig. 1. 661.67 keV photopeak ^{137}Cs spectrum

2. ANALYSIS OF EFFICIENCY OF CHARGE COLLECTION

One of the main problems of wide band-gap semiconductor detectors results from considerable spread of ($\mu\tau$) values for electron and holes. Transport parameters for electrons and holes directly influence on charge collection efficiency. The change in the charge collection efficiency, by turn, leads to distortions to the pulse height spectrum.

Therefore, to interpret correctly the investigated spectra it is necessary to analyze *CCE* [3]. We will consider uniformity of distribution of electric field within detector. In this case, the efficiency of charge collection in the planar detector irradiated by gamma-quanta from the negative contact is described by Hecht model [4]:

$$\eta(z,\mu_e,\tau_e,\mu_h,\tau_h,d,U)=\frac{Q_{ind}}{Q_{gen}}=$$
$$=\frac{(\mu\tau)_e U_b}{d^2}\left(1-\exp\left(-\frac{(d-z)d}{(\mu\tau)_e U_b}\right)\right)+ \qquad (1)$$
$$+\frac{(\mu\tau)_h U_b}{d^2}\left(1-\exp\left(-\frac{zd}{(\mu\tau)_h U_b}\right)\right).$$

Here, η is the charge-collection efficiency; Q_{ind} is the charge induced on the detector contacts; Q_{gen} is the average charge created at absorption energy E_{i}, $Q_{\text{gen}} = E_{\text{i}}/\varepsilon$; d is the detector's thickness; and z is the depth of the gamma-quantum interaction within the detector's material ($0 < z < d$).

In the following, we suppose that the values of $(\mu\tau)_e$, U_b, and d are constant. We use the notations $\lambda_e=\frac{(\mu\tau)_e U_b}{d}$ corresponding to the electron's mean-free-path which is assumed constant in this analysis, and $\kappa=\frac{(\mu\tau)_h}{(\mu\tau)_e}$, $0<\kappa<\infty$. Then, equation (1) can be rewritten in the equivalent form [3]:

$$\eta(\kappa,z)=\frac{\lambda_e}{d}\left(1-\exp\left(-\frac{d-z}{\lambda_e}\right)\right)+$$
$$+\frac{\kappa\lambda_e}{d}\left(1-\exp\left(-\frac{z}{\kappa\lambda_e}\right)\right). \qquad (2)$$

The first derivative of equation (2) $\left.\frac{d\eta(\kappa,z)}{d\kappa}\right|_{z=\text{const}}$ is equal to

$$\left.\frac{d\eta(\kappa,z)}{d\kappa}\right|_{z=const}=\frac{\lambda_e}{d}-\left(\frac{\lambda_e}{d}+\frac{z}{\kappa d}\right)\exp\left(-\frac{z}{\kappa\lambda_e}\right). \qquad (3)$$

The first derivative (3) is positive in the whole range, $\frac{z}{\kappa\lambda_e}>0$, so that the efficiency of charge collection is a monotonically increasing function of the ratio κ and respectively, $(\mu\tau)_h$. It is correct for all z in the range from 0 to d.

3. INFLUENCE OF TRANSPORT PARAMETERS OF TlBr- AND CdZnTe- DETECTORS ON ITS SPECTROSCOPIC CHARACTERISTICS

In the present work, we simulated 2.7×2.7×2 mm planar TlBr-detectors equipped with ohmic contacts. Given thickness of the TlBr crystal was selected as typical for detectors based on this material [5]. TlBr-detector with such thickness gives higher efficiency for detecting gamma-quanta with 122 and 136 keV energies from ^{57}Co (≈ 97 and ≈ 93%, respectively) compared with lower thickness detector (Fig. 2).

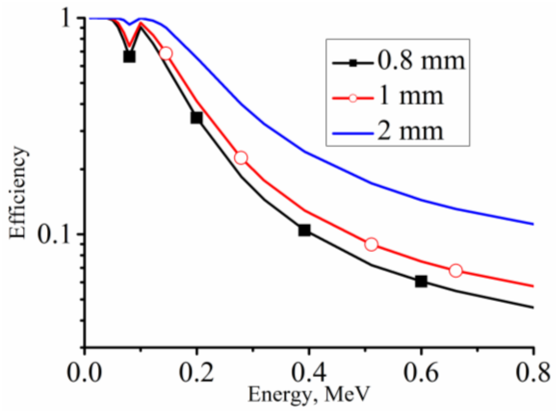

Fig. 2. Efficiency of gamma-ray TlBr-detectors with different thicknesses

In the range of energies of gamma-quanta less than 1 MeV, the gamma-ray detector efficiency of 2 mm TlBr-detector slightly exceeds this efficiency of 3 mm CdZnTe-detector (Fig. 3). At the same time, as evident from Fig. 3, efficiency of detection of 661.7 keV gamma-quanta from ^{137}Cs radioactive source does not exceed 15% for both materials with above mentioned thicknesses.

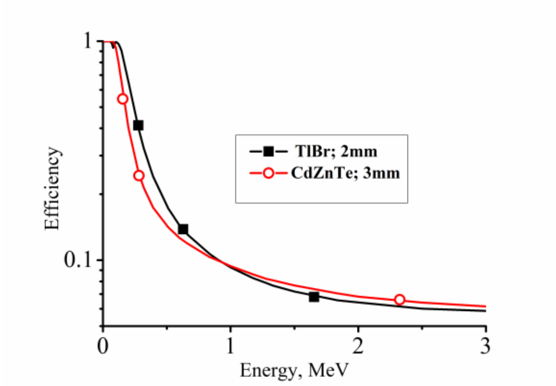

Fig. 3. Comparison of gamma-ray detector efficiency for TlBr- and CdZnTe-detectors

Fig. 4 shows the transformation of ^{57}Co spectrum obtained by simulation of TlBr-detector with decreasing κ value. The bias voltage, U_b, was 400 V. We specified the total level of noise in the TlBr spectrometry systems at about 400 e^-. It was assumed that the detector's dark current was 3 nA. We considered the material with values of the electron and hole mobility of 30 and 4 $cm^2/(V{\cdot}s)$, respectively, which reflect the measured μτ products for electrons and holes [5].

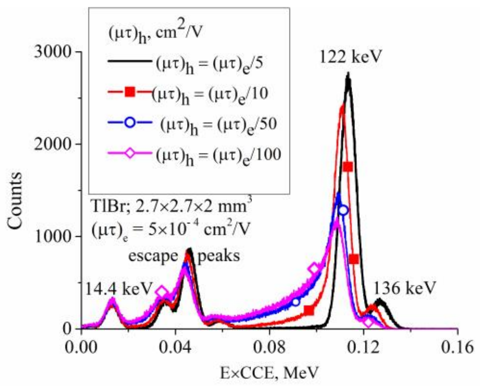

Fig. 4. Transformation of ^{57}Co spectrum obtained by TlBr-detector with decreasing κ value

The electron mobility-lifetime was fixed at $5{\cdot}10^{-4}$ cm^2/V. The mobility-lifetime values for holes were varied from $1{\cdot}10^{-4}$ [5] to $5{\cdot}10^{-6}$ cm^2/V. 10^7 gamma-quantum trajectories were simulated. From Fig. 4, we observe a little shift of the centroids of 122 and 136 keV photopeaks in the direction of lower energy with decreasing a value of κ i. e. with decreasing a value of $(\mu\tau)_h$ at const $(\mu\tau)_e$. Moreover, the theoretical energy resolution of the studied TlBr-detector for gamma-quantum energy at 122 keV declines from 5.7 to 7.6% with increasing 1/κ value from 5 to 100. 136 keV photopeak tends to full degeneration. 14.4 keV photopeak corresponded to third principal gamma-ray line of ^{57}Co almost does not change.

Spectrum of gamma-quanta from ^{57}Co source obtained by simulation of TlBr-detector was compared with such spectrum received by simulation of CdZnTe-detector [3].

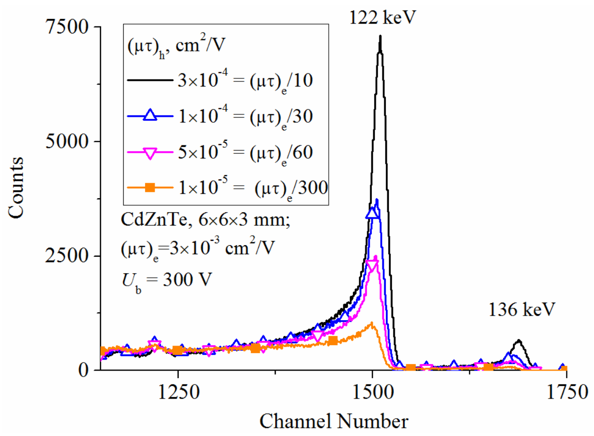

Fig. 5. Transformation of ^{57}Co spectrum obtained by CdZnTe-detector with decreasing κ value

From Figs. 4 and 5, it is evident that these spectra of gamma-quanta obtained by both detectors have similar tendency to decreasing and broadening of 122 and 136 keV photopeaks and similar shape in this range of energies with decreasing a value of hole mobility-lifetime product. The theoretical energy resolution of CdZnTe-detector for gamma-quantum energy at 122 keV drops from 1.8 to 2.3% when the value of 1/κ changes from 10 to 60. The spectrum obtained by CdZnTe also has almost constant 14.4 keV photopeak (it is not shown in Fig. 5). This reflects the fact that the depth of absorption of the main part of the gamma-quanta with 14.4 keV energy in both TlBr- and CdZnTe-materials is near to a hole-drift-length even at the worst $(\mu\tau)_h$ values. Qualitative changes in the simulated spectra of CdZnTe-detectors agree with the experimental data of Sato et al. [6].

However, irradiation of investigated TlBr-detector by gamma-quanta from ^{57}Co source gives high enough peaks in the spectrum in the range between about 30…50 keV in contrast with CdZnTe-detector. The centroids of these photopeaks also are shifted in the direction of lower energy with decreasing a value of κ. We suppose that they are escape peaks corresponding to gamma-radiation from *K*-shells of Tl. Also, our simulation results agree with results of real experiment for TlBr-detectors [5].

Basing on the data of the computer experiment, it can be concluded that for gamma-quantum energies less than 150 keV, planar CdZnTe-detectors of 3 mm thickness retain satisfactory spectrometric properties in the ratio range $(\mu\tau)_e/(\mu\tau)_h$ below 30. Energy resolution of the investigated TlBr-detectors of 2 mm thickness approximately in two times worse compared with CdZnTe-detectors in this range of gamma-quanta energies. It agrees with experimental data for TlBr-detectors which are obtained to the present time.

Fig. 6 presents the simulated spectrum of gamma-quanta from ^{137}Cs source obtained for investigated TlBr-detector.

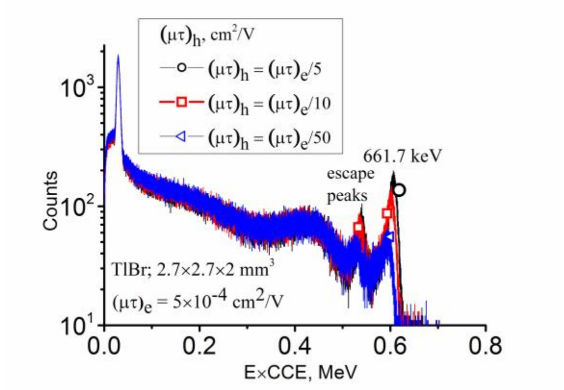

Fig. 6. Transformation of [137]Cs spectrum obtained by TlBr-detector with decreasing κ value

Because of low efficiency for detecting the gamma-quantum energy at 661.7 keV we needed to increase the number of simulated gamma-quantum trajectories of ^{137}Cs source compared with ^{57}Co to 10^8 to collect statistics. The theoretical energy resolution of the investigated TlBr-detector at a gamma-ray energy of 661.7 keV drops from 2.6 to 4.8%, when the value of $1/\kappa$ changes from 5 to 20.

From Fig. 6 we observe faster degeneration of 661.7 keV photopeak in TlBr-compared with 122 keV photopeak. These results agree with results of simulation of CdZnTe-detector irradiated by ^{137}Cs source. Fig. 7 shows the changes that occur around the 661.7 keV photopeak with the simulated spectrum of the ^{137}Cs source for a CdZnTe-detector [3]. The value of $1/\kappa = 20$ can be considered as the threshold level. The theoretical energy resolution of the investigated CdZnTe-detector at 661.7 keV declines from 1.1 to 1.5% in the range of $1/\kappa$ values from 10 to 20. The planar CdZnTe-detectors with higher value of $1/\kappa$ are unsuitable for the spectrometry of high-energy gamma-quanta, because even low accumulation of radiation traps can lead to the disappearance of the photopeak.

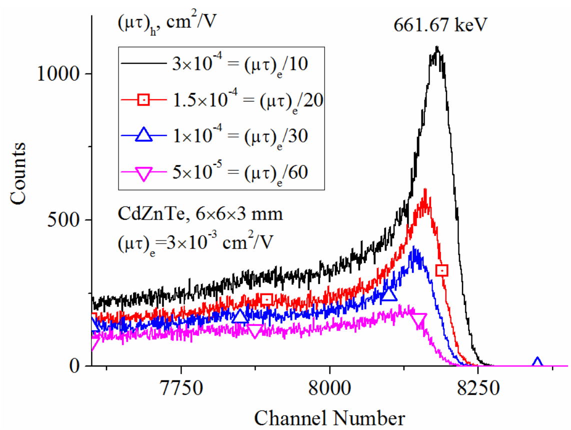

Fig. 7. Transformation of [137]Cs spectrum obtained by CdZnTe-detector with decreasing κ value

The faster degeneration of the 661.7 keV photopeak in CdZnTe- and TlBr-detectors compared with the 122 keV photopeak is connected with the fact that in the simulated detectors the interaction of 122 keV gamma-quanta within the detector material mainly occurs in the first one-third of its thickness. At the same time, gammas with energy of 661.7 keV uniformly interact with detector throughout its entire thickness. The efficiency of charge collection, Eq. (1), depends on interaction depth. Therefore, decreasing the hole-drift-length relative to the electron-free path more strongly reduces $\eta(\kappa, z)$ and the pulse amplitude at greater depths. The full absorption cross-section of CdZnTe and TlBr is small in the energy region E_γ above 100 keV. Therefore, this small total pulse-number from the full absorption of 661.7 keV gamma-quantum is spread therewith over a wider range of amplitudes.

It was determined that planar CdZnTe-detectors theoretically can ensure an energy resolution of better than 2% at 661.7 keV provided that the value of $1/\kappa$ is less than 20. In the range $1/\kappa$ from 20 to 60, the detector's resolution quickly deteriorates to 10…12% after the complete disappearance of the 661.7 keV photopeak.

From simulation of TlBr-detectors, we concluded that in the range $1/\kappa$ less than 10 we may receive energy resolution better than 3%. At a value of $1/\kappa$ more than 45 the 661.7 keV photopeak cannot be observed by TlBr-detector.

CONCLUSIONS

Basing on the mentioned model, response of semiconductor TlBr-detectors to gamma-quanta from ^{57}Co and ^{137}Cs sources was simulated and then was compared with response of CdZnTe-detectors to gamma-quanta from the same sources. The detection efficiency of both materials was investigated. We conclude that TlBr- and CdZnTe-detectors have the same detection efficiency in the range of energies to 60 keV. At gamma-ray energies of 122 and 136 keV (from ^{57}Co source) TlBr-detector has higher detection efficiency compared with CdZnTe-detector. For 661.7 keV energy for both investigated detectors the given value does not exceed 15%.

We determined that investigated detectors have similar tendency to broadening of 122, 136 and 661.7 keV photopeaks and deterioration of energy resolution with decreasing a value of $(\mu\tau)_h$ at a constant value of $(\mu\tau)_e$. It is concluded that the spectroscopic properties of the both kinds of detector are maintained when the range of the $(\mu\tau)_e/(\mu\tau)_h$ ratio is below 20. For CdZnTe if the $(\mu\tau)_e/(\mu\tau)_h$ ratio is above 60, then the 661.7 keV photopeak cannot be observed for planar detectors, even with very low levels of electronic noise. In the case of TlBr-detectors, complete degeneration of 661.7 keV photopeak is observed at a little less $(\mu\tau)_e/(\mu\tau)_h$ ratio. These criteria establish quality-growth requirements for spectrometric TlBr- and CdZnTe-materials.

ACKNOWLEDGEMENTS

We are very grateful to A.V. Rybka and V.E. Kutny for providing the experimental data for CdZnTe-detector and their help in the analysis of obtained results.

REFERENCES

1. M. Suzuki, M. Tashiro, G Sato, S. Watanabe, K. Nakazawa, T. Takahashi, Y. Okada, H. Takahashi, A. Parsons, S. Barthelmy, J. Cummings, N. Gehrels, D. Hullinger, H. Krimm, J. Tueller. Hard X-ray

response of CdZnTe-detectors in the swift burst alert telescope // *IEEE Trans. Nucl. Sci.* 2005, v. 52, p. 1033-1035.

2. A. Cavallini, B. Fraboni, W. Dusi, N. Auricchio, P. Chirco, M. Zanarini, P. Siffert, P. Fougeres. Radiation effects on II–VI compound-based detectors // *Nucl. Instr. and Meth. A.* 2002, v. 476, p. 770-778.

3. A. Zakharchenko, A. Rybka, V. Kutny, A. Skrypnyk, M. Khazhmuradov, P. Fochuk, A. Bolotnikov, R. James. Transport properties and spectrometric performances of CdZnTe gamma-ray detectors // *Proc. of SPIE.* 2012, v. 8507, p. 85071I-1-7.

4. W. Akutagawa, K. Zanio. Gamma response of semi-insulating material in the presence of trapping and detrapping // *J. Appl. Phys*. 1969, v. 40, p. 3838-3854.

5. M. Shorohov, M. Kouznetsov, I. Lisitskiy, V. Ivanov, V. Gostilo, and A. Owens. Member, IEEE. Recent results in TlBr-detector crystals performance // *IEEE Transactions on Nuclear Science.* 2009, v. 56, N 4, p. 1855-1858.

6. G. Sato, A. Parsons, D. Hullinger, M. Suzuki, T. Takahashi, et al. Development of a spectral model based on charge transport for the Swift/BAT 32 K CdZnTe-detector array // *Nucl. Instr. and Meth. A.* 2005, v. 541, p. 372-384.

Статья поступила в редакцию 28.05.2014 г.

ВЛИЯНИЕ ТРАНСПОРТНЫХ СВОЙСТВ НА ЭНЕРГЕТИЧЕСКОЕ РАЗРЕШЕНИЕ ПЛАНАРНЫХ TlBr- И CdZnTe-ДЕТЕКТОРОВ ГАММА-ИЗЛУЧЕНИЯ: ИССЛЕДОВАНИЕ МЕТОДОМ МОНТЕ-КАРЛО

А.И. Скрыпник, М.А. Хажмурадов

С помощью пакета Geant4 методом Монте-Карло промоделирован отклик TlBr- и CdZnTe-детекторов на гамма-излучение от ^{57}Co и ^{137}Cs. Изучено влияние транспортных свойств электронов и дырок на энергетическое разрешение детекторов. Исследована модификация фотопиков с изменением отношения произведений подвижности на время жизни для электронов и дырок. Все результаты, полученные для TlBr-детекторов, были сравнены с результатами для CdZnTe-детекторов. Исследована эффективность обеих систем детектирования гамма-квантов в диапазоне энергий от 10 кэВ до 3 МэВ.

ВПЛИВ ТРАНСПОРТНИХ ВЛАСТИВОСТЕЙ НА ЕНЕРГЕТИЧНУ РОЗДІЛЬНІСТЬ ПЛАНАРНИХ TlBr- ТА CdZnTe-ДЕТЕКТОРІВ ГАММА-ВИПРОМІНЮВАННЯ: ДОСЛІДЖЕННЯ МЕТОДОМ МОНТЕ-КАРЛО

А.І. Скрипник, М.А. Хажмурадов

За допомогою пакета Geant4 методом Монте-Карло було промодельовано відгук TlBr- і CdZnTe-детекторів на гамма-випромінювання від ^{57}Co і ^{137}Cs. Вивчено вплив транспортних параметрів електронів і дірок на енергетичну роздільність детекторів. Досліджено модифікацію фотопіків зі зміною відношення добутків рухливості на час життя для електронів і дірок. Всі результати, які було отримано для TlBr-детекторів, було порівняно з результатами для CdZnTe-детекторів. Досліджено ефективність обох систем детектування гамма-квантів у діапазоні енергій від 10 кеВ до 3 МеВ.