



**BNL-98465-2012-CP**

***Transport properties and spectrometric performances  
of CdZnTe gamma-ray detectors***

**Aleksey E. Bolotnikov**

*Presented at the 2012-SPIE Optics and Photonics Conference  
San Diego, CA  
August 12-16, 2012*

August 2012

**Nonproliferation and National Security Department**

**Brookhaven National Laboratory**

P.O. Box 5000  
Upton, N.Y. 11973-5000  
[www.bnl.gov](http://www.bnl.gov)

Notice: This manuscript has been authored by employees of Brookhaven Science Associates, LLC under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy. The publisher by accepting the manuscript for publication acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

This preprint is intended for publication in a journal or proceedings. Since changes may be made before publication, it may not be cited or reproduced without the author's permission.

## **DISCLAIMER**

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

# Transport properties and spectrometric performances of CdZnTe gamma-ray detectors

Alexandr A. Zakharchenko\*<sup>a</sup>, Alexandr V. Rybka<sup>a</sup>, Vladimir E. Kutny<sup>a</sup>, Anna I. Skrypnyk<sup>a</sup>,  
Manap A. Khazhmuradov<sup>a</sup>, Petro M. Fochuk<sup>b</sup>, Aleksey E. Bolotnikov<sup>c</sup>, Ralph B. James<sup>c</sup>

<sup>a</sup>National Science Ctr. “Kharkov Institute of Physics and Technology”, 1, Akademicheskaya St.,  
Kharkov, 61108, Ukraine; <sup>b</sup>Chernivtsi National University, 2, Kotsubinsky Str., 58012, Chernivtsi,  
Ukraine; <sup>c</sup>Brookhaven National Laboratory, Upton, NY 11973-5000

## ABSTRACT

We investigated the influence of the ratio of the electron and hole mobility-lifetime products,  $(\mu\tau)_{e,h}$  and  $(\mu\tau)_e/(\mu\tau)_h$ , on the resolution of CdZnTe planar radiation detectors via Monte-Carlo simulations. Preliminary results show that this ratio exercises a larger effect than that of any other parameter on the detector's peak-to-valley ratio and resolution. We determined the range of values of the ratio  $(\mu\tau)_e/(\mu\tau)_h$  where the fast degeneration of the photopeak in CdZnTe detectors takes place at a gamma-ray energy 661.7 keV (<sup>137</sup>Cs). We offer an explanation, based on the results of some of our experimental data, on the spectrometric performance of CdZnTe detectors.

**Keywords:** CdZnTe, semiconductor gamma-radiation detector, mobility-lifetime product, Monte-Carlo simulation, EGSnrc, photopeak degeneration

## 1. INTRODUCTION

The transport properties of electrons (e) and holes (h) determine the spectroscopic characteristics of CdZnTe planar gamma-radiation detectors. In applications of CdZnTe radiation detectors, the main focus of attention usually is given to the direct influence of their transport properties on the efficiency of charge collection, *CCE*. Such investigations can be relatively easy when carried out with planar detectors for which the Hecht equation can describe the relationship between the *CCE* and the mean free paths of charge carriers  $\lambda_{e,h}$ .<sup>[1]</sup>

Experiments showed<sup>[2]</sup> that in CdZnTe single-crystals, the ratio of charge transport parameters for electrons and holes within the same ingot may vary profoundly:  $(\mu\tau)_e/(\mu\tau)_h = 10 \dots 100$  ( $\mu$  – mobility and  $\tau$  – average life time of the charge carrier). 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<sup>[3]</sup>. The loss in spectroscopic properties over time is a characteristic feature of the processes of the creation of defects in the planar CdZnTe gamma-radiation detectors. At some level of the accumulated absorbed dose, the gradual decreases of the peak-to-valley ratio and the associated energy resolution cause the disappearance of the photopeak<sup>[3]</sup>. The centroid of the photopeak almost invariably remains up to the moment of its rapid degeneration, demonstrating that the  $(\mu\tau)_e$  value is almost constant. Evidently, the fluid broadening in the photopeak generally takes place due to a decreasing  $(\mu\tau)_h$  value.

In the present work, we investigated the influence of the  $(\mu\tau)_{e,h}$  products and  $(\mu\tau)_e/(\mu\tau)_h$  ratio on the spectroscopic characteristics of CdZnTe planar radiation detectors via simulation modeling. The results of our preliminary simulations show that the largest effect on the peak-to-valley ratio and resolution is exercised by the  $(\mu\tau)_e/(\mu\tau)_h$  ratio. We explored the dynamics of the CdZnTe detector's response function for gamma-ray energies of 122 keV (<sup>57</sup>Co source) and 661.7 keV (<sup>137</sup>Cs source). The value ranges of the  $(\mu\tau)_e/(\mu\tau)_h$  ratio are determined, wherein the faster degeneration of the photopeak in CdZnTe detectors takes place at a gamma-ray energy of 661.7 keV.

\*az@kipt.kharkov.ua; phone 38 095 367-4613; fax 38 057 335-1738; kipt.kharkov.ua

## 2. SIMULATION OF CdZnTe DETECTOR RESPONSE FUNCTIONS

We simulated  $6 \times 6 \times 3 \text{ mm}^3$  planar  $\text{Cd}_{0.9}\text{Zn}_{0.1}\text{Te}$  detectors, equipped with ohmic contacts. The bias voltage,  $U_b$ , was 300 V. The electron mobility-lifetime product  $(\mu\tau)_e$  was fixed at  $3 \times 10^{-3} \text{ cm}^2/\text{V}$  to assure the occurrence of a full absorption peak at the simulation of the registration of the high energy gamma-quanta. The hole mobility-lifetime product  $(\mu\tau)_h$  was varied in the range between  $(\mu\tau)_e/7$  and  $(\mu\tau)_e/100$ . 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.

We simulated the passage of gamma-quanta through the detector using the Monte-Carlo EGSnrc package for calculating photon- and electron-transport<sup>[4]</sup>. The user program code, embedded in this package, mimics the detector's response for every gamma-quantum, taking 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. At the first stage of simulation, the program calculates the value of ionization energy,  $E_i$ , absorbed in the detector for an initial energy of gamma-quantum  $E_\gamma$ .

At the second stage, we calculate the value of charge induced on the detector's contacts for every interacted photon. Also, we take into consideration the efficiency of charge collection, the contribution of noise to the induced signal, along with variations in charge-carrier capture by traps. The absorbed energy  $E_i$  is converted into the charge value using the mean energy of generation of an electron-hole pair,  $\varepsilon$ . Our assessments of the charge-collection efficiency, CCE, in the planar detectors are made using the basic Hecht model<sup>[1]</sup>. Controlling the model's parameters also are important in measuring channel characteristics: pulse shaping time, equivalent noise charge and the width of the analog-digital converter (ADC) channel. This supports our having an amplitude distribution of the pulses that most closely corresponds to the measured spectrum in the specific experiment.

Generally, three factors influence the amplitude of the induced charge: 1) Fluctuations in the generation of electron-hole pairs (Fano noise); 2) variations in the numbers of collected electrons and holes; and 3) electronic noise. The last factor depends on detector's dark currents  $I_d$ , bias currents, and the thermal noises of the circuit of the input-signal's amplifier. The variations in amplitude of these pulses is described satisfactorily by a Gaussian distribution<sup>[5]</sup> with  $E_i/\varepsilon$  mean and  $\sigma^2$  variance

$$\sigma^2 = F \frac{E_i}{\varepsilon} + \sigma_d^2 + \sigma_{el}^2 + G(E_i) \left( \frac{E_i}{\varepsilon} \right)^2. \quad (1)$$

Here,  $F$  is the Fano factor characterizing the statistical fluctuations of ionization, and the distinction between real statistics and Poisson statistics;  $\varepsilon$  is the mean energy required for generating electron-hole pairs;  $\sigma_d^2 \sim I_d \cdot \tau$  is the variance of the shot noise, depending on the detector's leakage current,  $I_d$ , and the pulse-shaping time  $\tau$ ;  $\sigma_{el}^2 \sim \frac{T}{\tau}$  the variance of thermal electronic noise depending on the temperature,  $T$ , and pulse shaping time  $\tau$ , and  $G(E_i)$  is the capture factor<sup>[6,7]</sup>.

The variance  $\sigma_{el}^2$  is obtained experimentally by measuring the signal broadening from a precision pulse generator. The variance  $\sigma_d^2$  can be calculated from measurements of the dark current-voltage.

The trapping of charge carriers drifting under the influence of the electric field is related to the different number of capture centers occurring along their paths, and the probabilistic nature of the capture process. Material non-uniformities influence the distribution of the internal field within semiconductor detectors and the volume profile of charge-carriers' lifetimes. Thus, fluctuations in charge collection are inevitable, even for the idealized case when the non-equilibrium depth of charge generation is fixed in the detector. The variance of the fluctuations in charge collection,

$\sigma_i^2 = G(E_i) \left( \frac{E_i}{\varepsilon} \right)^2$ , is proportionate to number of electron-hole pairs created and the ratio of carrier collection time,  $t_d$ , to life time,  $\tau_{e,h}$ <sup>[7]</sup>. The proportionality coefficient is a capture factor. In this work, we fixed the capture factor of the CdZnTe detector at  $1 \times 10^{-5}$ .

Figures 1 to 3 show the experimental- and calculated-response functions (probability of registration of the pulse whose amplitude corresponds to the specified energy  $E$ ) of the CdZnTe detectors measured with  $^{241}\text{Am}$ -,  $^{137}\text{Cs}$ -, and  $^{152}\text{Eu}$ -

sources. These data demonstrate that the described model is in good agreement with the experimental measurements. The qualitative trend of the calculated spectra corresponds to their spectral peculiarities. The location of the photopeaks, their amplitude and full-width-at-half maximum also correspond closely to the experimental data.

The observed differences in photopeak region may be influenced by a random factor. We can suppose that the main reason for the evident differences between theoretical- and experimental-spectra for  $^{137}\text{Cs}$  (Figure 2) and  $^{152}\text{Eu}$  (Figure 3) lies in the simplified description of the geometry and the chemical composition of scattered elements from the measuring bench. On simulation, it leads to some underestimation of the contribution in the output signal from high energy gamma-quanta scattered at angles more than  $135^\circ$  outside the sensitive volume of the detector.

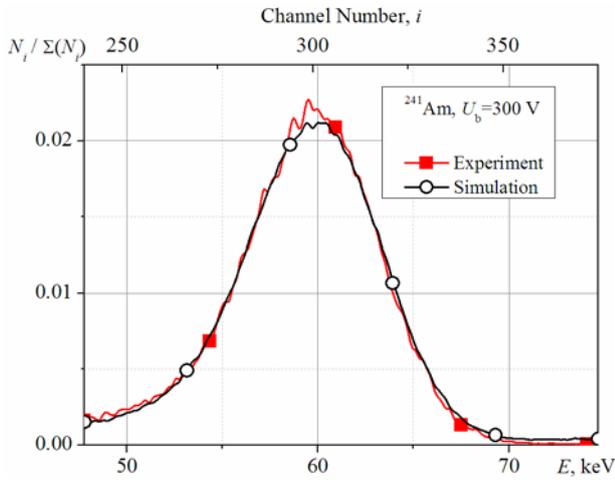


Figure 1. 60-keV  $^{241}\text{Am}$  spectrum

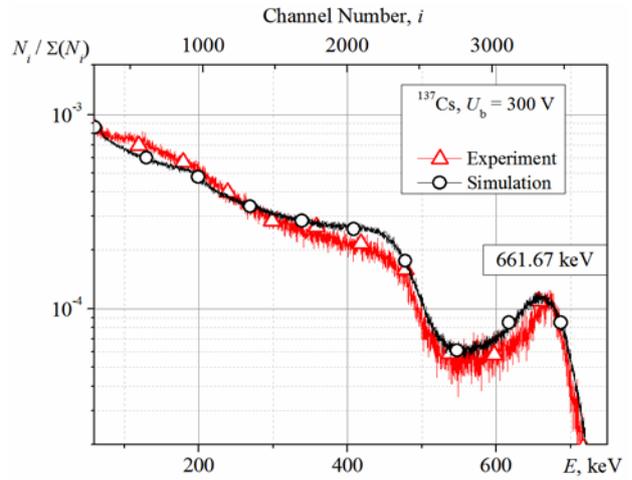


Figure 2. 661.67-keV  $^{137}\text{Cs}$  spectrum

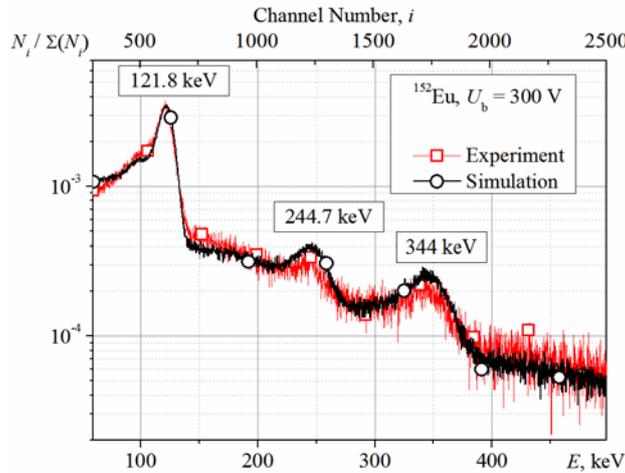


Figure 3.  $^{152}\text{Eu}$  spectrum

Ref. [8] contains examples of other applications of the described model.

### 3. HECHT EQUATION ANALYSIS

Next we consider the dependency of the efficiency of charge collection from the transport parameters of electrons and holes in the planar detector irradiated by gamma-quanta from the negative contact <sup>[1]</sup>

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

Here,  $\eta$  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  $E_i$ ,  $Q_{gen} = E_i/\varepsilon$ ;  $d$  is the detector's thickness; and  $z$  is the depth of 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 research, and  $\kappa = \frac{(\mu\tau)_h}{(\mu\tau)_e}$ ,  $0 < \kappa < \infty$ .

Then, equation (2) can be rewritten in the equivalent form

$$\eta(\kappa, z) = \frac{\lambda_e}{d} \left( 1 - \exp\left(-\frac{d-z}{\lambda_e}\right) \right) + \frac{\kappa\lambda_e}{d} \left( 1 - \exp\left(-\frac{z}{\kappa\lambda_e}\right) \right). \quad (3)$$

The first derivative of the equation (3)  $\left. \frac{d\eta(\kappa, z)}{d\kappa} \right|_{z=const}$  is equal to

$$\left. \frac{d\eta(\kappa, z)}{d\kappa} \right|_{z=const} = \frac{\lambda_e}{d} - \left( \frac{\lambda_e}{d} + \frac{z}{\kappa d} \right) \exp\left(-\frac{z}{\kappa\lambda_e}\right). \quad (4)$$

The first derivative (4) 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  $\kappa$  and respectively,  $(\mu\tau)_h$ . It is correct for all  $z$  in the range from 0 to  $d$ .

#### 4. ANALYSIS OF THE CHANGE OF SPECTROSCOPIC CHARACTERISTICS OF CdZnTe DETECTORS

Figure 4 demonstrates the change in the  $^{57}\text{Co}$  spectrum registered by CdZnTe detector with decreasing  $\kappa$  value. The centroid of the 122-keV photopeak is shifted marginally in the direction of lower energy. Therein the height of the 122-keV photopeak and the peak-to-valley ratio is decreased more than threefold. Degeneration of the 136-keV photopeak is observed. The theoretical energy-resolution of the investigated CdZnTe detector for gamma-quantum energy at 122 keV drops from 1.8% to 2.3%, when the value of  $1/\kappa$  changes from 10 to 60. From Figure 4, it is evident that with increasing  $1/\kappa$ , the gradual decreasing peak-to-valley ratio of CdZnTe detector takes place, corresponding with the data in Ref. [3]. If  $1/\kappa$  is above 150, the 122-keV photopeak is broad.

The results of simulation agree with the data from Ref. [9] (Sato et al.). Figure 8 from Ref. [9] confirms that the peak-to-valley ratio for the 122-keV photopeak is higher for detectors with a lower  $1/\kappa$  value, even if their electron-transport characteristics  $(\mu\tau)_e$  are worse. Similarly, for the same  $(\mu\tau)_e$  value, detectors with a higher  $\kappa$  value demonstrate better resolution and peak-to-valley ratio.

The simulation also confirms the experimental findings (Figure 8, Ref. [9]) deducing that the parameters of the 14.4-keV photopeak of the  $^{57}\text{Co}$  radioactive source remain constant with a changing  $\kappa$  value. This reflects the fact that the depth of absorption of the main part of gamma-quanta with 14.4-keV energy in CdZnTe (reduction intensity in  $e$  times) is near to a hole-drift-length even at the worst  $(\mu\tau)_h$  values, viz., that is  $z \cong \lambda_h$ . In this case, the second member of the equation (3) can be neglected, and the efficiency of the charge collection of a CdZnTe detector for 14.4-keV gamma-quanta appears practically constant ( $\eta(\kappa, z) \approx const$ ).

Overall, we conclude that for gamma-quantum energies less than 150 keV, planar CdZnTe detectors of 2–3 mm

thickness retain satisfactory spectrometric properties in the ratio range  $(\mu\tau)_e/(\mu\tau)_h$  below 30.

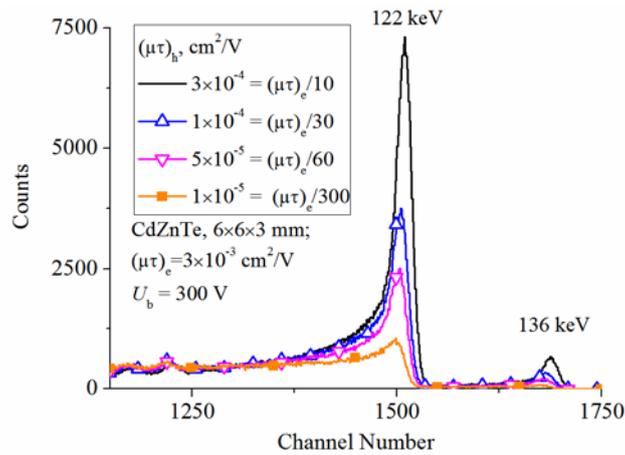


Figure 4. <sup>57</sup>Co spectrum transformation with decreasing  $\kappa$  value

Figure 5 shows the changes that occur around the 661.7-keV photopeak with the spectrum of a <sup>137</sup>Cs source registered by a CdZnTe detector. The degeneration of the 661.7-keV photopeak occurs faster than that of the 122-keV photopeak. 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 the accumulation of radiation traps can lead to the disappearance of the photopeak.

The faster degeneration of the 661.7-keV photopeak in CdZnTe detectors compared with the 122-keV photopeak is connected with the fact that in the simulated detector the interaction of 122-keV gamma-quanta within the detector material mainly occurs in the first one-third of its thickness (Figure 6). Gammas with energy of 661.7 keV uniformly interact with detector through its entire thickness. The efficiency of charge collection (equation 3) 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 is small in the energy region  $E_\gamma$  above 100 keV. Therefore, this restricted total pulse-number from the full absorption of 661.7-keV gamma-quantum is spread over a wider range of amplitudes.

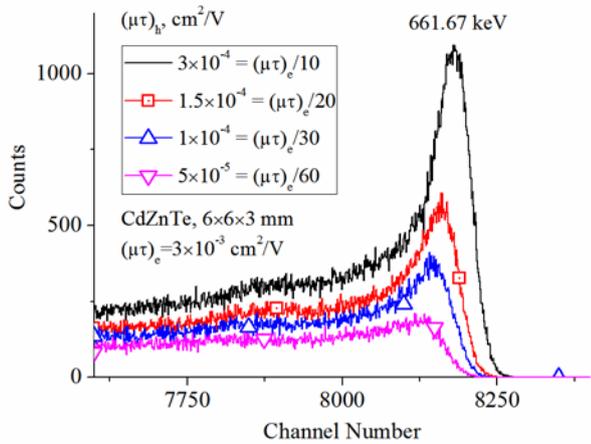


Figure 5. <sup>137</sup>Cs spectrum transformation with decreasing  $\kappa$  value

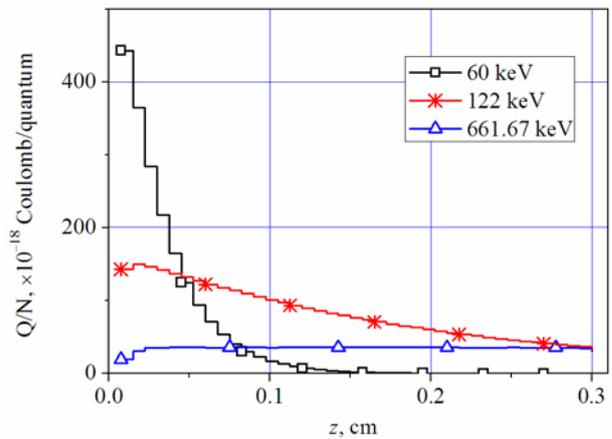


Figure 6. Normalized distribution of created charge with thickness in  $6 \times 6 \times 3$  mm<sup>3</sup> CdZnTe detectors for different energies of gamma-quanta

As our preliminary calculations show (Figure 7), a planar CdZnTe detector theoretically can ensure an energy resolution of less 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.

More precise data can be obtained by modifying the model of the CdZnTe detector, so to account for a changing capture factor  $G(E_i)$  at decreasing  $(\mu\tau)_h$ , because the increase of the number of hole traps is the main factor driving the degradation of the hole-transport property.

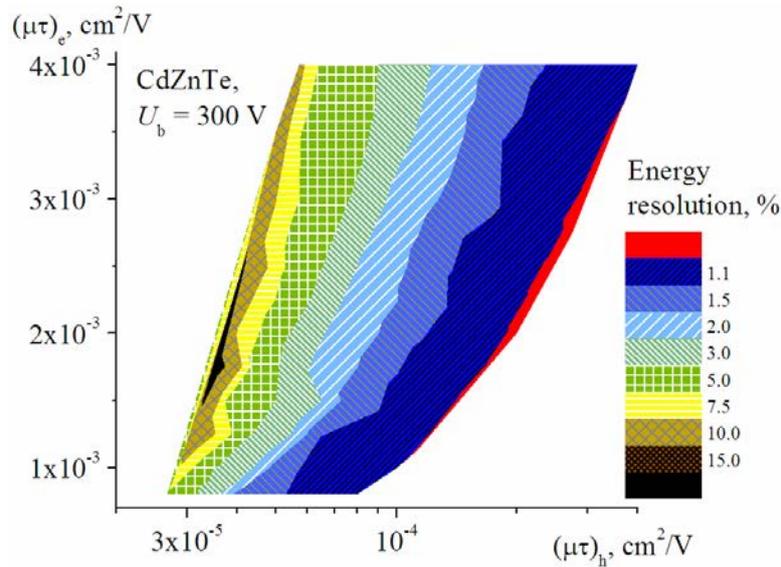


Figure 7. Energy resolution of CdZnTe detector versus ratio  $(\mu\tau)_e/(\mu\tau)_h$

## 5. CONCLUSION

The spectroscopic properties of the CdZnTe detectors are maintained when the range of the  $(\mu\tau)_e/(\mu\tau)_h$  ratio is below 20. 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. These criteria establish quality-growth requirements for spectrometric CdZnTe material. Finding a relationship between the mobility-lifetime product for the holes and the capture factor, and modifying the model of the CdZnTe detector would allow us to explain experimental data on the degradation of the detector's spectrometric performance when exposed to large doses of different kinds of ionizing radiation.

## REFERENCES

- [1] Akutagawa W., Zanio K., "Gamma response of semi-insulating material in the presence of trapping and detrapping," J. Appl. Phys. 40, 3838–3854 (1969).
- [2] Suzuki M., Tashiro M., Sato G., Watanabe S., Nakazawa K., Takahashi T., Okada Y., Takahashi H., Parsons A., Barthelmy S., Cummings J., Gehrels N., Hullinger D., Krimm H., Tueller J., "Hard X-Ray Response of CdZnTe Detectors in the Swift Burst Alert Telescope," IEEE Trans. Nucl. Sci. 52, 1033–1035 (2005).
- [3] Cavallini A., Fraboni B., Dusi W., Auricchio N., Chirco P., Zanarini M., Siffert P., Fougères P., "Radiation effects on II–VI compound-based detectors," Nucl. Instr. and Meth. A 476, 770–778 (2002).
- [4] Kawrakow I., Mainegra-Hing E., Rogers D., "EGSnrcMP, the new multi platform version of EGSnrc," Med. Phys. 31, 1731 (2004).
- [5] Devanathan R., Corrales L.R., Gao F., Weber W.J., "Signal variance in gamma-ray detectors - A review," Nucl. Instr. and Meth. A 565, 637–649 (2006).

- [6] Kozorezov A., Wigmore J., Owens A., den Hartog R., Peacock A., Hala A Al-Jawhari, "Resolution degradation of semiconductor detectors due to carrier trapping," *Nucl. Instr. and Meth. A* 546, 209–212 (2005).
- [7] Bolotnikov A., Camarda G., Wright G., James R. B., "Factors limiting the performance of CdZnTe detectors," *IEEE Trans. Nucl. Sci.* 52, 589–598 (2005).
- [8] Skrypnyk A., Zakharchenko A., Khazhmuradov M., "Comparison of GEANT4 with EGSnrc for simulation of gamma-radiation detectors based on semi-insulating materials," *Problems of atomic science and technology, Series: Nuclear Physics Investigations* 5 (56), 93–100 (2011).
- [9] Sato G., Parsons A., Hullinger D. Suzuki M., Takahashi T., Tashiro M., Nakazawa K., Okada Y., Takahashi H., Watanabe S., Barthelmy S., Cummings J., Gehrels N., Krimm H., Markwardt C., Tueller J., Fenimore Ed, Palmer D., "Development of a spectral model based on charge transport for the Swift/BAT 32K CdZnTe detector array," *Nucl. Instr. and Meth. A* 541, 372-384 (2005).