RECONSTRUCTION OF ENERGY DEPENDENCE OF THE SENSITIVITY OF CdZnTe- AND TlBr-DETECTORS THROUGH THE RESTRICTED DATA

A. I. Skrypnyk*

National Science Center "Kharkov Institute of Physics and Technology", 61108, Kharkov, Ukraine

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Monte-Carlo method is used for investigating the energy dependence of sensitivity of CdZnTe- and TlBr-detectors of gamma-radiation, which operate in the mode of pulse-amplitude analysis. We researched the approximate formulae that describe this dependence in the range of gamma-quantum energies from 30 keV to 3 MeV. It is proposed a method for determining the fitting parameters for approximate formulae through gamma-radiation spectra measured experimentally by several reference sources of gamma-radiation. In particular, it can be ^{241}Am, ^{137}Cs and ^{60}Co gamma-radiation sources. It is also discussed the measurements with additional radiation sources that can be used for improving an accuracy of reconstruction of energy dependence of detectors' sensitivity.

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1. INTRODUCTION

The study of wide-band gap semiconductor radiation detectors is of great interest for far more than one year. Cd(Zn)Te-, TlBr-, HgI_2-materials are ones of the most suitable candidates for creating commercially available radiation detection systems with quite good spectroscopic properties in the cases of operating at room temperatures [1, 2]. However, some features of these semiconductor materials create problems in determining a detector's main operating characteristics such as the dependence of their sensitivity, δ, on the energy of the detected gamma-rays. The variety of electrophysical characteristics of wide-band gap semiconductor detectors results in the significant variations in the sensitivity of identical detectors working under the same bias condition. It causes a necessity of detailed measurements of energy dependence of the sensitivity for every detector.

Considerable assistance in answering these problems may spring from first principles' simulations of material and detector operation. It could be of help in developing semi-experimental methods for estimating and measuring detector parameters, such as the energy dependence of the detectors' sensitivity. Simulation will be especially useful for multi-detector systems wherein the sensitivity of all components must be known and taken into account for optimal system performance.

In the present work, simulation of response of CdZnTe- and TlBr-detectors was researched. Analysis of energy dependence of detectors' sensitivity was made. It was considered the simple approximation formulae for determining the dependence of the sensitivity for CdZnTe- and TlBr-detectors on the energy for gamma-rays in the energy range from 30 keV to 3 MeV. Fitting parameters for these formulae can be determined with a satisfactory accuracy basing on the measurements of gamma-quantum spectra from several reference sources. Analysis of results from simulation of response functions and energy dependence of sensitivity for CdZnTe-detectors allowed to propose a method for calculating the fitting parameters of approximate formulae based on the experimentally measured gamma-ray spectra from ^{241}Am, ^{137}Cs and ^{60}Co reference sources. This method was used for reconstructing the energy dependence of sensitivity of CdZnTe-detector. Numerical experiment allowed us to confirm a validity of the obtained approximate formulae for TlBr-detectors. Overall, it was concluded that the sensitivity of CdZnTe- and TlBr-detectors can be adequately reconstructed using approximation formulae which, therefore, appreciably simplify the procedures of their calibration.

2. MODEL VERIFICATION

To investigate characteristics of TlBr- and CdZnTe-detectors Geant4 v.4.9.6 package – universal toolkit for the simulating the passage of charged particles, neutrons and gamma-quanta through matter [3] was used. We simulated the passage of gamma-quanta through the detectors by Monte-Carlo method via the user program code described detail in [4], embedded in Geant4-package.

The user program code mimics the detector's response for every gamma-quantum. Firstly, program calculates the value of the ionization energy, E_i,

*Corresponding author E-mail address: belkas@kipt.kharkov.ua

transferred to the detector by the absorbed gamma-quantum with the initial energy of Eγ, and, secondly, it computers the value of charge induced on the detector's contacts for every interacted photon.

To obtain from Monte-Carlo simulation the detector's response function that will be in a good agreement with the experimental response function of real detector the user program code takes into account the great number of factors which influence on the amplitude of the induced charge including fluctuations in the generation of electron-hole pairs, variations in the numbers of collected electrons and holes and electronic noise [4].

Previously, for calculating the response functions of CdTe- and Cd(Zn)Te-detectors with this model, the EGSnrc Monte-Carlo code was used. In [5, 6] we compared results of Monte-Carlo simulation obtained by EGSnrc- and Geant4-packages. We obtained a good agreement between calculated- and experimental-data for gamma-ray lines that can be considered almost monochromatic.

3. DETERMINATION OF ENERGY DEPENDENCE OF TlBr- AND CdZnTe-DETECTORS' SENSITIVITY

One of the critical characteristics that determines the operating the semiconductor gamma-radiation detectors at room temperatures is their sensitivity, δ, that is defined as the ratio of the number of pulses, N, produced by the detector to the value of exposure (X) or absorbed (D) radiation dose: $\delta_X = N/X$ or $\delta_D = N/D$. A sharp dependency of sensitivity from the gamma-radiation energy, $\delta_{X,D}(E_\gamma)$, is a characteristic feature of all wide band-gap semiconductors used for detecting gamma-quanta.

The measurement of sensitivity of detectors is a laborious problem. To determine this value for semiconductor detectors in the range of gamma-quantum energies from 30 keV to 3 MeV it is necessary about 10 reference gamma-radiation sources. In some cases, it is not possible to conduct experiment with such number of reference sources. Monte-Carlo simulation of semiconductor detectors can be used as solution of this problem. However, for obtaining correct values of sensitivity via Monte-Carlo simulation it needs to have accurate characteristics of detectors some of which, for example, electrophysical parameters, are not always known.

Analytic formulae exist for only the simplest geometries of measurement setup in which the influence of the Compton scattering of gamma-rays is negligible. In such cases, the user can easily calculate the radiation dose created by the gamma-quantum flow. The principal reason is that the Compton scattering changes the energy spectrum of gamma-rays in a manner that is highly dependent on the detector dimensions. It does not allow to obtain analytical expressions for calculating the energy dependence of sensitivity of semiconductor detectors in the wide range of energies of gamma-quanta.

In the present work, we used Monte-Carlo method for simulating the response functions of two types of planar semiconductor detectors of gamma-radiation: CdZnTe and TlBr. Firstly, we considered 6 × 6 × 3 mm^3 CdZnTe-detector. Fig. 1 plots $\delta_X(E_\gamma)$, the energy dependency of sensitivity of such detector, calculated by the Geant4 code at a zero-noise discrimination threshold. At gamma-ray energies between 10 and 60 keV the sensitivity, $\delta_X(E_\gamma)$, increases by more than one order-of-magnitude. In contrast, at gamma-ray energies between 80 keV and 1 MeV, the sensitivity drops by more than two orders of magnitude. An analytical form for the energy dependency, $\delta_X(E_\gamma)$, in the entire range of gamma-quantum energies between 10 keV and 3 MeV cannot be obtained. Thus, the curve of sensitivity was divided into 3 parts. The behavior of $\delta_X(E_\gamma)$ in CdZnTe-detectors in the different energy ranges was approximated by three different functions. In Fig.1 and the following ones, the names of fitting functions correspond to the names that are used in the Origin 9 software [7]. The log-log scale of Fig.1 specifies the visible shape of the fitting curves.

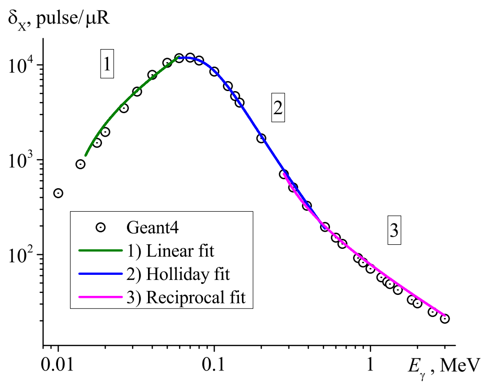

Fig.1. *Approximate description of the dependency, $\delta_X(E_\gamma)$, in three ranges of gamma-ray energies*

It is easy to determine an analytical form of functions that approximates a dependency of $\delta_X(E_\gamma)$ in regions 1 and 3. At gamma-ray energies between 10 and 60 keV (region 1), the sensitivity of the CdZnTe-detector can be approximated by a linear function such as

$$\delta_X(E_\gamma) \approx a_1 + b_1 \times E_\gamma,\ E_\gamma < 60\,keV. \quad (1)$$

At gamma-quantum energies more than 0.3 MeV (region 3), the inverse dependency is evident in the form

$$\delta_X(E_\gamma) \approx \frac{1}{a_3 + b_3 \times E_\gamma},\ E_\gamma > 0.3\,MeV. \quad (2)$$

In Eqs. (1) and (2), the values of a_1, b_1, a_3, and b_3 are the fitting parameters that can be determined from the data of the experimental measurements of the energy dependency, $\delta_X(E_\gamma)$. The difference between units for measuring energy (keV and MeV) in Eqs. (1) and (2) is related to the method of determining the fitting parameters.

In region 1, good accuracy was achieved in evaluating the parameters for the linear fitting Eq. (1) with only three experimental points. For example, they could be measurements of $\delta_X(E_\gamma)$, the sensitivity of CdZnTe detectors, for gamma-ray energies of 31.6 keV (^{133}Ba source, multiplet) or 32.9 keV (^{137}Cs source, multiplet) plus 39.9 keV (^{152}Eu source, doublet) and 59.54 keV (^{241}Am source, monoenergetic line). For gamma-ray energies up to approximately 80 keV, the Compton scattering in CdZnTe is insignificant, and the probability of the photoelectric absorption is very high. The process of reconstructing the functional dependency of $\delta_X(E_\gamma)$ and determining the sensitivity of CdZnTe-detectors in the range of gamma-ray energies between 25 and 60 keV is sufficiently easy. Below 25 keV the results of linear fitting with only three experimental points are doubtful in that it is apparently connected with a near-vertical slope of the approximation curve.

The sensitivity of the investigated CdZnTe-detectors reaches a maximum value at gamma-rays between 60 and 80 keV. Moreover, in this energy range, the value of sensitivity, $\delta_X(E_\gamma)$, changes only within 5%, so for the given approximations, it is assumed that it is constant. It was shown [6] that the determination of the fitting parameters for Eq. (2) can be simplified by rewriting it in the form

$$\frac{1}{\delta_X(E_\gamma)} \approx a_3 + b_3 \times E_\gamma,\ E_\gamma > 0.3\,MeV. \quad (3)$$

In this case, a linear function can be fitted through three experimental points. In reconstructing the high-energy region for the dependency of the sensitivity of CdZnTe-detectors from the gamma-ray energy, we can use experimental data for ^{241}Am-, ^{137}Cs- and ^{60}Co-sources.

In Table 1, we compare the coefficients of fitting functions Eq. (1) and (3) obtained by analyzing an array of values of the simulated functions, $\delta_X(E_\gamma)$, and using only three points in regions 1 and 3 of this function (see Fig.1).

According to the data from Table 1, the variation in the coefficients of the slope of linear dependencies used for approximating the energy dependency of the sensitivity of detectors is no more than 9%. Hence, we can, with satisfactory accuracy, reconstruct the dependency of $\delta_X(E_\gamma)$ in regions 1 and 3 (see Fig.1) through three measured values of sensitivity.

Table 1. *Coefficients of approximation Eqs. (1) and (3) for CdZnTe detector*

Approximation formula	Slope, $b_{1,3}$		Ratio, b_{full}/b_{three}
	Whole array of data, b_{full}	Three points, b_{three}	
$\delta_X(E_\gamma) \approx a_1 + b_1 \times E_\gamma$, $E_\gamma < 60$ keV	250 ± 10, $pulse/(\mu R \times keV)$	230 ± 28, $pulse/(\mu R \times keV)$	1.09
$\frac{1}{\delta_X(E_\gamma)} \approx a_3 + b_3 \times E_\gamma$, $E_\gamma > 0.3$ MeV	0.01891 ± 0.00021, $\mu R/(MeV \times pulse)$	0.01869 ± 0.00025, $\mu R/(MeV \times pulse)$	1.01

From Fig.1 it is evident that the regions 2 and 3 of the $\delta_X(E_\gamma)$ dependency partially overlap in the energy range from 300 to 400 keV. The analysis of the calculated dependency of $1/\delta_X(E_\gamma)$ showed that in considering gamma-ray energies between approximately 0.08- and 0.4 MeV, it is convenient to use the next approximation formula with less number of fitting parameters

$$\frac{1}{\delta_X(E_\gamma)} \approx a \times E_\gamma^b,\ 0.08\,MeV < E_\gamma < 0.4\,MeV. \quad (4)$$

Fig.2 demonstrates the result of using Eq. (4) for fitting the calculated dependency of $1/\delta_X(E_\gamma)$ in the range of low gamma-ray energies. As illustrated, employing Eq. (4) for fitting the dependency of $\delta_X(E_\gamma)$ through three energies is equally effective as modeling the sensitivity in detail by a Monte-Carlo method. The data from Table 2 show that the difference between the coefficients of Eq. (4) obtained by approximating the different sets of data is 1...3%.

In deciding on the experimental points for the fitting, we take into account first those as follows from the data in Fig. 1 $\delta_X(60\,keV) \approx \delta_X(80\,keV)$. The choice of a gamma-ray energy of 122.06 keV as the second point is conditioned by the fact that for a ^{57}Co source, the contribution in the measured sensitivity of CdZnTe-detectors from this line considerably exceeds the contribution from all other high-energy lines, and the contribution in the measured sensitivity from 14.4 keV line is subtracted easily. The quality of the fitting in the energy range from 0.08 to 0.4 MeV depends on the possibility of measuring the third point. A monoenergetic ^{203}Hg (E=279.2 keV) source is a very good candidate; however, the ^{203}Hg isotope has a half-life of only 46.6 days. For the ^{51}Cr isotope that also has an intensive single line, E=320.1 keV, the half-life is 27.7 days.

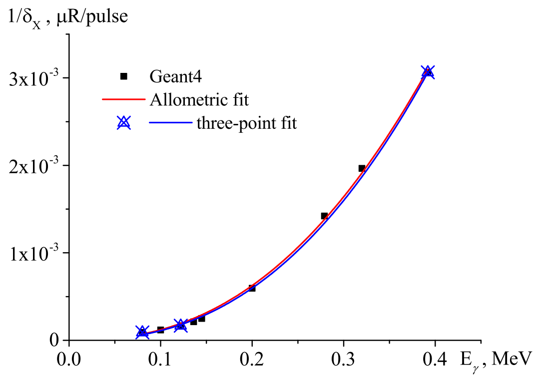

Fig.2. *Fitting of the dependency of $1/\delta_X(E_\gamma)$ of CdZnTe-detector in the range of gamma-ray energies between 90 and 400 keV*

Table 2. *Fitting parameters for Eq. (4)*

Parameter	Whole array of data	Three points	Ratio
b	2.38 ± 0.05	2.4 ± 0.1	0.99
a	0.029±0.002	0.03±0.003	0.97

For an approximate calculation, the partial overlapping in regions 2 and 3 of the energy dependency of the sensitivity, $\delta_X(E_\gamma)$, was used. For the third point needed to obtain an approximation in region 2, the value for δ_X (at 0.4 MeV) obtained by Eq. (3) can be used. However, in this case, the discrepancy in the fitting through three points with detailed Monte-Carlo simulation may reach up to several tens of percents. For example, for the CdZnTe-detector we investigated, the sensitivity, $\delta_X(E_\gamma)$, obtained by Eq. (4) for the range of gamma-quantum energies from 0.2 to 0.4 MeV is understated by no less than one third.

Fig.3 presents the difference between the approximate $1/\delta$ calculation with investigated formulae and the Monte-Carlo simulation data for CdZnTe-detectors. It is evident that the maximum discrepancy is about 10%. TlBr-detector was simulated via Geant4 package for verification of possibility of using the formulae investigated above for TlBr-material.

The Fig.4 shows the $1/\delta$ dependence for 7 mm^2×1 mm TlBr-detectors in the energy range E_γ below 0.3 MeV and its fitting by the formula (4). It is evident that sensitivity of TlBr-detectors can be reconstructed with a good accuracy.

Fig.5 presents the total $1/\delta$ dependence for TlBr-detector. As we can see TlBr-detector does not have a linear energy dependence of sensitivity in the high energy region as it was shown for CdZnTe-detector [4]. Thus, we cannot use the formula (3) for reconstructing the sensitivity in the range of gamma-quantum energies above 0.3 MeV. However, in this case we can apply the more complicated formula, which is also correct for CdZnTe-detector:

$$\frac{1}{\delta_X(E_\gamma)} = \frac{a \times b \times E_\gamma^{1-c}}{1 + b \times E_\gamma^{1-c}}, \; E_\gamma > 0.3\,MeV. \quad (5)$$

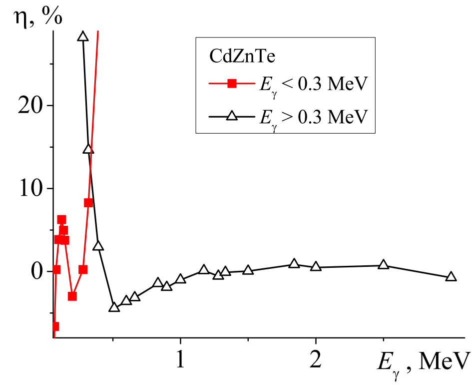

Fig.3. *The difference between the approximate $1/\delta$ calculation with investigated formulae and the Monte-Carlo simulation data for CdZnTe-detectors*

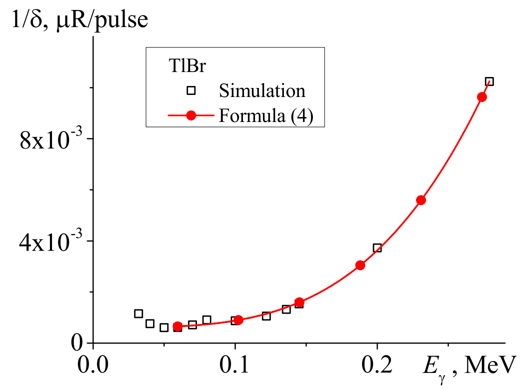

Fig.4. *The $1/\delta$ dependence at $E\gamma$ below 0.3 MeV for TlBr-detector*

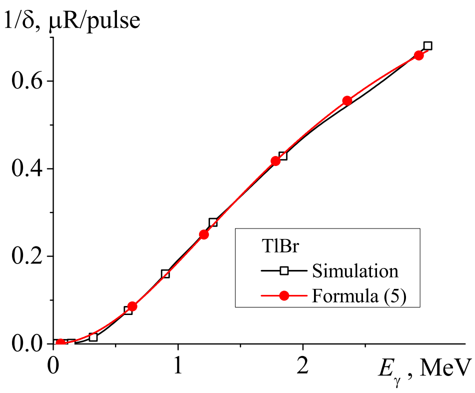

Fig.5. *The total $1/\delta$ dependence for TlBr-detector*

The difference between the approximate $1/\delta$ calculation with investigated formulae and the Monte-Carlo simulation data for TlBr-detectors is shown in Fig.6. We can conclude that maximum discrepancy between values of $1/\delta$ obtained by formulae and simulation is in the range about from 0.32 MeV to 0.38 MeV.

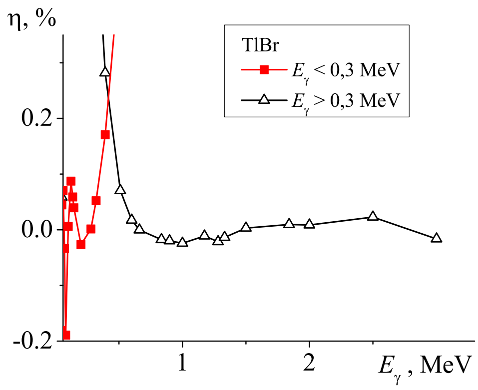

Fig.6. *The difference between the approximate* $1/\delta$ *calculation with investigated formulae and the Monte-Carlo simulation data for TlBr-detectors*

Overall, the sensitivity of CdZnTe- and TlBr-detectors can be restored by the investigated approximate formulae in the range of gamma-quantum energies from 30 keV to 3 MeV.

4. EXAMPLE OF RECONSTRUCTING THE SENSITIVITY OF CdZnTe-DETECTOR THROUGH EXPERIMENTAL DATA

Basing on data of Ref. [6] we considered the example of reconstruction of CdZnTe-detector's sensitivity. To reconstruct the sensitivity by investigated formulae described above it was used the experimental data derived from 5×5×1.8 mm^3 CdZnTe-detector with known values of transport parameters for electrons and holes. Its sensitivity was measured in the reference points through gamma-quantum spectra with 59.54 keV (^{241}Am), 122.06 keV (^{57}Co), 661.67 keV (^{137}Cs), and 1.28 MeV (^{60}Co) energies. For evaluating the spectrum of gamma-rays from the ^{241}Am source, the chosen discrimination threshold of noise was at a level of 40 keV. Other spectra were obtained at the 60 keV discrimination threshold for noise. The bias voltage of detectors in all measurements was 300 V. In detailing the results of fitting in Fig.7, the respective dependency, $\delta_X(E_\gamma)$, obtained by simulating the response of CdZnTe-detectors using the Geant4 toolkit was shown.

Fig.7 reveals that the maximum difference between the function of $\delta_X(E_\gamma)$ reconstructed through experimental measurements and data of simulation is evident at the edges of the fitting region, i.e., in the range of gamma-ray energies below 90 keV and in the energy range from 0.3 to 0.5 MeV. Additional experimental measurements of sensitivity, $\delta_X(E_\gamma)$, in these ranges of gamma-quantum energies essentially should improve the quality-of-fit.

In Table 3, it was compared the values of the parameters of approximation functions for the reconstructed dependency, $\delta_X(E_\gamma)$, and for the dependency, $\delta_X(E_\gamma)$, obtained from the findings of our detailed Monte-Carlo simulation. The parameters of approximation function in region 3 agree with the results of the simulation much better than in region 2. This may reflect the absence of the experimental measurements for the sensitivity of the CdZnTe-detector in the range of gamma-ray energies from 300 to 400 keV. For obtaining parameters for the approximation function in region 2, a value of $\delta_X(E_\gamma = 0.4\,MeV)$ calculated from the approximate dependency, $\delta_X(E_\gamma)$, in region 3 was used. The essential difference between the ADC step size in the measurements (about 0.7 keV) and for the simulation (50 eV) of the response of CdZnTe detectors may be another factor affecting the quality-of-fit in region 2.

It was concluded that using the presented methodology gives satisfactory results for reconstructing the energy dependency of the sensitivity for CdZnTe-detectors. From the considered example we see that this method can be applied to the cases of high electronic noise and a lack of extensive experimental data.

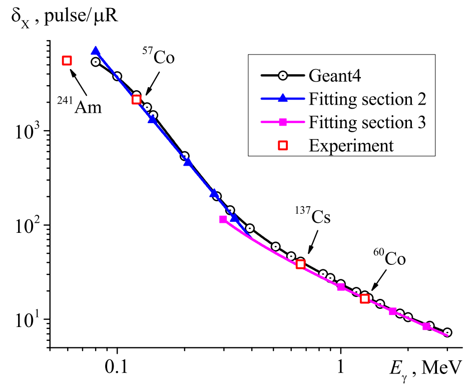

Fig.7. *Example of reconstruction of dependency,* $\delta_X(E_\gamma)$*, for the* $5\times5\times1.8\,mm^3$ *CdZnTe detector*

5. CONCLUSIONS

We investigated the dependence of energy sensitivity of CdZnTe- and TlBr-detectors. The approximate formulae for reconstructing the sensitivity of CdZnTe were researched. It was shown that the greater part of the curve of sensitivity may be reconstructed using measurements with three reference sources. However, presence of other measurements can significantly improve the accuracy of reconstruction.

In region 1 ($E_\gamma < 60\ keV$) the sensitivity can be reconstructed through three experimental reference points, such as with ^{137}Cs (32.9 keV), ^{152}Eu (39.9 keV) and ^{241}Am (59.54 keV) sources. The reconstruction of sensitivity in region 2 (90 keV< E_γ < 0.3 MeV) require measurements with ^{241}Am (59.54 keV) and ^{57}Co (122.06 keV) sources. Also, short-lived isotope of ^{203}Hg ($E_\gamma = 279.2$ keV) can be used. In region 3 ($E_\gamma > 0.3$ MeV) the energy dependence of the sensitivity, $\delta_X(E_\gamma)$, for planar CdZnTe-detectors can be reconstructed based on experimental measurements of sensitivity also at three reference points with ^{241}Am (59.54 keV), ^{137}Cs (661.67 keV), and ^{60}Co (about 1.28 MeV) sources.

Table 3. *Fitting parameters for reconstructed dependency, $\delta_X(E_\gamma)$, for the $5 \times 5 \times 1.8$ mm^3 CdZnTe-detector*

Approximation formula	Parameters	
	Experiment	Simulation
$\frac{1}{\delta_X(E_\gamma)} \approx a \times E_\gamma^b$, $0.08\,MeV < E_\gamma < 0.4\,MeV$	$a = 0.19 \pm 0.01$ $pulse/(\mu R \times MeV)$ $b = 2.84 \pm 0.06$	$a = 0.12 \pm 0.01$ $pulse/(\mu R \times MeV)$ $b = 2.51 \pm 0.09$
$\frac{1}{\delta_X(E_\gamma)} \approx a_3 + b_3 \times E_\gamma$, $E_\gamma > 0.3\,MeV$	$b_3 = 0.052 \pm 0.002$ $\mu R/(pulse \times MeV)$ $a_3 = -0.007 \pm 0.002$, $\mu R/pulse$	$b_3 = 0.0502 \pm 0.0006$ $\mu R/(pulse \times MeV)$ $a_3 = -0.0081 \pm 0.0008$, $\mu R/pulse$

Maximum discrepancy of $1/\delta$ values in the total range from 30 keV to 3 MeV obtained by the investigated formulae and Monte-Carlo simulation is about 10%.

We used the investigated formula obtained for CdZnTe-detectors for reconstructing the sensitivity of TlBr detectors. Our analysis allows us to conclude that more quantity of these formulae can be useful for receiving TlBr-detectors' sensitivity. Maximum discrepancy of $1/\delta$ values obtained by the investigated formulae and Monte-Carlo simulation is in the range about from 0.32 MeV to 0.38 MeV.

The energy dependence of the sensitivity for CdZnTe-detector was reconstructed by approximate formulae within a satisfactory accuracy through the experimental measurements in the reference gamma-quantum spectra with 59.54 keV (^{241}Am), 122.06 keV (^{57}Co), 661.67 keV (^{137}Cs), and 1.28 MeV (^{60}Co) energies.

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ВОССТАНОВЛЕНИЕ ЭНЕРГЕТИЧЕСКОЙ ЗАВИСИМОСТИ ЧУВСТВИТЕЛЬНОСТИ CdZnTe- и TlBr-ДЕТЕКТОРОВ ПО ОГРАНИЧЕННЫМ ДАННЫМ

А. И. Скрыпник

Метод Монте-Карло использован для исследования энергетической зависимости чувствительности CdZnTe- и TlBr-детекторов гамма-излучения, которые работают в режиме анализа амплитуд импульсов. Мы изучили приближенные формулы, описывающие эту зависимость в диапазоне энергий гамма-квантов от 30 кэВ до 3 МэВ. Предлагается метод определения параметров подгонки для приближенных формул по спектрам гамма-излучения, которые экспериментально измерены с помощью нескольких стандартных источников излучения. В частности, это могут быть источники гамма-излучения ^{241}Am, ^{137}Cs и ^{60}Co. Обсуждаются также измерения с дополнительными источниками излучений, которые могут быть использованы для улучшения точности восстановления энергетической зависимости чувствительности детекторов.

ВІДНОВЛЕННЯ ЕНЕРГЕТИЧНОЇ ЗАЛЕЖНОСТІ ЧУТЛИВОСТІ CdZnTe- і TlBr-ДЕТЕКТОРІВ ЗА ДОПОМОГОЮ ОБМЕЖЕНИХ ДАНИХ

А. І. Скрипник

Метод Монте-Карло використаний для дослідження енергетичної залежності чутливості CdZnTe- і TlBr-детекторів гамма-випромінювання, котрі працюють в режимі аналізу амплітуд імпульсів. Ми дослідили наближені формули, які описують цю залежність в діапазоні енергій гамма-квантів від 30 кеВ до 3 МеВ. Пропонується метод визначення параметрів підгонки для наближених формул за спектрами гамма-випромінювання, які експериментально виміряні за допомогою декількох стандартних джерел випромінювання. Зокрема, це можуть бути джерела гамма-випромінювання ^{241}Am, ^{137}Cs та ^{60}Co. Обговорюються також вимірювання з додатковими джерелами випромінювань, які можуть бути використані для поліпшення точності відновлення енергетичної залежності чутливості детекторів.