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THE STUDY OF RESPONSE OF WIDE BAND GAP SEMICONDUCTOR DETECTORS USING THE GEANT4

by

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The energy dependence on the intrinsic efficiency, absolute efficiency, full energy peak absolute efficiency and peak-to-total ratio have been studied for various wide band gap semiconductor detectors using the Geant4 based Monte Carlo simulations. The detector thickness of 1-4 mm and the area in 16-100 mm^2 range were considered in this work. In excellent agreement with earlier work (Rybka *et al*., [20]), the Geant4 simulated values of detector efficiencies have been found to decrease with incident γ-ray energy. Both for the detector thickness and the detector area, the increasing trends have been observed for total efficiency as well as for full-energy peak efficiency in 0.1 MeV-50 MeV range. For $Cd_{1-x}Zn_xTe$, the detector response remained insensitive to changes in relative proportions of Zn. For various wide band gap detectors studied in this work, the detection efficiency of TlBr was found highest over the entire range of energy, followed by the HgI_2, CdTe, and then by CZT.

Key words: semiconductor detector, Geant4, absolute full-peak efficiency, wide band gap

INTRODUCTION

The wide band-gap (WBG) compound semiconductors have attracted a great deal of attention recently due to their room temperature operation capability, high energy resolution, and simple operation. In recent past, the appreciable growth has been observed in their use in bio-medical, radiation monitoring and control, industrial imaging, and in space science technologies [1, 2]. Since the advent of AgCl radiation counters by van Heerden [3] and CdS room temperature semiconductor detectors by Frerichs [4], the search for high performance radiation detector has continued. Among the desirable characteristics of radiation detector are high efficiency, high resolution and stable operation at room temperature. While the early radiation detectors had poor characteristics, the discovery of the *p-n* Germanium (Ge) semiconductor diode detectors by McKay [5] proved to be of landmark importance. Mayer extended this work and designed Schottky diode surface barrier detectors of Ge that found wide range of practical uses [6]. Subsequently, the Silicon (Si) and high purity Germanium (HPGe) based semiconductor detectors were discovered and they made a profound impact on detection of low energy γ-ray and X-ray detection [7]. However, both of these detectors need to be operated at low temperature.

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The compound semiconductor detectors (CSD) have a distinct advantage over the semiconductor or scintillation detectors. They exhibit higher efficiency values especially at low energies where only a few millimeter thicknesses of these materials have been found sufficient. The low leakage current and better energy resolution operating at room temperature are the other attractive features of WBG compound semiconductor detectors. The work on WBG compound semiconductor detectors started in the mid-forties with AgCl being the first candidate studied. This was followed by CdS and GaAs which exhibited γ-ray energy resolution at room temperature conditions [8]. However, preparation of GaAs in liquid phase with high purity epitaxial material proved highly expansive and non-repeatable. Consequently, its commercial use has been limited.

The γ-ray detection properties of CdTe were first reported in the late sixties [9]. It has a cubic zinc blende structure and a number of different methods exist for high purity crystal growth including the solution growth, the Bridgeman method and the travelling heater method (THM). The HgI_2 as CSD was first time reported in 1971. It has CsCl like layered crystalline structure. It has a large value of the band-gap energy and consequently small value of thermal dark current, rendering it suitable for room temperature operation. The cadmium zinc telluride $Cd_{1-x}Zn_xTe$ (x 0.2) is relatively more recent contender for the room temperature semiconductor detectors. The CZT has zinc blende structure with large energy band-gap which reduces dark current. Also, it has lower intrinsic carrier concentration as compared to CdTe [10, 11].

Caroli *et al.*, in 1992 modeled a γ-ray spectrometer capable of imaging for astronomical applications with the help of the Geant3 based Monte Carlo simulations [12]. Their study was centered upon finding the detection efficiency of CdTe in 0.05-5 MeV energy range and predicting the spatial resolution of the detector, both as a function of the incident γ-energy and their angle of incidence. Their simulations produced satisfactory results for γ-spectroscopy. The outstanding problems included: (1) the packing such type of bar detectors together so that their resolution may not get affected and (2) the improvement of the detector response at higher energies.

Coupat *et al.*, in 1987 studied the HgI_2 semiconductor detector response for γ-ray photons using the Monte Carlo simulations. They were able to match the two corresponding spectra within the acceptable limits for simulated and experimental results. However, their study lacked results for important parameters including efficiency and the spectral comparisons were limited to few sources [13].

Jung *et al.*, reported a new method to evaluate the transport properties of CdTe and CdZnTe detectors [14]. The simulations were carried out for collection efficiency of CdTe γ-ray detector by Vittone *et al.*, using ISIDE based Monte Carlo simulations [15]. They obtained collection efficiencies for different bias voltages and shaping times. They used ion-beam induced charge (IBIC) technique and simulated ^{57}Co spectra using the ISIDE code and concluded that spectral resolution of CdTe improves as collection efficiency peak flattens. Jung *et al.*, studied cadmium zinc telluride CZT detectors as 3-D γ-radiation calorimeters [16]. They simulated the energy dependence of the detector efficiency along with the spectra for 0.662 and 5 MeV incident γ-rays and found the detection efficiency of CZT in between those of HPGe and scintillation detector.

Tan *et al.*, examined the response of cadmium tellurie (CdTe) and cadmium zinc telluride (CdZnTe) detectors of different thicknesses in strong magnetic field both experimentally and using the Geant4 Monte Carlo simulations [17]. Skyrpnyk *et al.*, compared Geant4 (version 4.9.4), predictions with the corresponding EGSnrc Monte Carlo simulations [18]. The detectors under the study were the HgI_2 and thallium bromide (TlBr), covering the 0.026 MeV-3 MeV energy range. For a wide energy range of γ-rays (0.026 MeV-3 MeV), the EGSnrc results matched only with Geant4 Penelope 2008 EM-package. Apart from the energy loss, many additional parameters must be studied for the WBG compound semiconductor detectors to fully explore their properties and scope. Cheves *et a*l., (2012), performed the CdTe detector efficiency calibrations with different thickness targets using the induced X-ray emission (PIXE) technique [19]. They studied the spectra of a cooled CdTe detector in energy range 8.047 keV-98.439 keV. The results indicate that the CdTe could be the useful candidate for spectrum studies of especially rare earth elements. But, the PIXE technique can be of use only in some limited areas.

A lot of research work on CSD has been carried out in the past, for their characterization, spectral studies, and their applications to astrophysics, nuclear medicine and other fields. Rybka *et al.*, investigated some of the aspects of γ-dosimetry, thermal effects and I-V characteristics of CdTe and CdZnTe detectors experimentally and the detection efficiency with the Geant3 simulation code [20]. But, in the view of the huge scope for the application of WBG compound semiconductor detectors, a detailed study of the basic aspects of the compound semiconductor detector performance is needed. In regard to this, the intrinsic efficiency, absolute efficiency, full peak efficiency, Compton-to-peak and Compton-to-total ratio of detector are among the prominent detector characteristics to be studied. The dosimetric studies and energy deposition aspects were also needed to be explored for the compound semiconductor detectors for their medical and nuclear safety applications.

In this work, a comparative study of γ-ray detection properties of various WBG compound semiconductor detector has been performed using the Geant4 toolkit. The detectors include the CdTe, CdZnTe, HgI_2 and TlBr. The variation of the intrinsic- and full-peak efficiencies, along with the peak-to-total ratios with energy of γ-ray photons and with detector dimensions has been studied for the three types of detector materials. This work encompasses much wider energy range: 0.01 MeV-50 MeV. The effect of the detector response to the changes of zinc composition in CdZnTe detector has also been performed in this work and the corresponding results are reported. Finally, the results for energy deposition and dose correction factor for all detectors are also included.

MATERIALS AND METHODS

In this work, the Geant4 toolkit has been used to simulate and track γ-ray photons through matter [21]. It is based on four essential features: (1) Geometry, (2) Interaction physics, (3) tracking, and (4) scoring.

The Detector Construction class in Geant4 allows users to setup a world volume containing a radiation source and sensitive detector along with the remaining environment. In these simulations, the material for sensitive detector was taken from the Geant4 built-in database manager G4NistManager. The world volume was taken as 50 cm × 50 cm × 50 cm. The detector was placed at such origin that the source to detector front-surface distance was 10 cm.

In these simulations, the Standard model was employed for the inclusion of the electromagnetic and electron/positron processes. Therefore, all photon interactions including the Photo-electric effect, the Compton scattering and the Pair-production were considered. The electron interactions cover the ionization, multiple, and Rayleigh scatterings. For positrons, the annihilation process is included additionally. The Range Cuts or threshold values covering 0.01-1 μm range have been used in this study. The optimum value which maintains the accuracy of the results while conserving computational time, has been found as 1 μm which is equivalent to the 990 eV energy cut-off for photons.

The general particle source (GPS) was employed for the description of spatial, spectral and angular distribution of primary particles, due to its provided flexibility. The GPS was also used to specify the position, type (point, surface or volume) and nature (isotropic, beam, *etc*.) and energy of emitted particles.

The run action class

As the Geant4 carries out the particle tracking, the essential information regarding interactions and energy deposition is collected in the RunAction Class. Using these data, the values of the detector efficiency are determined using the following relations [22]

$$\text{int} \quad \frac{N_{\text{detected}}}{N_{\text{incident}}} \tag{1}$$

$$\text{abs} \quad \frac{N_{\text{detected}}}{N_{\text{source}}} \tag{2}$$

In the Geant4 program execution cycle, the user specifies the total number of histories to be tracked. The simulations loop through generation, tracking, and scoring of individual photon. Subsequently, the necessary statistics regarding the particle are collected including the type of interaction and total energy deposited by the particle, *etc*. The RunManager loops through all emitted particles and when it finishes, various quantities of interest such as the intrinsic and the absolute efficiency, peak-to-total and the peak-to-Compton ratios, *etc*., are computed and the results are finally printed.

RESULTS AND DISCUSSIONS

First, the validation of the Geant4.9.3 physics model developed in this work has been performed by comparing it's predictions with the simulated absorption (intrinsic) efficiency, with the earlier published data. The detector response was studied by placing a point isotropic γ-ray source at 10 cm from the detector's front face. The energy dependence of the absorption efficiency of the CdTe detector over 0.01 MeV-1.2 MeV energy range was simulated using the 10^6 histories employing source biasing technique to improve the statistical accuracy of the computed values. These results compared with the corresponding data by Rybka *et al*., [20] are shown in fig. 1. The ex-

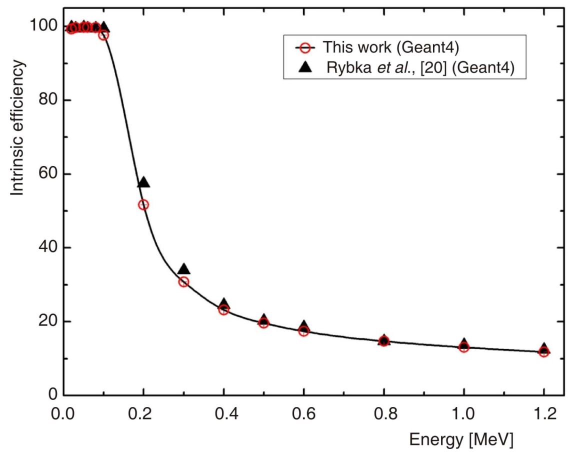

Figure 1. The comparison of the Geant4.9.3 (this work) computed variation of the intrinsic efficiency of the CdTe detector with γ-ray energy with the corresponding data from literature

cellent agreement is found between the Geant4 computed values with earlier data throughout the energy range, validating the current model used for the simulations. The detector response has the initial low-energy photoelectric dominant region where the efficiency remains maximum and exhibits flat response. This is followed by a Compton dominant region where some contribution due to the photoelectric effect remains but continues to decrease with the increase in γ-ray energy. Consequently, the detector efficiency also shows a decreasing trend in this region. As the energy of incident γ-ray photon increases beyond the 1.022 MeV, the pair production also starts contributing and since the pair production cross-section increases with energy, a corresponding increase in the detector efficiency is observed.

In the second study, a perforated filter of Cu-W alloy was used at the entrance window of the CdTe detector while the detector dimensions and source-to-detector distance values were kept identical to the previous case. As shown in fig. 2, the resulting variation of the in-

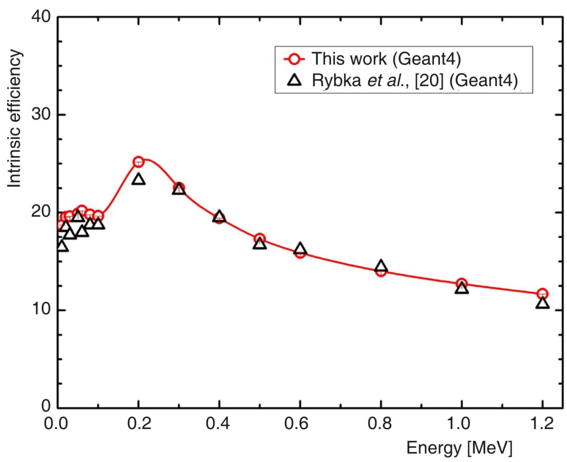

Figure 2. The comparison of the Geant4.9.3 (this work) computed variation of the intrinsic efficiency of the CdTe with the Cu-W alloy with γ-ray energy with the corresponding data from literature

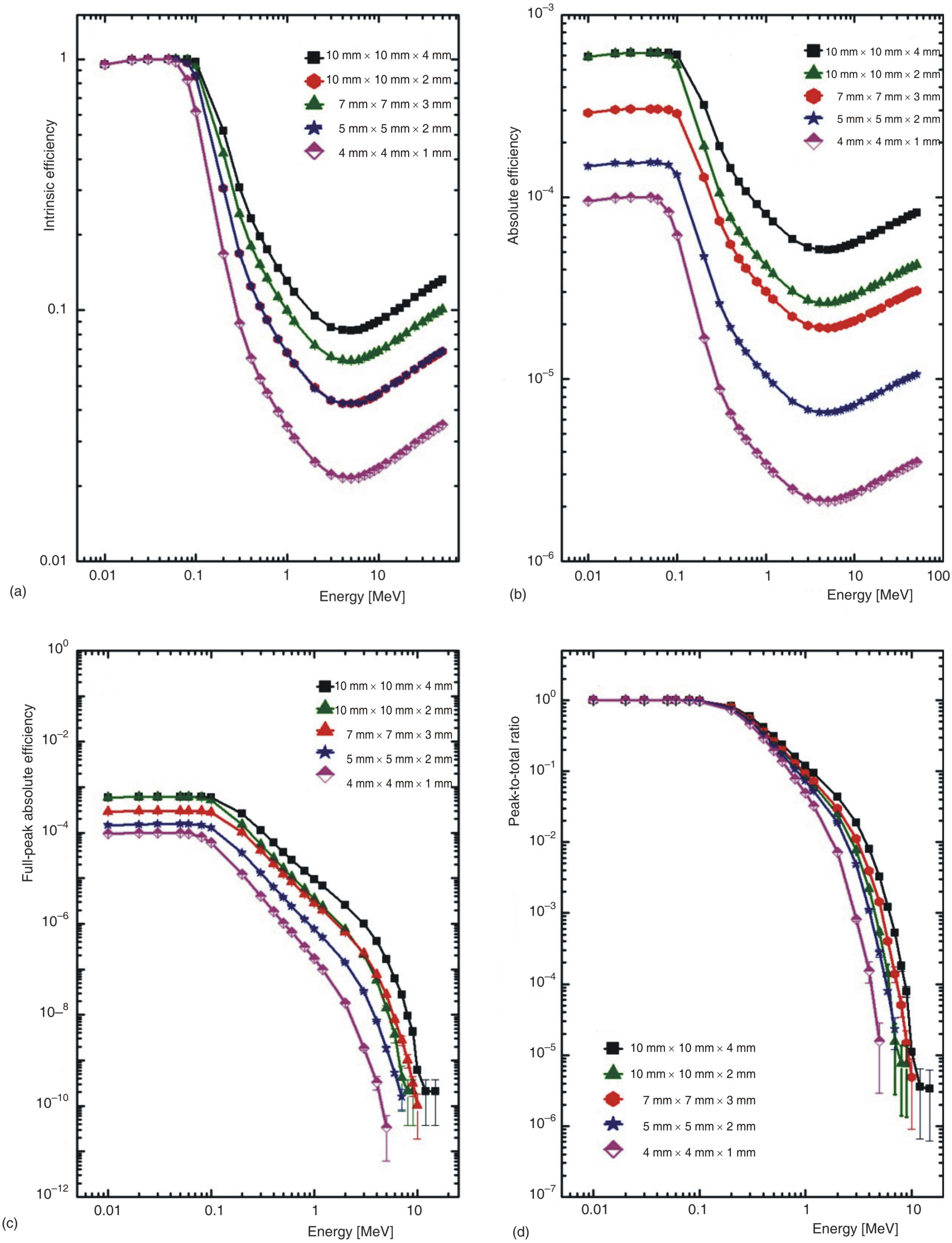

Figure 3. The variation of the intrinsic, absolute, full-peak efficiency values and peak-to-total ratio of CdTe detector with γ-ray energy for various indicated values of the detector thickness

trinsic efficiency with the energy of γ-rays computed using the Geant4.9.3 (this work) has a good agreement with the corresponding published data throughout the 0.01 MeV-1.2 MeV energy range again validating the effectiveness of model used. The results clearly show the high-pass nature of Cu-W alloy filter as it absorbs the low energy photons making the overall response of the detector relatively flat over the specified energy range. The Cu-W filter effectively absorbs the substantial fraction of low energy photons that would have normally contributed towards the photoelectric events in the detector. The reduction in the number of incidence

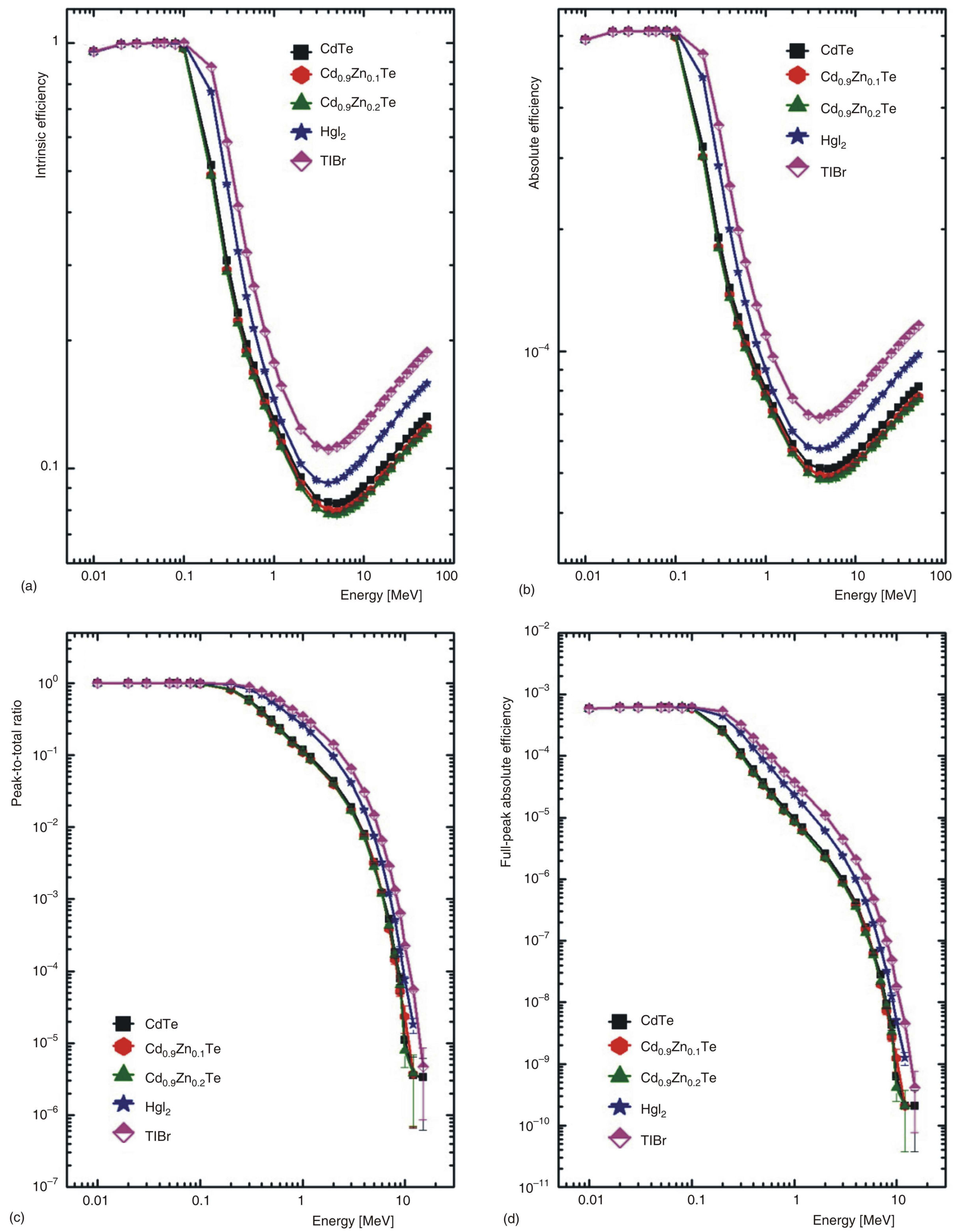

Figure 4. Variation of the intrinsic, absolute, full-peak efficiency values and peak-to-total ratio of detectors with γ-ray energy for various indicated detector materials

of these photons, leads to a relative flattening of the detector response towards the desired range.

The intrinsic detector efficiency, the absolute efficiency, and full-energy peak (FEP) efficiency values along with the peak-to-total ratios show sensitivity towards the detector thickness. The current Geant4.9.3 simulations show in fig. 3, an increasing behavior of the CdTe detector efficiency with thickness in 0.1 MeV-50 MeV energy range. The γ-rays of this energy range have high penetration power in CdTe and by increasing the detector thickness, larger fraction of the incident γ-ray photons undergoes interaction with the detector material which results in the observed increasing behavior. Also, as the detector thickness is increased, the relative number of full energy deposition events is higher than the partial energy deposition events. Subsequently, the peak-to-total ratio also shows increasing trend with the detector thickness.

A comparative study of the dependence of the detector material of intrinsic, absolute and full-energy peak (FEP) efficiency as well as of the peak-to-total ratio has been performed with geant4.9.3. Since the interaction probabilities of detector material depend on the *Z*-number, the values of efficiencies are therefore expected to increase with the rise in the *Z*-number of detector. In agreement with the expected behavior, the detection efficiency and the peak-to-total values are dominant for the TlBr which is followed by the HgI_2, CdTe, and then by CZT as shown in fig. 4.

The $Cd_{1-x}Zn_xTe$ with x 0.2 allows various values of relative Zn amount in the composition. In order to study the sensitivity of this composition variation on the detector properties, the energy dependence of intrinsic, absolute, FEP absolute efficiency values for $x = 0.1$ were compared with the corresponding data for $x = 0.2$. A similar comparison was also performed for the peak-to-total ratio. The results clearly indicate the independence of the detector response with the respect to a relative amount of Zn in the detector composition. It may be noted that these results are preliminary in the sense that these do not incorporate the corresponding changes in the density and the temperature dependence of the compositions.

CONCLUSIONS

A comparative study of the response of some wide band-gap compound semiconductor detectors has been performed including the CdTe, CdZnTe, TlBr, and HgI_2 detectors. The response including the intrinsic efficiency, absolute efficiency, full energy peak (FEP) absolute efficiency and peak-to-total ratio have been studied using the Gean4 toolkit for 0.01 MeV to 50 MeV energy range. The dependence of the detector response on the detector dimensions including the detector area covering 16-100 mm^2 range and the detector thickness in 1-4 mm range has been studied. The following may be concluded from this study:

– the detection efficiency has been found to increase with the detector thickness in 0.1 MeV to 50 MeV energy range,
– the total and full energy peak efficiency also increases with the detector area in the 0.1 MeV to 50 MeV energy range,
– the detector response remained relatively insensitive towards the changes in relative proportions of Zn in $Cd_{1-x}Zn_xTe$ with x 0.2, and
– over medium and high range of energy range studied in this work, the detection efficiency of TlBr remained leading, followed by the HgI_2, CdTe, and then CZT. In the low energy range, all detectors exhibited the same value of the detection efficiency.

AUTHOR CONTRIBUTIONS

The computational work was carried out by S. M. Mirza and R. Hussain. All authors analyzed and discussed the results. Figures were prepared by N. M. Mirza, S. M. Mirza and R. Hussain.

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ПРОУЧАВАЊЕ ОДЗИВА ПОЛУПРОВОДНИЧКИХ ДЕТЕКТОРА ШИРОКОГ ПРОЦЕПА КОРИШЋЕЊЕМ ПРОГРАМА GEANT4

Користећи Монте Карло симулације засноване на програмском пакету Geant4, испитивана је енергетска зависност параметара полупроводничких детектора широког пропусног процепа – унутрашње ефикасности, апсолутне ефикасности, апсолутне ефикасности енергије пуног пика и односа пика и целине. Разматране су дебљине детектора од 1 mm до 4 mm и површине од 16 mm^2 до 100 mm^2. Уз одлично слагање са ранијим резултатима (Rybka *et al*., [20]), ефикасности детектора добијене симулацијом смањивале су се при порасту енергије упадног гама зрачења. У опсегу енергија од 0.1 MeV до 50 MeV, уочен је растући тренд за укупну ефикасност и ефикасност детекције енергије пуног пика са порастом дебљине и површине детектора. За $Cd_{1-x}Zn_xTe$ детектор, одзив детектора остао је неосетљив на промене релативног удела Zn. У целом опсегу енергија, највећу ефикасност детекције имао је TlBr детектор, а затим HgI_2, CdTe и на крају CZT детектор.

Кључне речи: полупроводнички детектор, Geant4, апсолутна ефикасност пуног пика, широки пропусни процеп