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Original Article

The effect of front edge on efficiency for point and volume source geometries in p-type HPGe detectors

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ABSTRACT

Monte Carlo (MC) simulations are increasingly being used as an alternative or supplement to the gamma spectrometric method in determining the full energy peak efficiency (FEPE) necessary for radionuclide identification and quantification. The MC method is more advantageous than the experimental method in terms of both cost and time. Experimental calibration with standard sources is difficult, especially for specimens with unusually shaped geometries. However, with MC, efficiency values can be obtained by modeling the geometry as desired without using any calibration source. Modeling the detector with the correct parameters is critical in the MC method. These parameters given to the user by the manufacturer are especially the dimensions of the crystal and its front edge, the thickness of the dead layer, dimensions, and materials of the detector components. This study aimed to investigate the effect of the front edge geometry of the detector crystal on efficiency, so the effect of rounded and sharp modeled front edges on the FEPE was investigated for <300 keV with three different HPGe detectors in point and volume source geometries using PHITS MC code. All results showed that the crystal should be modeled as a rounded edge, especially for gamma-ray energies below 100 keV.

1. Introduction

Gamma spectrometry is one of the fast, practical, and reliable methods for measuring radioactivity. Compared to other nuclear analytical techniques, the sample preparation process is less laborious, and simple, and it is a non-destructive method [1]. Since the energies of γ-rays emitted by a nuclide are specific to the nuclide, the gamma spectrometric method can be used to identify nuclides in the sample by measuring the energy of photons emitted from the sample, and then to determine the activity or concentration of that radionuclide [2]. In this method, HPGe detectors are widely used because of their high-energy resolution and detection efficiency. In radiation detection systems, full energy peak efficiency (FEPE) calibration of the system to be used for the identification of radionuclides and determination of activity concentrations should be performed accurately and precisely [2,3]. The FEPE value can be determined experimentally or by the Monte Carlo (MC) method. Since the FEPE of any sample can be obtained in a short time without the use of calibration sources with the MC method, it is advantageous in terms of both cost and time, but the correct modeling of the detector is critical. The most critical step in modeling is modeling the germanium crystal because it is in the crystal where photon interactions occur, and accumulate energy, and modeling it round or sharp is important as it will change the active crystal volume. In the coaxial detectors used in this study, the crystals were initially manufactured with a whole cylindrical shape, but as the crystal size increased, and it was understood that there were weak field regions at the sharp corners. It has been noticed that the interactions occurring at these corners cause pulses with much higher rise times than the average and these pulses cannot be collected in the average times required for collecting the pulses. To eliminate these weak field regions that reduce the detector performance and to improve the charge collection, the edges of the front face of the crystal in coaxial detectors are rounded in a process known as “bulletization” [4]. Modeling the front edge of the detector as a sharp edge will increase the active volume and the solid angle, causing the FEPE value to be higher than it should be [5]. This effect changes the detector efficiency in the range of 5%–10%, especially for gamma-ray energies below 100 keV [5–7]. In the study by Cornejo Díaz and Jurado Vargas, it was stated that there are deviations greater than 10% for energies below 60 keV when

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rounding is not taken into account [8].

In our previous paper, the effect of front edge geometry on the efficiency of point source geometry at a distance with a p-type detector was investigated [9]. In this study, the methodology was expanded, and the effect of modeling the front edge of the crystal as a rounded or a sharp edge in point and volume source geometries using three different p-type detectors on the efficiency was examined in more detail. For this purpose, this effect has been determined primarily by point sources at different distances and volumetric source geometry counted on the detector's endcap, experimentally and with the PHITS MC program. Volumetric geometry prepared in cylindrical or Marinelli geometries is often used for radioactivity analysis in gamma spectrometry laboratories. For this reason, the effect of front edge shape on efficiency is important in volumetric source geometry.

2. Materials and methods

2.1. Gamma-ray spectrometers (The HPGe detectors)

In this study, three different p-type HPGe detectors were used. The p-type detectors, named HPGe-1, HPGe-2 and HPGe-3 with a relative efficiency of 150%, 58.5% and 54.7%, respectively. The geometric characteristics of the detectors provided by the manufacturer are given in Table 1. HPGe-1 detector was connected to an Ortec DSPEC jr 2.0 digital signal processing analyzer with a 16 k ADC/MCA operating through Gamma Vision spectroscopy software. The HPGe-1 detector was shielded with 10 cm thick Pb and graded with 1.6 mm Cu and 0.5 mm Sn liners. HPGe-2 and HPGe-3 detectors were connected to a Canberra DSA 1000 (16 k channel) digital multi-channel analyzer operating through Genie 2000™ spectroscopy software. HPGe-2 and HPGe-3 detectors were shielded with 10 cm thick Pb and graded with a 5 mm Cu liner. Genie 2000™ and Gamma Vision spectroscopy software were used for spectral analysis and peak area calculations [9,10].

2.2. Point sources and certified reference materials

Two different geometries were used in this study, point source and volume source geometries. Since the effect of the crystal front edge shape is dominant in the low energy region [9], sources with gamma energies around 300 keV were selected. The used point sources are ^{241}Am (59.5 keV) purchased from Amersham, ^{133}Ba (81 keV and 302.9 keV), and ^{152}Eu (121.8 keV) purchased from PTB. They have a total uncertainty, of less than ±2% at a 99% confidence level for the certified activities 21.6 kBq (^{133}Ba), 54.5 kBq (^{152}Eu), and 381.6 kBq (^{241}Am). In this study, the efficiency values obtained from the simulation of the detectors modeled as rounded and sharp-edged using the energies of the specified point sources were given at different source-detector distances. A standard volume source was used to examine the effect of the crystal front face on efficiency, which is the International Atomic Energy Agency (IAEA) certified reference standard RGU-1 [10]. The uranium reference material RGU-I was prepared by the Canadian Certified Reference Materials Project (CCRMP) on behalf of the IAEA in 1984. RGU-1 was the first to be prepared by dilution with silica sand of CCRMP Uranium ore BL-5 (7.09% U). Certified activity values and the elemental composition of the reference material are given in Table 2.

2.3. Monte Carlo simulations

PHITS (Particle and Heavy Ion Transport code System, version 3.24) was used for the simulations in this paper. PHITS is a multi-application MC simulation program that deals with the transport of all particles in a wide energy range using various nuclear data libraries and nuclear reaction models [11]. It has been shown in our previous publications that PHITS can be successfully used to calculate the HPGe detector efficiency [9,12]. The T-deposit tally, which gives the deposited energy distribution in a specific region where the HPGe detector operates in pulse-height mode, is used to obtain FEPE values. While the rounded edge germanium crystal shown in Fig. 1a consists of a cylinder, sphere, and torus geometric shapes, the sharp edge germanium crystal shown in Fig. 1b consists of cylinders. The "detector end radius" value provided by the manufacturer is used in modeling the torus, which is the geometric shape used for rounding the front edge. However, while some manufacturers report this value, others do not. It has been seen that this value is given as "hole diameter/2" in the p-type detector diagrams reported as in the HPGe-1 detector. Therefore, since this value was not given by the manufacturer of the HPGe-2 and HPGe-3 detectors used in this study, since the hole diameter of both detectors was 9 mm, the end radius, that is torus radii, was taken as 4.5 mm. In the volume calculation in PHITS, the source type is

Table 1
The geometric characteristics of the detectors provided by the manufacturer.

	Basic and Miscellaneous Physical Characteristics			
Description		HPGe-1	HPGe-2	HPGe-3
Crystal polarity		p-type	p-type	p-type
Relative efficiency		150%	58.49%	54.71%
Crystal diameter		94.8 mm	65.8 mm	65.8 mm
Crystal length		87.2 mm	65.9 mm	65.8 mm
Core diameter		11.2 mm	9 mm	9 mm
Core length		73.4 mm	53 mm	53 mm
Crystal to window distance		5 mm	5 mm	5 mm
End cap window		1.5 mm/Al	0.5 mm/Al	0.5 mm/Al
Dead layer thickness	Outside contact	700 µm Li	<1 mm	<1 mm
	Hole contact	0.3 µm/B		
Electrical Characteristics				
Detector bias and polarity		+3300 V	+2500 V	+3000 V
Measured Performances				
Peak-to-Compton ratio (@1332.5 keV)		90/1	71.27/1	67.15/1
Resolution at 1332.5 kev		2.11 keV	3.61 keV	3.83 keV
Resolution at 122.1 keV		0.89 keV	1.07 keV	1.22 keV

Table 2
Elemental composition, gamma-ray energy, and certified activity values of related radionuclides of reference material.

Reference material	Elemental composition (%)[a]	Gamma-ray energy (Radionuclide/Parent radionuclide)[b]	Certified activity values for radionuclides (Bg kg^{-1})[b]
RGU-1	O: 53.4 Si: 46.4 Al: 0.10 U: 0.04 Ca: 0.03 Fe: 0.03 Na: 0.02 C: 0.01 Pb: 0.008 K: 0.002	46.5 keV (^{210}Pb/^{238}U) 63.3 keV (^{234}Th/^{238}U) 143.8 keV (^{235}U)	^{235}U: 224 ± 5 ^{238}U: 4941 ± 99

[a] Elemental compositions of the reference material derived from XRF data.
[b] Gamma-ray energies and certified activity values within the energy range examined in this study are given.

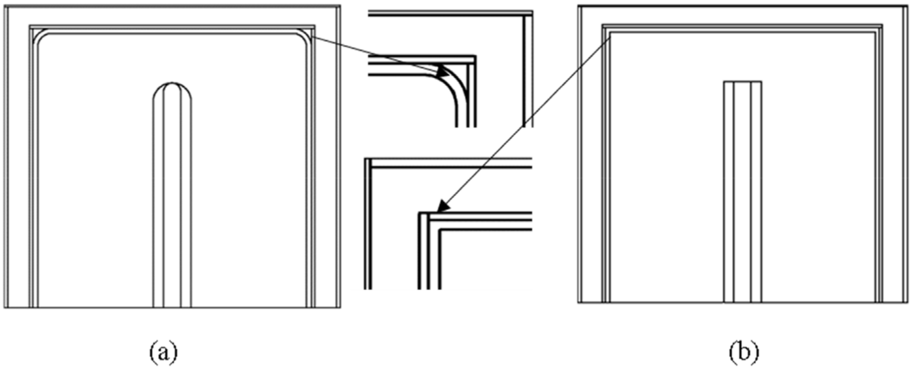

Fig. 1. Diagram of HPGe detector modeled as rounded (a) and sharp (b) edges in PHITS.

specified by s-type. In s-type = 1, the source generates on a sphere of the center coordinates (x_θ, y_θ, z_θ) and the radius r_θ with the inward direction. IAEA RGU-1 certified reference material prepared in a 5.6 cm × 5 cm cylinder shape container was modeled in PHITS using s-type = 1. Point source models were made by choosing s-type = 9, which is the source definition for the spherical surface. The number of histories in each simulation was chosen at 10 million to achieve statistical uncertainty lower than 1%.

2.4. Experimental

The experimental part of the study includes the investigation of the effect of the front edge shape of the crystal on the efficiency in the case of a volume source. For this purpose, measurements were made using the IAEA RGU-1 source in all detectors. Since the effect is dominant in the low energy region, the 46.5 (^{210}Pb/^{238}U), 63.3 keV (^{234}Th/^{238}U) and 143 keV (^{235}U) peaks in the RGU-1 spectrum were studied. The reference material, dried to a constant weight at 80–105 °C to remove its moisture content, was filled into a plastic beaker with a fill height of 5 cm and an internal diameter of 5.6 cm. To avoid losses of ^{222}Rn and ^{220}Rn from a sample, a hermetically sealed container was left for at least 30 days to reach radioactive equilibrium. In the study, measurements for reference material were repeated at least thrice until sufficient count statistics were obtained on the endcap of the detectors. It is necessary to carefully examine the correction factors that affect the measurement accuracy obtained in the gamma spectrometer. If high-quality gamma spectrometric measurements are to be performed, corrections for self-absorption effects and true coincidence summing (TCS) correction for multi-cascading gamma-ray transitions should be made for gamma rays with close count geometry and energies below 300 keV, as in the study by Yücel et al. [1]. Self-absorption correction factors were determined using the mass attenuation coefficients (μ) achieved using the XCOM: Photon Cross-Section Database application [13]. TCS correction factors were obtained using the GESPECOR program.

3. Results and discussion

Efficiency values were obtained from the simulation of each detector modeled as a rounded and sharp edge at different distances by using the energies of the point sources. These distances are on the end cap and at a distance of 1 cm, 2 cm, 3 cm, 4 cm, 5 cm, 10 cm, 15 cm, and 20 cm from the end cap. The relative difference graphs between rounded and sharp edges modeling according to source-detector distance are given in Table 3 for four distances and Figs. 2–4 for all distances. It can be seen that all detectors exhibit similar behavior (Figs. 2–4). The figures show that the relative differences are greater at lower energies (<100 keV) (except for the measurement on the end cap). At 59.5 and 81 keV, the relative differences in the endcap and at 1 cm distance are around 2%, while the differences increase as the source-detector distance increases. Differences up to 5 cm distance increased up to 5.7% in HPGe-1, 7.4% in HPGe-2, and 6.4% in HPGe-3 detector at further distances where they are independent of the source-detector distance (Table 3).

In all three detectors, it is seen that the values with the least percentage difference between the rounded edge and the sharp edge are in the geometry on the end cap distance. The reason for this is that photons reach the crystal and they are absorbed in a short time at this distance. The relative differences in all source-detector distances can be explained by the solid angle difference. In addition, these differences are due to differences in the optimum distance of each detector and flux differences in addition to the solid angle.

Table 3
Efficiency values calculated using PHITS for different source-detector distances in sharp and rounded edge geometries with point sources.

	Nuclide	Energy (keV)	On the end cap			@ 5 cm distance			@ 10 cm distance			@ 20 cm distance		
			Sharp edge	Rounded edge	% Diff.[a]	Sharp edge	Rounded edge	% Diff.[a]	Sharp edge	Rounded edge	% Diff.[a]	Sharp edge	Rounded edge	% Diff.[a]
HPGe-1	^{241}Am	59.54	0.03618	0.03617	0.0	0.01929	0.01825	5.7	0.00809	0.00756	7.1	0.00249	0.00234	6.6
	^{133}Ba	81.00	0.11425	0.11409	0.1	0.04596	0.04411	4.2	0.01819	0.01728	5.2	0.00553	0.00531	4.2
	^{152}Eu	121.78	0.20659	0.20593	0.3	0.06414	0.06280	2.1	0.02497	0.02441	2.3	0.00769	0.00754	2.0
	^{133}Ba	302.85	0.18899	0.18864	0.2	0.04743	0.04713	0.6	0.01920	0.01908	0.6	0.00626	0.00622	0.6
HPGe-2	^{241}Am	59.54	0.06005	0.05987	0.3	0.01818	0.01693	7.4	0.00631	0.00588	7.4	0.00181	0.00170	6.3
	^{133}Ba	81.00	0.14749	0.14633	0.8	0.03368	0.03214	4.8	0.01148	0.01098	4.5	0.00328	0.00316	3.7
	^{152}Eu	121.78	0.20506	0.20364	0.7	0.03878	0.03798	2.1	0.01343	0.01316	2.1	0.00394	0.00387	1.8
	^{133}Ba	302.85	0.13740	0.13701	0.3	0.02409	0.02395	0.6	0.00892	0.00886	0.6	0.00277	0.00276	0.5
HPGe-3	^{241}Am	59.54	0.03368	0.03363	0.1	0.01134	0.01065	6.4	0.00401	0.00376	6.5	0.00115	0.00109	5.9
	^{133}Ba	81.00	0.11064	0.11008	0.5	0.02688	0.02587	3.9	0.00923	0.00889	3.8	0.00265	0.00256	3.4
	^{152}Eu	121.78	0.17381	0.17300	0.5	0.03373	0.03321	1.6	0.01174	0.01156	1.6	0.00346	0.00341	1.4
	^{133}Ba	302.85	0.12591	0.12572	0.2	0.02226	0.02218	0.4	0.00827	0.00823	0.4	0.00258	0.00257	0.4

[a] It is the percentage difference between sharp and rounded edges.

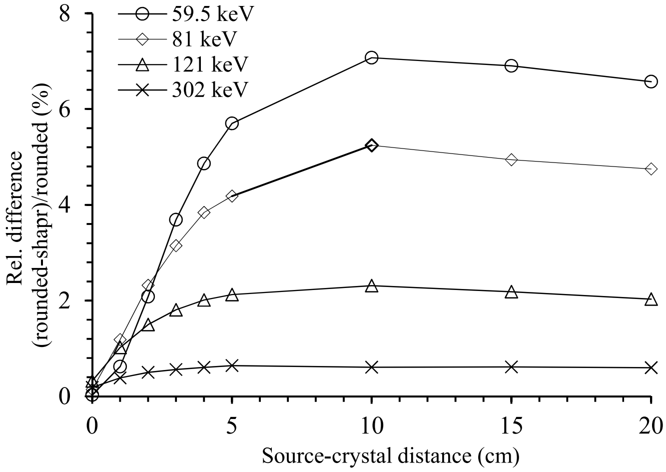

Fig. 2. Variation of percentage relative differences between rounded and sharp edges with source-crystal distance at different energies for HPGe-1 detector.

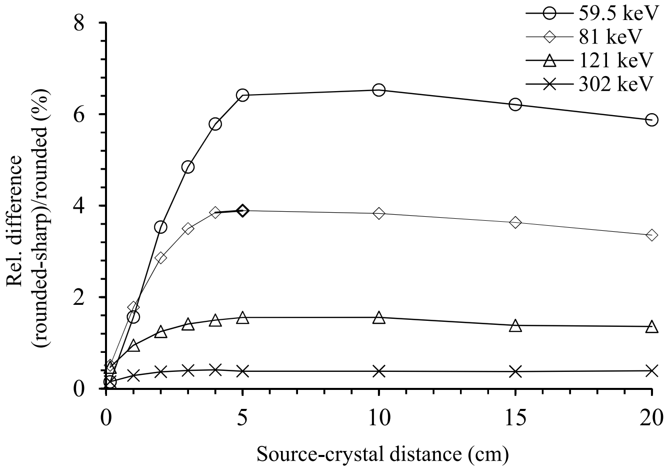

Fig. 4. Variation of percentage relative differences between rounded and sharp edges with source-crystal distance at different energies for HPGe-3 detector.

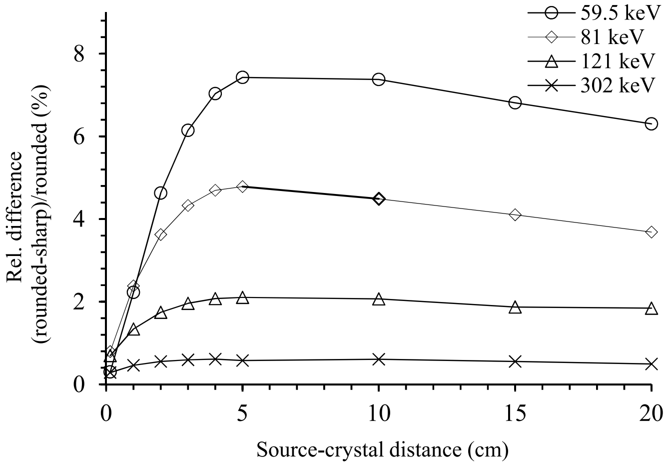

Fig. 3. Variation of percentage relative differences between rounded and sharp edges with source-crystal distance at different energies for HPGe-2 detector.

In addition, the difference between the experimental efficiencies with point sources and the MC calculations were compared at the appropriate source-detector distances for each detector. These distances were determined by controlling the dead time of the systems depending on the activities of the radioactive sources and minimizing the count rate losses caused by random summing at high count rates. Accordingly, experimental FEPE values were determined at a distance of 12.5 cm for HPGe-1, 7 cm for HPGe-2, and 8 cm for HPGe-3. As seen in Table 4, the differences between experimental and MC efficiencies in point source geometries were between 7 and 8% at below 100 keV in all three detectors.

The effect of rounded edge on FEPE was also investigated using a volumetric source. Experimental and simulated efficiency values of RGU-1 reference material were obtained using all the detectors. As shown in Table 5, when the crystal was modeled as a rounded edge, the absolute differences from the experimental values were at most 2.2%, while this difference increased to 3.8% at the sharp edge. It is seen that the percentage error of the sharp edge results in the volumetric geometry counted on the detector end cap mostly falls within the experimental percentage error. However, in gamma spectrometric measurements where there are many uncertainty sources, the crystal should be rounded to avoid such an error due to the geometry of the crystal. The relative difference between the rounded edge and the sharp edge reached 5.5% below 100 keV (Fig. 5).

It can be seen that the simulated FEPE curve with the rounded edge is within the uncertainty limits of the experimental efficiency curve and in good agreement with those of the experiments.

Table 4
Comparison of experimental and calculated FEPEs with point source[a].

	Nuclide	Energy (keV)	Experimental efficiency (U_{exp} %)	Sharp edge	Rounded edge	Difference from experimental efficiency, %	
						Sharp edge	Rounded edge
HPGe-1[b]	^{241}Am	59.54	0.00465 (1.2)	0.00516	0.00483	11.0	3.9
	^{133}Ba	81.00	0.01113 (1.6)	0.01148	0.01098	3.1	1.3
	^{152}Eu	121.78	0.01536 (1.6)	0.01580	0.01545	2.9	0.6
	^{133}Ba	302.85	0.01237 (1.5)	0.01244	0.01237	0.6	0.0
HPGe-2	^{241}Am	59.54	0.00924 (1.7)	0.01019	0.00947	10.2	2.5
	^{133}Ba	81.00	0.01806 (1.5)	0.01960	0.01774	8.5	1.8
	^{152}Eu	121.78	0.02151 (1.6)	0.02165	0.02106	0.7	2.1
	^{133}Ba	302.85	0.01395 (1.4)	0.01419	0.01380	1.7	1.1
HPGe-3	^{241}Am	59.54	0.00489 (1.8)	0.00541	0.00503	10.8	3.0
	^{133}Ba	81.00	0.01321 (1.5)	0.01429	0.01288	8.2	2.5
	^{152}Eu	121.78	0.01643 (1.7)	0.01676	0.01664	2.0	1.3
	^{133}Ba	302.85	0.01168 (1.5)	0.01178	0.01159	0.9	0.8

[a] Point sources were measured at a distance of 12.5 cm for HPGe-1, 7.5 cm for HPGe-2, and 8 cm for HPGe-3.
[b] From Bölükdemir et al., 2021.

Table 5
Comparison of experimental and calculated FEPEs with volume source.

	Nuclide	Energy (keV)	Experimental efficiency (U_{exp} %)	Sharp edge	Rounded edge	Difference from experimental efficiency, %	
						Sharp edge	Rounded edge
HPGe-1	^{210}Pb/^{238}U	46.54	0.00375 (9.7)	0.00385	0.00372	2.7	0.8
	^{234}Th/^{238}U	63.29	0.02992 (3.3)	0.03099	0.02997	3.6	0.2
	^{235}U	143.76	0.10462 (3.6)	0.10827	0.10691	3.5	2.2
HPGe-2	^{210}Pb/^{238}U	46.54	0.00397 (4.2)	0.00412	0.00390	3.8	1.6
	^{234}Th/^{238}U	63.29	0.02601 (3.4)	0.02679	0.02558	3.0	1.7
	^{235}U	143.76	0.07383 (4.1)	0.07484	0.07376	1.4	0.1
HPGe-3	^{210}Pb/^{238}U	46.54	0.00111 (3.9)	0.00115	0.00109	3.0	1.8
	^{234}Th/^{238}U	63.29	0.01436 (2.9)	0.01482	0.01431	3.2	0.4
	^{235}U	143.76	0.06529 (3.1)	0.06592	0.06524	1.0	0.1

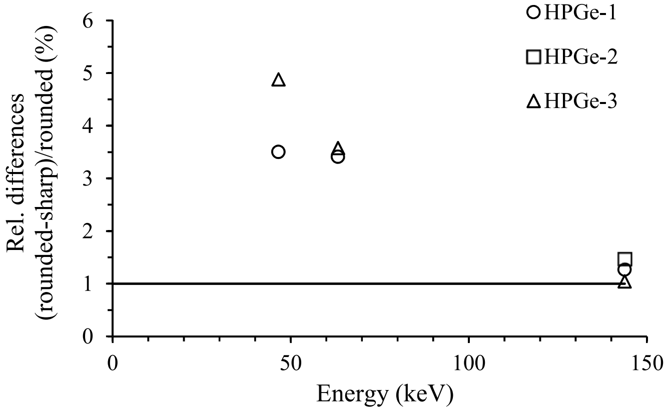

Fig. 5. The variation of percentage relative difference in simulated efficiency values with RGU-1 reference material in all detectors with rounded and sharp edges.

4. Conclusions

In our previous publication [9], it was determined that the front edge effect would cause up to 8% variation at <100 keV for a p-type detector at a certain distance from the point source geometry. In this study, this effect was investigated in detail at different distances and geometries using three different p-type detectors. In this study, as seen in three different detectors, it was observed that the front edge shape in the point source geometry similarly led to differences of up to 8%. The relative difference at source-detector distances can be explained by the differences in solid angles. The efficiency results obtained from the PHITS MC simulation method agreed well with the experimental values. With this study, it has been shown that the PHITS MC simulation program can be used confidently in volume and point samples. The rounded and sharp edge results were compared according to the results of all detectors and geometries, and it was determined that the bulletization affects the efficiency at low photon energies. Therefore, especially when dealing with radionuclides in the low energy region (especially <100 keV), the detector should be modeled with rounded edges.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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