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Determination of Energy Resolution for YSO:Ce Detector Modelled with FLUKA Code

G. M. Nadeera Hemamali, D. R. Smith, P. R. Hobson

Abstract–**In this paper, a 5×5×5 mm^3 YSO:Ce scintillator detector was modelled with FLUKA code, and calculations for the determination of energy resolution are reported using energies of 59.5, 81, 356, and 661.7 keV. We measured the energy resolution of the scintillator detector in the photon energy range of 59.5 to 661.7 keV using radioactive Am-241, Ba-133, and Cs-137 sources and compared the results with the computed energy resolution obtained using FLUKA, the comparison between simulated and measured resolution showing good agreement. This study shows that the FLUKA code can be used to determine the expected energy resolution successfully, saving both financial cost and time in the development of new scintillators and radiation sensors.**

I. Introduction

INORGANIC scintillators play a major role in many fields of radiation detection, mainly in medical imaging, astrophysics, and high energy physics because high detection efficiency can be obtained at room temperature [1-7]. The last decade has seen the introduction of several new high luminosity scintillators based on cerium doped complex oxide crystals, such as cerium doped yttrium orthosilicate, Y_2SiO_5:Ce (YSO:Ce) [6]. In YSO crystal, the effective atomic number (Z) is 35 and the density is 4.4 g/cm^3 resulting in high stopping power. Due to these properties, YSO detectors are expected to have high detection efficiency and better energy resolution.

The energy resolution of any detector is defined as the ability to distinguish between two peaks which is dependent on the FWHM (Full Width at Half Maximum) value. The lower the FWHM value, the greater the resolution.

The calculation of resolution can also be done by using simulation techniques. A variety of simulation approaches are available in the literature [1-5]. For this purpose, Monte Carlo based programs such as FLUKA, GEANT4, MCNPX are beneficial. In this study, the resolution calculations were done with FLUKA for a 5×5×5 mm^3 YSO:Ce detector. The energy spectra were obtained for energy deposited at 59.5, 81, 356, and 661.7 keV from Am-241, Ba-133, and Cs-137 radiation sources. FWHM and energy resolution values were calculated from the data generated in FLUKA, based on Poisson statistics. The results from the presented work were then compared with experimental data.

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II. Material and Method

A. Experimental Work

In this study, to measure the emission spectra, we coupled a YSO:Ce scintillator crystal from Epic Crystal, China, with a custom designed SiPM MCA from Bridgeport Instruments, USA, (model no: SIPM 1K_BC36_H50) with peak spectral sensitivity at around 420 nm which matches closely with the peak emission of the scintillator crystal used in this study. According to the manufacturer, the nominal cerium doping level of YSO:Ce is 0.5 mol%.

Radiation sources used for experimental activities are listed in Table I.

TABLE I. Radioactive sources used in experimental activities

Radiation Source	Expected γ-ray or X-ray Energy (keV)	Current Activity (μCi)
Cs-137	32.2, 661.7	0.445
Am-241	59.5	0.998
Ba-133	31, 81, 276.4, 302.9, 356	0.129

B. FLUKA Simulation

FLUKA is a Fortran-based Monte Carlo code used to calculate particle transport and interactions with matter and can be applied in many different fields such as nuclear physics, high-energy physics, and particle physics, developed by CERN (European Organization for Nuclear Research) and INFN (Italian National Institute for Nuclear Physics) [9-10]. FLUKA has the FLAIR interface for editing the input file, executing the code, and visualizing the output files. The presented study was done with FLUKA version 4.2.0 and FLAIR 3.1-15 version installed in Centos (Linux based operating system).

FLUKA offers numerous different estimators that can be used to score for various quantities of interest. FLUKA cards, BEAM and BEAMPOS were used to introduce the energy type, position/direction, and the energy spectrum of the chosen radiation sources, respectively. The DETECT card was used for acquiring energy deposition spectrum. The EMF (electromagnetic interactions) card was active and the EMF cut-off energy for photons was set to 10^{-6} GeV.

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All these functions (cards) were used for finding the response function of the scintillator. The DETECT card output gives a spectrum distributed over a fixed number of channels. In this study, 1024 channels were used. The light produced in the scintillator material is emitted in all directions. Only a limited fraction of it reaches the surface where the SiPM detector is mounted, the USRBDX card being used to calculate the light passing through the boundary. To obtain a reasonable statistical error (<2%), 10^8 particles were run with five cycles.

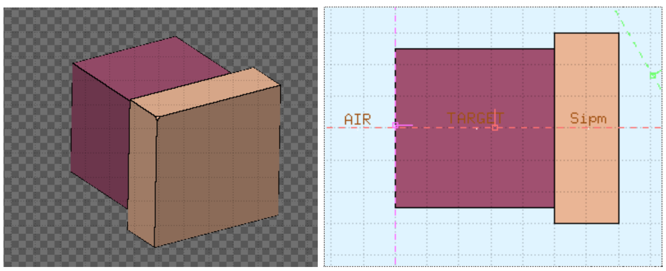

Fig. 1. Geometry of detector used for simulation, the purple color representing the scintillator target.

In simulations, Am-241, Ba-133, and Cs-137 point sources were defined as isotopic gamma sources. Each gamma source was placed 5 cm away from the YSO:Ce detector and a simulation were performed by obtaining results from the DETECT card which scores energy deposition on an event by event basis. Fig. 1 shows images of the detector geometry used for the simulation.

C. Conversion Process of Photons to Pulse Height Spectrum in FLUKA

As explained in the previous section, the DETECT card records the amount of deposited energy for each scintillation pulse. The number of counts generated in the YSO:Ce crystal dependent on the energy, is obtained in FLUKA by calculations that assume the energy deposition spectrum of the detector follows Poisson statistics.

If the mean number of scintillator events generated is $\overline{N}$, the standard deviation (σ) is given as [8]:

$$\sigma = \sqrt{\mathrm{N}} \tag{1}$$

The standard deviation can be also described in terms of deposited energy as follows:

$$\sigma(E) = \sqrt{E_m} \cdot \sqrt{E_{avg}} \tag{2}$$

Where E_{m} is the smallest energy value measured by the FLUKA simulation (1 keV), and E_{avg} is the average energy deposited in the crystal for a given scintillation pulse.

The response function is approximately Gaussian in shape. The FWHM for a Gaussian distribution is given by:

$$FWHM = 2\sqrt{2\ln 2} \, . \, \sigma \tag{3}$$

The energy resolution (R) is often expressed as a percentage and evaluated using the following formula:

$$R = \frac{FWHM}{E_0} \, . \, 100 \tag{4}$$

Where E_0 is the energy of the photopeak.

The Gaussian distribution fits for the photopeak in the simulated spectra were made with MATLAB version R2022a using σ values calculated from (2).

III. Results and Discussion

A. Determination of Energy Resolution

In this work, the energy resolution and FWHM values calculated for the 59.5 to 661.7 keV energy range are given in Table II.

The calculated results were compared with experimental results obtained, using Am-241, Ba-133, and Cs-133 radiation sources listed in Table I.

The photon pulse height distribution, the energy resolution, and other effects related to the SiPM detector have not been considered in the FLUKA simulation. The obtained values by the FLUKA simulation were converted to a real detector response using the sigma values calculated theoretically.

The broadening of the photopeak expected is not included in the spectra obtained by the DETECT card in FLUKA due to one of the main factors impacting the broadening coming from the electronic circuit used for the detector [1, 4].

Fig. 2. (b), (d), and (f) show the simulated photon spectra for YSO:Ce crystal with SiPM and without resolution correction for 662, 356, and 59.5 keV, respectively while Fig. 2 (a), (c), and (e) show the actual radiation spectrum obtained by experiment.

In the experimental results, the energy resolution (FWHM) for an electron energy (E) was obtained using the following equation by assuming the square root of the energy dependency:

$$FWHM = \frac{FWHM_0}{\sqrt{E/E_0}} \tag{5}$$

Table II. Comparison of Energy resolution and FWHM

Energy (keV)	FLUKA FWHM (Calculated)	FLUKA Energy Resolution (R%)	Experimental Peak Energy (keV)	Experimental FWHM	Experimental Energy Resolution (R%)	Difference in Energy Resolution (R%)	Relative Difference (RD%)
59.5	19.04	32.0	48	15.3	31.8	0.2	0.6
81.0	21.60	26.7	70	18.6	26.5	0.2	0.7
356.0	31.02	8.7	354	33.9	9.5	0.8	8.4
661.7	43.70	6.7	660	48.8	7.4	0.7	9.4

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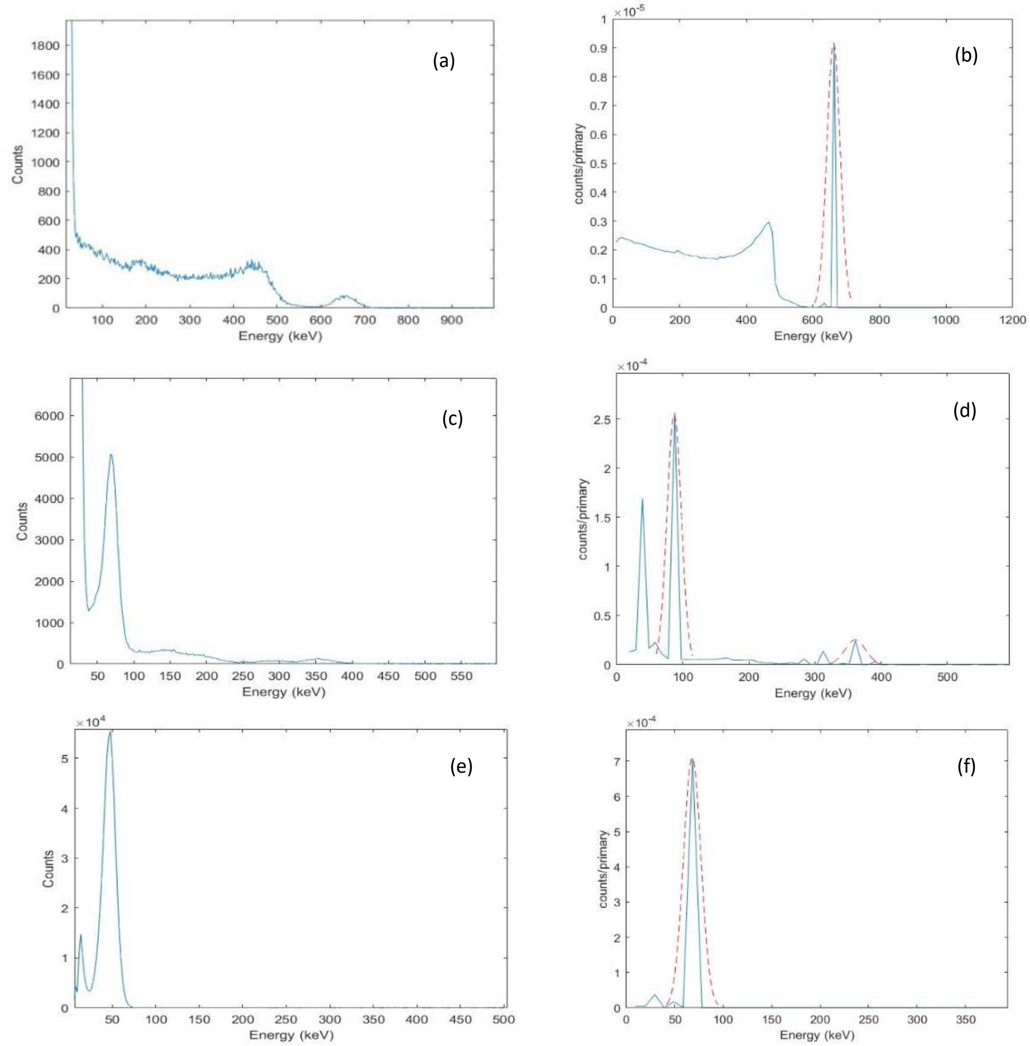

Fig. 2. (a) Measured Cs-137 spectrum, (b) simulated spectrum for Cs-137, (c) measured Ba-133 spectrum, (d) simulated spectrum for Ba-133, (e) measured Am-241 spectrum, (f) simulated spectrum for Am-241. The blue line in each plot represents the spectrum generated by the DETECT card and the red dotted line indicates the spectrum generated after adding calculated sigma values.

Where E_0 is the peak centroid respectively for the peak width of the source.

The energy resolution and FWHM values obtained for the 59 to 661.7 keV peaks in the experimental results are also given in Table II.

B. Comparison of Experimental and Simulation Results

In comparison with the experimental data, a small discrepancy in energy resolution can be seen at 356 and 661.7 keV as shown in Fig. 3. This may be due to the fact that in the simulation data there are no photons scattered by the surrounding material.

The relative difference (RD%) between the resolution calculated from FLUKA (A) and the resolution obtained by experimental results (B), were determined using the following equation:

$$RD\% = \frac{A-B}{B}.100 \qquad (6)$$

It is observed from Table II that the FLUKA results are in good agreement with experimental results, although there is a small discrepancy (<10%) observed in energies above 356 keV.

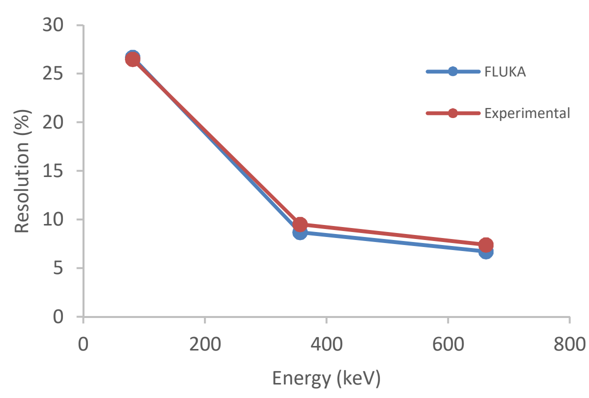

Fig. 3. Energy resolution comparison.

In this study, the simulation value for the energy resolution at 661.7 keV is 6.7% while the obtained value from experimental results is 7.4%. As it is known, the simulation

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uncertainties are small and only statistical. The simulation program was run with 10^8 primary particles for each isotope.

IV. Conclusion

In this study, a 5×5×5 mm^3 YSO:Ce detector was modelled using the FLUKA Monte Carlo code. The simulation parameters and information related to the FLUKA code used have been presented in detail. The pulse height distributions of a YSO:Ce detector were obtained for each point gamma source in the energy range 59.5 to 661.7 keV, and the energy resolution was calculated. Relative percentage differences between the experimental and simulation results are less than 10%.

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Data Access Statement

Supplementary data to this article can be found online at DOI: 10.6084/m9.figshare.20521047.

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