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Energy and resolution calibration of NaI(Tl) and LaBr₃(Ce) scintillators and validation of an EGS5 Monte Carlo user code for efficiency calculations

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ABSTRACT

The radiation detectors yield the optimal performance if they are accurately calibrated. This paper presents the energy, resolution and efficiency calibrations for two scintillation detectors, Nal(Tl) and LaBr₃(Ce). For the two former calibrations, several fitting functions were tested. To perform the efficiency calculations, a Monte Carlo user code for the EGS5 code system was developed with several important implementations. The correct performance of the simulations was validated by comparing the simulated spectra with the experimental spectra and reproducing a number of efficiency and activity calculations.

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1. Introduction

Scintillation detectors, with a special emphasis on the Nal(Tl) detectors, have been broadly used in many fields over the last 50 years [1]. Recently, the new lanthanum-based scintillators have become commercially available [2]. Compared with the Nal(Tl) detectors, the lanthanum detectors have better scintillation properties, including energy resolution, temperature performance, decay time, light yield and material density [2]. All of these capabilities make lanthanum detectors good candidates to substitute the Nal(Tl) scintillators in most applications.

Nonetheless, the correct performance of all radiation detectors requires the correct calibration. When the scintillation detectors are used for gamma spectrometry, the calibration procedure can be divided into three sub-calibrations [3]: the energy calibration, the resolution calibration and the efficiency calibration. These calibrations make it possible to correctly identify and determine the activity of the involved isotopes.

However, while the energy and the resolution calibrations are easily performed experimentally, the efficiency calibration can be a demanding task, especially for complex and extended source geometries. Thus, a common approach to perform the efficiency calibration is to use the Monte Carlo (MC) simulation techniques, which must be experimentally validated at least for the simple source geometries. This validation enables one to extrapolate the simulations to obtain the efficiency curves for other sources that would be difficult or impossible to obtain in a laboratory.

In this study, we perform the energy and the resolution calibrations for the Nal(Tl) and LaBr₃(Ce) scintillators, and we test several fitting functions used in both calibrations. For the efficiency calculations, we present an MC user code, which is validated with certified calibration sources. The details of the more important implementations of the MC code are also discussed.

2. Materials and methods

2.1. Experimental setup

The detectors used in this study were a $2'' \times 2''$ Nal(Tl) and a $2'' \times 2''$ LaBr₃(Ce) scintillation detectors. The Nal(Tl) detector was an ORTEC[®] Model 905-3 and the LaBr₃(Ce) detector was a BrilLanCeTM380 from Saint-Gobain Crystals. Both detectors were coupled to a preamplifier (ORTEC[®] Model 276) and an amplifier (ORTEC[®] Model 575A), which were connected to a multichannel pulse-height analyser ORTEC[®] TRUMPTM-PCI-2k. The spectrum analysis software that we used was ScintiVisionTM from ORTEC[®].

The experimental data were obtained from five radioactive sources that allowed the coverage of all gamma energies up to 1408 keV. Table 1 shows the current activity (deduced from the

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 Table 1

 Radioactive sources used in this study with their current activity and their active dimensions.

Radionuclide	Current activity ^a (kBq)	Source shape	Active dimensions (mm)
²⁴¹ Am	3.2 ± 0.3	Squared	Side=55
¹³³ Ba	1.0 ± 0.1	Circular	Radius=47
¹³⁷ Cs	4.0 ± 0.4	Circular	Radius=0.5
⁶⁰ Co	1.40 ± 0.14	Circular	Radius=1.0
¹⁵² Eu	Unknown	Unknown	Unknown

^a At the time of measurement.

certifications) and the active dimensions of each source. In all measurements, the background spectra were subtracted. The data related to the decay, the energies and the emission probabilities were taken from [4].

2.1.1. Energy calibrations

The energy calibration consists of establishing a relationship between the channels C and the corresponding gamma-ray energies E in the spectrum. Because this relationship is not always linear [5], as expected, its nonlinearity may produce inaccuracies in the determination of the peak energies and the comparison of real spectra with the MC simulations. This nonlinearity is produced as a consequence of the different uncertainties introduced in the measured energies that come from the different processes involved in the detection of gamma-rays [1].

Thus, the relationship between the energy *E* and the peak position *C* should be extended to a polynomial with n > 1:

$$E = \sum_{k=0}^{n} a_k \cdot C^k \tag{1}$$

where *n* is the degree of the polynomial.

2.1.2. Resolution calibrations

The non-proportional light response in scintillation detectors is the main cause of the limited energy resolution [1,6-8]. This limitation makes it necessary to perform a peak width calibration, which establishes a correspondence between the peak width and its energy. Resolution calibrations are necessary as an input not only for the peak-analysis software but also for the MC simulations to obtain realistic spectra. Because the peak width is often given by the Full Width at Half Maximum (FWHM), this calibration establishes the dependence of the FWHM on the energy *E*, i.e., it sets the function FWHM(*E*). However, there is no consensus in the literature on the mathematical form of this function. Thus, we tested several functions to identify one that provides the best fit (see Table 3).

2.1.3. Experimental efficiency calibrations

The relationship between the number of counts under a peak and the activity of a radioactive source is set by the efficiency calibration. Whereas the two previous calibrations only depended on the gamma-ray energy, the efficiency calibration depends on many other factors, such as the source-to-detector distance, the source geometry and the materials surrounding the setup. Consequentially, the efficiency calibration is only valid for identical calibration and measuring conditions.

If the efficiency calibrations are performed with certified sources, the experimental efficiencies ε_{exp} are calculated using the following equation:

$$\varepsilon_{\exp} = \frac{N}{A \cdot t \cdot p} \tag{2}$$

where N is the number of net counts under the full-energy peak, A is the known radionuclide activity, t is the counting time and p is the emission probability of the particular gamma-ray being measured.

The uncertainty propagation gives the following equation for the efficiency uncertainty $\delta \varepsilon_{exp}$:

$$\delta \varepsilon_{\exp} = \varepsilon_{\exp} \sqrt{\left(\frac{\delta N}{N}\right)^2 + \left(\frac{\delta A}{A}\right)^2 + \left(\frac{\delta p}{p}\right)^2} \tag{3}$$

2.2. Monte Carlo simulation

The MC simulations were performed with the EGS5 code system [9]. This general-purpose package enables the simulation of the coupled transport of electrons and photons in an arbitrary geometry. The EGS5 subroutines are controlled by a user code, which must be written in Fortran 77. The user code must contain all of the information about the radiation source (the type of particles, the energy and the probabilities of emission, the position and the geometry, the direction of emission, etc.) and the detector geometry (the components, the sizes, the materials, etc.). In addition, the user code must contain all of the calculations related to the quantities to be obtained.

In this study, we were interested in reproducing real gammaray spectra and performing the efficiency calculations. A user code for EGS5 was prepared for this purpose, where the radioactive isotopes comprising the emitting source were modelled through their gamma emission energies and associated probabilities. The source spatial distribution and the emitting directions are set in each simulated history (i.e., in each simulation of the primary source-particles and all of the secondary particles produced by it). Thus, it is possible to define extended sources that emit in the desired directions. Meanwhile, the geometry where the radiation interacts was defined using the combinational geometry package [9], which allows the definition of multiple geometries by combining 14 elemental bodies.

Fig. 1 shows the geometry of the Nal/LaBr₃ detectors. The dimensions were adapted to the manufacturer technical specifications. Basically, the geometry was modelled with the corresponding scintillation crystal with a case of 0.5 mm of aluminium. The space between the case and the crystal was filled with air. A glass light guide after the crystal was also considered, and the photomultiplier tube was modelled as a filled-of-air cylinder of aluminium. The material information (density and composition) were taken from [10], and the cut-off energy for the photons and the electrons was set at 10 keV.

2.2.1. Simulation of gamma-ray spectra

When some energy E' is deposited into the detector, a count in the corresponding channel of the spectrum is recorded. However, the gamma-ray spectra obtained in the simulations are very



Fig. 1. Cross-section of the detector geometry used in the simulations. The modelled parts are: scintillation crystal (green), aluminium (grey), glass light guide (red) and air (yellow). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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