MONTE CARLO SIMULATION OF THE IBA END-STATION'S GAMMA SPECTROMETRY SYSTEM OF THE 3 MV TANDETRON ACCELERATOR AT IFIN-HH

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Abstract. The quality of the results of the experiments planned at the Ion Beam Analysis (IBA) end-station of the 3 MV Tandetron accelerator at IFIN-HH depends critically on the accurate evaluation of the detectors efficiency. A reliable tool for calculating the efficiency is the Monte Carlo simulation, which can be applied to determine parameters difficult to evaluate using calibration sources. Monte Carlo simulation is more flexible than experimental calibration and can provide a realistic simulation of complex configurations. In this work, the PENELOPE simulation code was employed for the calibration of the gamma-spectrometer of IBA. In a first step we have expanded the capabilities of the `penmain` steering program. Then the geometry of the beam-line, gamma-ray detector and reaction chamber assembly was implemented and the HPGe crystal shape and size was optimized in respect to the experimental data. Realistic spectra were simulated and analyzed with the same tools and methods as the experimental spectra. Comparison of the simulation results with the experimental data validates the simulations, which will be used further on for a comprehensive calibration of the spectrometer.

Key words: Monte Carlo simulation, PENELOPE, gamma-ray spectrometry, germanium detectors, detector efficiency.

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1. INTRODUCTION

In 2012, at the Horia Hulubei National Institute for Physics and Nuclear Engineering, began the installation of a new Cockcroft–Walton 3 MV Tandem Accelerator [1]. The main application of the accelerator is material characterisation, and, for this purpose, the accelerator has been fitted with three dedicated end-stations, one for Ion Implantation, one for Cross Section Measurements (CMS) and one for Ion Beam Analysis (IBA).

The IBA end-station is designed for elemental analysis, achieved through one of the following methods: PIXE and μPIXE - Particle Induced X-ray Emission, PIGE

- Particle Induced γ-ray Emission, RBS - Rutherford Backscattering Spectrometry, ERDA - Elastic Recoil Detection Analysis and NRA - Nuclear Reaction Analysis. This type of analysis depends critically on an accurate evaluation of the detectors efficiency. A complete efficiency calibration of the gamma spectrometry system by purely experimental methods is impossible. The available calibration sources have limited geometries and contain few nuclides, thus the experimental calibration doesn't have the flexibility and extension necessary to cover all the situations of interest.

A reliable tool for calculating the efficiency is the Monte Carlo simulation [2], which can be applied to solve difficult calibration problems. Monte Carlo simulation is more flexible than experimental calibration and can provide a realistic simulation of complex configurations.

From all the Monte Carlo programs of general use in this field PENELOPE [3] is seeing an increased usage [4–6]. In order to apply PENELOPE for a particular problem, the user has the task of implementing the geometry model of the experiment and of specifying the problem (*i.e.* defining the source, the detection medium).

In this context, this paper anticipates the need for the characterisation of the efficiency of IBA's spectrometry system and provides a first solution to the problem, with the possibility for the expansion of the model in view of a more realistic calibration in future complex experimental configurations.

2. THE DEVELOPMENT OF THE `penmain` PROGRAM

For the present paper the PENELOPE Monte Carlo code was employed to perform the simulation of the IBA end-station and of Tandetron's gamma spectrometry system for the first time. Also, for further applications, an extension of the `penmain` code was realised, in order to simulate the coincidence-summing effects, while preserving the functionality of the `penmain` program. The extension will prove important when measuring nuclides with complex decay schemes, in the case of a high detection efficiency. For this purpose, the `penmain` code was programmed to tally the deposited energy of two particles emitted in cascade, as well as the individual spectrum of each particle (*i.e.* as if coincidence-summing effects were negligible), enabling thus the computation of the coincidence-summing correction factor.

`penmain` is a program written in Fortran and it has approximately 3600 lines of code. To preserve the way the program is initialized, in the input file, where the monoenergetic source is defined, a second energy, needed for the simulation of the coincidence-summing effects, has been added. In the code, in the section where the radiation source definition is read, a new variable has been declared and the maximum energy required for constructing the material database was re-evaluated. At the beginning of the shower, before sampling the coordinates of the emission point and

the direction of photon momentum, four new variables have been declared. Three of them are used to retain the coordinates of the emission point (information required when simulating coincidence summing effects in a volume source [7]), while the fourth is used as a counter. Before tallying the deposited energies in the detectors declared in the input file, the value of the counting variable is tested. If it has the
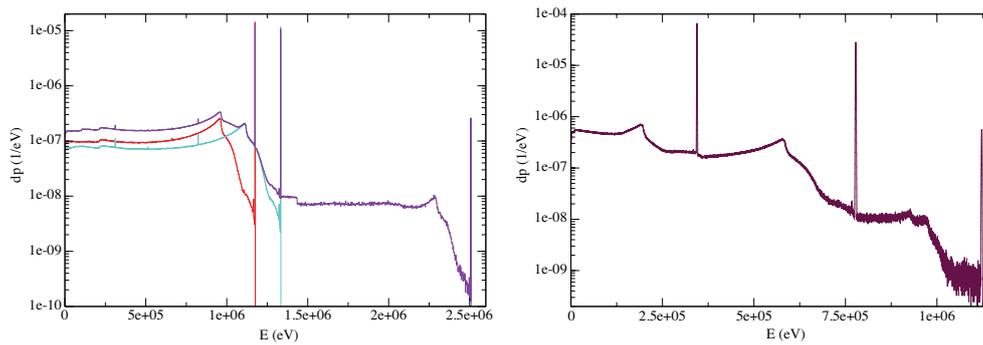

Fig. 1 – (Color online) On the left: The spectra of a simulated ^{60}Co point source. On the right: The simulated spectrum for the 778 and 344 keV photons of ^{152}Eu.

original value, this value is increased by one unit and the program begins to simulate a new particle with an energy equal to the second energy. This is accomplished without incrementing the number of simulated events, and by starting the simulation of the track from the same position as the first particle, but on a randomly sampled direction. The spectrum that has been obtained by simulating a point source of ^{60}Co, that emits the 1.173 and 1.332 MeV photons in cascade, detected with a coaxial detector enclosed in an aluminium endcap, is showed in Fig. 1.

To calculate the coincidence-summing correction factor we also need the spectrum of each individual particle, in the absence of the coincidence-summing effects. These have been obtained by saving in a vector the energy deposited in the detectors body by the first simulated particle and, after the simulation of the second particle, by subtracting this energy from the total deposited energy, obtaining thus the three necessary spectra. In order to preserve the functionality of the `penmain` program, *i.e.* the ability of resuming from where it was interrupted, two vectors have been added to the code, vectors that store the additional spectra. In Fig. 1 the most striking feature is the presence of the pure sum peak at the energy 2.505 MeV, which is not associated with a photon emission with the same energy, but also the decrease, due to the coincidence-summing effects, of the full-energy peaks at 1.173 and 1.332 MeV, can be observed.

To simulate realistic spectra, the implementation of the detector resolution was

required. To accomplish this, the widths of the measured peak were fitted with [8]:

$$f(x) = \sqrt{a_0 + a_1 \cdot x}, \tag{1}$$

where x is the energy corresponding to the peak and $f(x)$ is the full width at half maximum (FWHM). The values of the a_0 and a_1 are read from the input file of the `penmain` program, these parameters being added at the beginning of the file. Using the relation between FWHM and the standard deviation σ of the distribution of counts in the peak, assumed of gaussian shape, and by generating a gaussian distribution with the formula [9]:

$$y = \sqrt{-2 \cdot \ln(Rand_1)} \cdot \cos(2\pi \cdot Rand_2), \tag{2}$$

where $Rand_1$ and $Rand_2$ are two random generated numbers, the energy becomes:

$$E_s = E_d + \sigma \cdot y, \tag{3}$$

where E_d is the deposited energy. This is computed before the deposited energy is tallied, thus achieving a correct counting of the spectra. The spectrum in which the detector resolution can be observed, simulated for a point source that emits in cascade the 778 and 344 keV photons of ^{152}Eu, is represented in the right panel of Fig. 1.

3. THE DEFINITION OF THE GEOMETRY

Whereas the full-energy peak efficiency, in the absence of the coincidence-summing effects, depends only on the source, on the detector and on the materials located between the two of them, in the cases when the coincidence-summing effects come into play the whole geometric configuration becomes important. The radiation scattered from the materials that are not necessary interposed between the source and the detector can contribute to the coincidence-summing effects, implicitly to the value of the detection efficiency. Also, to determine the detection limit it is necessary to know the number of signals from the Compton region of the spectrum, region to which all the radiation scattered from the materials located in the vicinity of the source and of the detector contributes. Therefore in the general case it is not sufficient to include in the geometry definition only the source, the detector and the materials interposed between them, but it is necessary to completely describe the geometry and to simulate the complete spectrum.

In view of the above, a complex and realistic model of the experimental installation was defined and implemented - beam line, γ-ray detector, end-station. This geometry definition includes all the elements essential for a precise simulation, the quadrupole lens, the target holder and the detector. These complex elements of the

geometry have been defined in separated files. All of them were defined using the z-axis symmetry, and all the surfaces (except the cylinders) were defined south of the origin of the geometry coordinate system. The center of the station is placed in the origin of the final geometry. This method of constructing the geometry has enabled a more convenient procedure for placing the element in the final position, including its rotation and translation. In each external definition file, after the definition of the element, a module containing the element has been defined, rotated and placed in the position that it would occupy in the actual configuration.

The module defined to contain the detector enables the control of the distance between the detector and the target holder by adjusting only his position on the z-axis, the central symmetry axis of the definition file.

The elements were not created in a random order. The structure of the geometry used in PENELOPE demands that the bodies are defined in "ascending" order. For example, the wall of the chamber cannot be defined before defining the quadrupole lens and the detector, also, the space inside cannot be defined before defining the target holder.

The definition of the final geometry began from the top of the chamber, after which the quadrupole lens, the detector and the target holder definitions have been included, one by one, in the complete geometry definition file using the "INCLUDE" option available in the PENELOPE code. After the inclusion of each element, the file was read with the GVIEW2D program, and the output file, `geometry.rep`, was edited into a new definition file before including the next element.
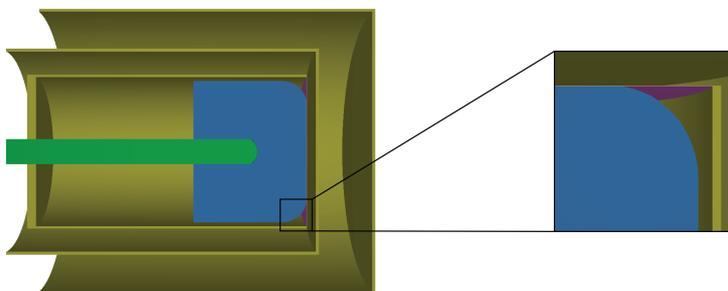

Fig. 2 – (Color online) The detector as rendered by the GVIEW3D program.

A difficult task of geometry modelling was the description of the rounding of the HPGe crystal. It was achieved by joining successive spherical surfaces, in the following way. First a sphere was defined at the edge of the crystal, to serve as a visual guide. Then, using the GVIEW2D program, the head of the crystal was cut with a spherical surface, smoothly connected with the first. The procedure was repeated until a very good representation of the actual shape of the rounded edges

was obtained. This procedure, which is original, is more realistic and superior to the procedures adopted in other papers published in the field, such as a succession of cylindrical surfaces, a truncated cone, a step-wise or even a straight cut [10–12]. The outer surface of the dead layer of the detector was approximated with the same method.
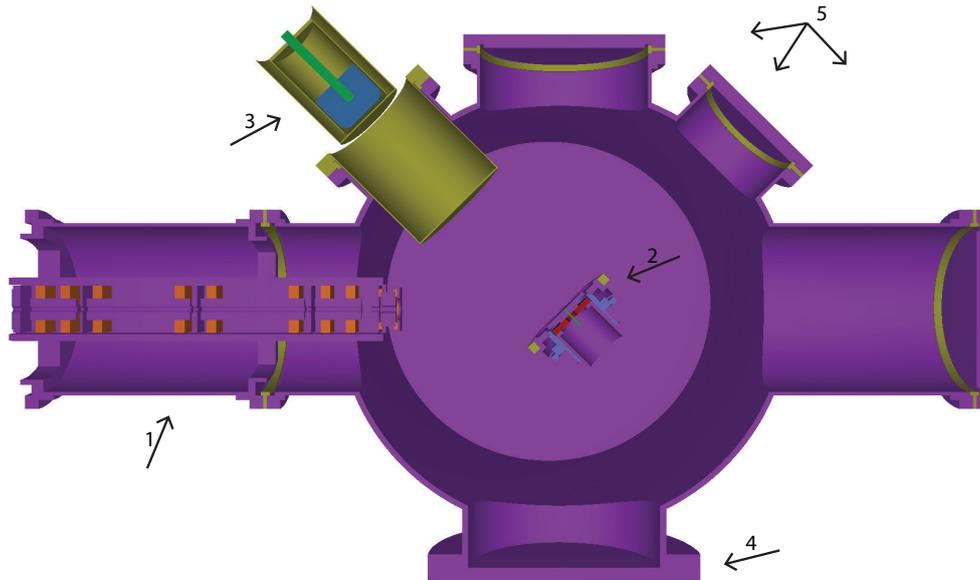

Fig. 3 – (Color online) Horizontal section of the IBA station geometry: 1 - beam line and quadrupole lens, 2 - target holder, 3 - detector, 4 - chamber door, 5 - extensions.

As it often happens in the Monte Carlo simulations of the germanium detectors, it was necessary to optimise the detector parameters in order to reproduce by simulation test experimental values of the efficiency. The parameters that made the object of the optimisation were the dimensions of the crystal and the thickness of the dead layer. The fact that the detector geometry was defined in a separated file proved to be extremely useful, *i.e.* the adjustments were done in the definition file of the detector, then the values were transferred to the definition of the complete geometry. In the first simulations, using detector dimensions taken from the detector specification sheet, the computed values of the full-energy peak efficiency were up to 20% bigger than the experimental values. The computed and the simulated values were in accordance when the crystal radius was decreased by 2 mm. For obtaining simulated values of the efficiency close to the experimental values at low energies, it was necessary to increase the thickness of the dead layer with 0.7 mm. Of course, each time when the crystal radius was modified, the procedure to describe the rounding of the detector was repeated.

After the optimisation, the Monte Carlo simulation can be applied to calculate the detection efficiency for measurement conditions that make the experimental calibration impossible. On this basis, a calibrating procedure, employing Monte Carlo simulation of the detection efficiency of the installation's spectrometry system, was developed.

4. DATA ANALYSIS

After the definition of the experimental installation's geometric model, a point source of ^{152}Eu was simulated. To compare the results of the simulations with the measured data for a point source of ^{152}Eu, the `penmain` program was extended to include the detector's experimental resolution. By these means, realistic spectra were simulated and analysed with the same programs as the measured spectra, in order to lower the uncertainty induced by the way the data is analysed.

36 simulations were done (12 energies at three detector-source distances - 15.1, 19.6 and 24.4 cm) with $2 \cdot 10^9$ showers for each simulation. The time necessary for these simulations was around 120 hours. The initial tests, in which the dimensions and the shape of the crystal were adjusted, were run with an absorption energy (for all the particles) of 1 keV; this is the energy limit below which the particle is locally absorbed. In order to lower the simulation time in the runs carried out for obtaining the ^{152}Eu spectrum, an absorption energy of 100 keV was employed for electrons and positrons in all the materials that where not found in the definition of the detector and of the detector holder, obtaining thus a simulation speed up to 10 times greater.

The measured and simulated spectra were analysed with `track`, part of the `GASPware` package [13]. The counting rate was determined by subtracting the background and fitting the peaks with a gaussian shape.

The realistic spectrum was constructed with the help of a small computer code, written in Fortran, using the formula:

$$R(E) = \sum_{i=1}^{12} \Lambda \cdot t \cdot I_i \cdot \eta_i(E), \qquad (4)$$

where Λ is the activity of the ^{152}Eu source at the time of the measurements, t is the live time, I_i is the intensity of the photons with the energy i and $\eta_i(E)$ is the normalized spectrum simulated for the i-th photon emitted by ^{152}Eu. The ^{152}Eu simulated spectrum is represented in Fig. 4, on top of the measured spectrum. The difference between the two spectra, visible in the figure, is due to the fact that only the twelve most intense photon emissions were simulated. The difference in the high energy region is due to the absence of simulated energies above 1408.013 keV, while in the low energy region it is primarily due to the absence of simulated X-

rays emitted by the source, and also to the missing contribution of the low intensity gamma photons that were not simulated.
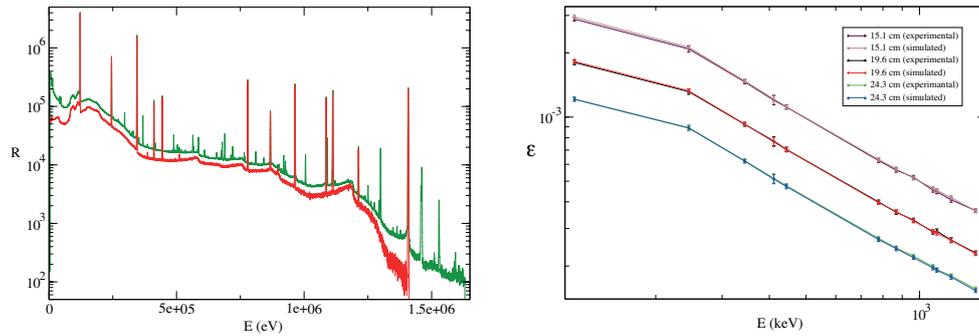

Fig. 4 – (Color online) On the left: The measured spectrum (green) and the simulated spectrum (red). On the right: The simulated and the measured efficiencies, the lines are drawn to guide the eye.

The simulated spectra were tallied in the same energy interval and using the same number of channels (8192), as in the case of the measured spectra. The measured and the simulated efficiency of the gamma spectrometer of the IBA end-station, represented in Fig. 4, are in very good accord.

5. CONCLUSIONS

In the present paper, for the first time, a general procedure to simulate the IBA end-station's gamma spectrometry system was developed and tested. The simulation includes all the details of the experimental setup, the detector resolution and the possible coincidence-summing effects.

The `penmain` program was extended to simulate two particles emitted in cascade and the detector's experimental resolution. The geometric model of the end-station was defined in PENELOPE, the beam-line, gamma-ray detector and reaction chamber assembly. The crystal parameters were adjusted in order to obtain a good agreement between the simulated efficiencies and test experimental values. The crystal rounding was implemented as a succession of spheric surfaces, which is a more realistic description of the crystal curvature than that applied in other works. All these features enabled a realistic simulation of the spectra, that can be analysed with the same programs as the measured spectra, limiting thus the uncertainties of the simulation results.

REFERENCES

1. D.G. Ghiţă *et al.*, *Modernizations and developments of the tandem accelerators in IFIN-HH*, EuNPC2012, 17-21 September, Bucharest, Romania (2012).

2. O. Sima, *Efficiency Calculation of Gamma Detectors by Monte Carlo Methods* in *Encyclopedia of Analytical Chemistry* (John Wiley & Sons, 2012).

3. F. Salvat *et al.*, *PENELOPE-2008: A Code System for Monte Carlo Simulation of Electron and photon Transport*, Workshop Proceedings, Barcelona, Spain, 30 June-3 July (2008).

4. E. García-Toraño, M. Pozuelo, F. Salvat, *Monte Carlo calculations of coincidence summing corrections for volume sources in gamma-ray spectrometry with Ge detectors*, Nuclear Instruments and Methods, A **544** (2005) 577–583.

5. J. Plagnard, J. Hamon, M. C. Lepy, *Study of scattering effects in low-energy gamma-ray spectrometry*, Applied Radiation and Isotopes **66** (2008) 769–773.

6. K. Agrafiotis, L. Karfopoulos, M. J. Anagnostakis, *Calibration of an in-situ BEGe detector using semi-empirical and Monte Carlo techniques*, Applied Radiation and Isotopes **69** (2011) 1151–1155.

7. D. Arnold, O. Sima, *Total versus effective total efficiency in the computation of the coincidence-summing corrections in gamma-ray spectrometry of volume sources*, Journal of Radioanalytical and Nuclear Chemistry **248** (2001) 365–370.

8. G. Gilmore, *Practical Gamma-ray Spectrometry* (2nd end. ,Wiley, 2008).

9. O. Sima, *Simularea Monte Carlo a transportului radiaţiilor* (Bucureşti, ALL, 1994).

10. R.G. Helmer *et al.*, *The use of Monte Carlo calculations in the determination of a Ge detector efficiency curve*, Applied Radiation and Isotopes **67** (2009) 2057–2061.

11. T. Vidmar and J. Gasparro, *Crystal rounding and the efficiency transfer method in gamma-ray spectrometry*, Nuclear Instruments and Methods in Physics Research A **511** (2003) 360–381.

12. N.C. Díaz and M.J. Vargas, *Improving the trade-off between simulation time and accuracy in efficiency calibrations with the code DETEFF*, Applied Radiation and Isotopes **68** (2010) 1413–1417.

13. D. Bazzacco and N. Mărginean, *Private Communication*, INFN Sezione di Padova, Italy (1997).