

## MONTE CARLO SIMULATION OF P-TYPE HPGe DETECTORS – THE DEAD LAYER PROBLEM\*

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*Abstract.* The Monte Carlo method is increasingly applied for simulation of germanium detectors. It can be successfully used for the evaluation of full energy peak efficiency or of the efficiency corrections due to self-attenuation, coincidence summing and geometry effects. Usually the simulation task is to evaluate the energy deposited in the sensitive volume of the detector, assuming that the detector signal is strictly proportional with this quantity. In this work it is shown that simulations of the energy deposition in a p-type HPGe detector for low energy photons, carried out with GEANT3 and PENELOPE, do not describe correctly experimental data that depend on the interactions taking place in the dead layer. Specifically, the effects of coincidence summing with low energy photons on peak shape and on coincidence summing correction factors, observed in the experimental spectra, are not reproduced by simulations. The reason is that the charge produced in specific regions of the dead layer is partly, but not completely, collected, and this fact is not taken into account in the simulations. A simplified procedure to avoid this problem is described, but the general solution requires the incorporation of the charge collection process into the simulation codes.

*Key words:* Monte Carlo simulation, GEANT 3, PENELOPE, germanium detectors, dead layer, detector efficiency, peak shape.

### 1. INTRODUCTION

Gamma-ray spectrometry is a highly appreciated multi-elemental analysis technique, currently applied in a variety of fields. Gamma spectrometry using germanium detectors is the best technique for identifying and quantifying radionuclides.

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This is due to the very sharply defined and characteristic energies of gamma-rays which are emitted by the great majority of radionuclides.

Accurate knowledge of detector efficiency appropriate to the specific measurement conditions of each sample is required in order to obtain high quality results. In view of the variety of these conditions (geometry of the measurement, sample type, volume and matrix) it is not possible to achieve a complete calibration purely on an experimental basis. Due to its flexibility, Monte Carlo simulation can be used to calculate the efficiency in cases in which experimental calibration is not available [1]. Sophisticated computer programs are currently available [e.g. 2–8] for the simulation of the detection process and on this theoretical basis for the computation of the full energy peak efficiency and of the total efficiency of the detector. The quality of the computed results depends on the quality of the input data and on the accuracy of various approximations that are applied in the physical model to take into account processes that are not fully simulated, such as charge collection.

The detector efficiency is strongly influenced by the thickness of any absorber layer surrounding the germanium crystal – especially the thickness of the inactive germanium layer, since the linear attenuation coefficient of the photons in Ge is high. In particular, the calculated full energy peak efficiency at low energies is very sensitive to the thickness of the germanium dead layer adopted in the computation. But the properties of the dead layer can be important also for higher energy peaks, for example in the case when the photon responsible for that peak is accompanied in the decay process by X-Rays. Accurate measurements and computations have shown [9] that in specific cases apparently it is not possible to describe simultaneously the low energy peak efficiency and the coincidence losses from peaks of higher energies with the same value of the thickness of the dead layer. Furthermore, in the case of p-type detectors, with a thick dead layer, the shape of the peaks affected by high coincidence summing effects with X-rays [9] cannot be reproduced by usual Monte Carlo simulations. Finally, the value of the total efficiency of a p-type detector, evaluated by Monte Carlo simulations, even in simple experimental conditions, underestimates the experimental value at low photon energies, if the thickness of the dead layer is chosen to obtain by simulation values of the peak efficiency close to the experimental data [10].

In this work a detailed study of the effects of the thickness of the dead layer on the peak efficiency  $\varepsilon(E)$ , total efficiency  $\eta(E)$ , as well as on the spectrum and peak shape in the presence of coincidence summing is presented. The study comprises simulations carried out for a measurement configuration for which experimental data have been published [9].

## 2. MONTE CARLO SIMULATIONS

The simulations have been done for a p-type closed end coaxial HPGe detector, with crystal radius 2.9 cm, length 5.9 cm; inner hole radius 0.5 cm and length 4 cm. The detector end cap is made from Al with a thickness of 0.1 cm, radius 7 cm and length 7 cm. The distance from end cap to crystal is 0.5 cm. The

detector system was supposed to have cylindrical symmetry. A set of values of the thickness of the dead layer were used in the detector model in order to observe the dependence of the simulation results on this parameter. A point source placed on the symmetry axis was considered.

GEANT 3.21 [2] and PENELOPE 2011 [7] were used. PENELOPE was developed more recently than GEANT 3.21 and has the following main features. Photon transport is simulated by means of the standard, detailed simulation scheme. Electron and positron histories are generated on the basis of a mixed procedure, which combines detailed simulation of hard events with condensed simulation of soft interactions. A geometry package called PENGEOM permits the generation of random electron-photon showers in material systems consisting of homogeneous bodies limited by quadratic surfaces, *i.e.* planes, spheres, cylinders, etc. In both cases, GEANT and PENELOPE, the programs were extended in order to include the spectral resolution and the evaluation of coincidence summing effects; a description of the extension in the case of the PENELOPE system of codes is given elsewhere [11].

Extensive computations were carried out with GEANT. A first run consisted in the simulation of the spectrum, the evaluation of the peak and total efficiency, for a set of energies between 30 keV and 3000 keV. For each energy, the simulations were carried out for several values of the thickness of the dead layer. In the second run coincidence summing effects were implemented. For each primary energy included in the first run, several values of the energy of the coincident photon were selected, spanning the same energy range. Preliminary results of these simulations have been presented elsewhere [12].

Less extensive simulations were carried out with PENELOPE [7], in order to check the GEANT simulations for test cases; this procedure was applied because simulations with GEANT 3.21 may have some problems, especially at low energies [13], while PENELOPE seems to be better tuned for simulation of germanium detectors.

As usually, in all the simulations the quantity finally evaluated for each simulated track was the energy deposited in the sensitive volume of the detector.

### 3. FULL ENERGY PEAK EFFICIENCY AND TOTAL EFFICIENCY

The full energy peak efficiency (FEPE)  $\varepsilon$  is defined as the ratio of the number of counts in the full-energy peak to the total number of gamma rays emitted from the source. It is roughly proportional with the solid angle subtended by the detector, and thus depends on the source-to-detector distance. Because photon interaction coefficients depend on photon energy, FEPE is a function of energy. In order to register a count within the full-energy peak it is necessary to collect all the charges produced in the detector when the complete energy of the photon was deposited in the detector, either as a single photoelectric interaction or as a multiple event. The total efficiency  $\eta$  is defined as the ratio of the number of counts in the integral spectrum due to the detection of events following the emission of photons from the source, and the number of photons emitted.

At low energies, the dependence of the efficiency on energy is dominated by the attenuation of the photons in the materials located between the photon emission point and the sensitive volume of the detector. In the case of detectors with a thick dead layer, the attenuation in this layer is usually the most important factor reducing the efficiency. As the thickness of the dead layer is not easily measured, frequently its value is fixed by adjustment in such a way as to reproduce by simulation the value of the FEPE at low energies [14].

In Fig. 1 the dependence of the efficiency curve on energy, obtained by simulations with GEANT 3.21, is represented for several values of the thickness of the dead layer. The particularly strong dependence on the thickness of the dead layer at low energies is obvious.

In Fig. 2 the same dependence is represented for the case of the total efficiency. Whereas many studies have been carried out for observing the effect of the thickness of the dead layer on the peak efficiency, comparatively few studies were devoted to the effect on the total efficiency. By detailed simulations carried out with MCNP, Dryak and his colleagues [10] observed that in the case of p-type detectors at low energies the simulated values of the total efficiency are significantly lower than the measured values if the thickness of the dead layer which gives a good accord between the simulated and the measured values of FEPE is used in the simulation. Furthermore, using a coincidence circuit, the same authors observed a dead layer signal, increasing the value of the total efficiency.

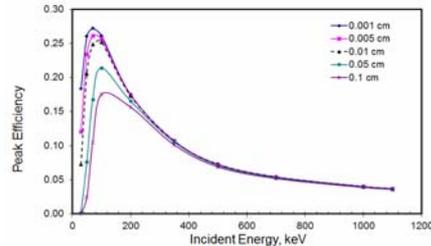


Fig. 1 – Peak efficiency curves for several values of the thickness of the dead layer (colored online).

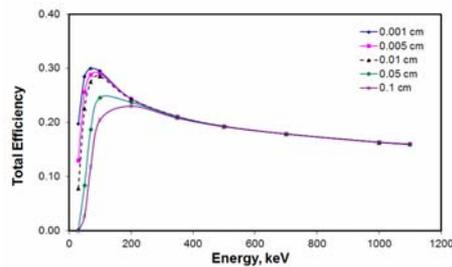


Fig. 2 – Total efficiency curves for several values of the thickness of the dead layer (colored online).

The strong dependence of the peak efficiency on the thickness of the dead layer is frequently used for fixing the value of this thickness in the Monte Carlo model of the detector. It should be mentioned that reliable data about the dead layer are hardly available either from the detector manufacturer or from direct measurement. The dependence of the total efficiency on the thickness of the dead layer is not so pronounced, but it is sufficiently strong to be observed in coincidence summing effects with low energy photons.

#### 4. PEAK SHAPE AND COINCIDENCE SUMMING EFFECTS

The spectra of sources emitting with high probability X-rays in coincidence with gamma photons, measured with a p-type detector, show distinctive features. Peaks corresponding to photons which are emitted together with X-rays have a specific tail in the high energy side of the peaks when measured in conditions enhancing coincidence summing effects. This feature was observed [9] in the measurement of point sources of  $^{133}\text{Ba}$  and  $^{152}\text{Eu}$  close to a p-type detector. Each peak from the spectrum of  $^{133}\text{Ba}$  presented the tail. However, in the spectrum of  $^{152}\text{Eu}$  only the peaks resulting from the electron capture decay presented the tail, whereas the peaks resulting from  $\beta^-$  decay had the typical symmetric shape. It should be mentioned that the gamma photons resulting from the electron capture decay are accompanied with high probability by X-rays, while the gamma photons from the other decay branch have low probability for being in coincidence with X-rays. The same measurements were repeated with an n-type detector. In this case all the peaks had the typical symmetric shape. Furthermore, if an absorber that stops the X-rays was interposed between the source and the detector, all the peaks, measured with both detectors, presented the typical symmetric shape.

In Fig. 3 the spectra (restricted to higher energies) of the  $^{133}\text{Ba}$  source measured with the p-type detector are represented. In Fig. 4 the spectra measured with the n-type detector are displayed. The tails are evident in the case of the measurement with the p-type detector without the absorber. The prominent peaks that are present only in the case of the measurement with the n-type detector without absorber are pure sum peaks due to summing effects between gamma photons and X-rays (see a complete description in [15]). The spectrum of  $^{152}\text{Eu}$  measured with the p-type detector in the absence of the absorber showed that the shape for the peaks corresponding to electron capture decay differs from the shape of peaks corresponding to  $\beta^-$  decay (see *e.g.* the comparison between the peak at 964 keV from the electron capture decay and the peak at 778 keV from  $\beta^-$  decay in Fig. 2 from reference [9]).

Clearly the asymmetric peak shape is due to coincidence summing effects between the gamma photons and the X-rays and also, that the asymmetry is present only in the case of the detector with a thick dead layer. The conclusion is that the asymmetric shape is due to coincidence summing effects between gamma photons and X-rays that have interacted in the dead layer. Considerations based on electron

range and X-ray interaction length [9] indicate that the shape cannot be explained as a result of the partial energy deposition in the sensitive volume due to photoelectrons originating in interactions taking place in the dead layer and ending their path in the sensitive volume. In order to check more rigorously this conclusion, detailed simulations with GEANT 3.21 and PENELOPE were carried out.

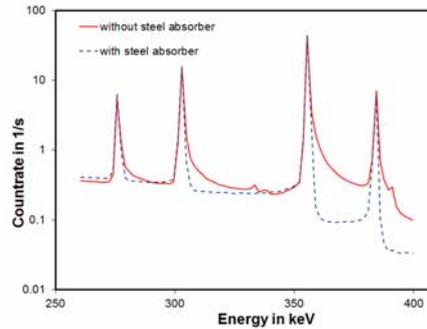


Fig. 3 – Part of the spectra of  $^{133}\text{Ba}$  measured with the p-type detector with and without a steel absorber of 1 mm thickness. The spectra were normalized to the same peak amplitude for 356 keV (colored online).

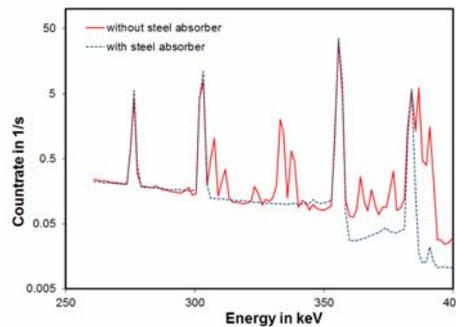


Fig. 4 – Same as Fig. 3, but in the case of measurements with n-type detector.

Both in GEANT 3.21 and in PENELOPE the simulation of the energy deposition due to coincident emission of photons was implemented. Also, for each case two spectra have been recorded. The first corresponds to the energy absorbed in the sensitive volume of the detector as given by the simulation. The second spectrum was constructed by replacing the absorbed energy  $E$  by a variable energy, selected randomly from a normal distribution with mean value  $E$  and standard deviation chosen so as to reproduce the experimental resolution of the detectors as a function of peak energy. The first spectrum is an ideal representation, whereas the second should be a realistic representation of the measured spectra.

The simulations have been done for each experimental case presented above. Simulated peak shapes describe well the experimental peak shape, with the

exception of the measurements with the p-type detector without absorber. In this case the high energy tail is missing in the simulation. As an example in Fig. 5 the shape of the peak of  $^{152}\text{Eu}$  at 964 keV (which presents the tail in the measured spectra) is represented for the case of p-type detector measurements, both in the presence and in the absence of the attenuator. The significant difference between the experimental peak shape in the two cases is missing in the simulation. Thus the tail cannot be explained by the energy deposited in the sensitive volume of the detector by the electrons produced by photon interactions in the dead layer and injected in the sensitive volume due to the initial momentum at the interaction point. The tail can be explained considering that a fraction of the charge carriers produced in the dead layer contributes to the detector signal, in contradiction with the common assumption in Monte Carlo simulation, that only the charge carriers produced in the sensitive volume of the detector contribute to the signal.

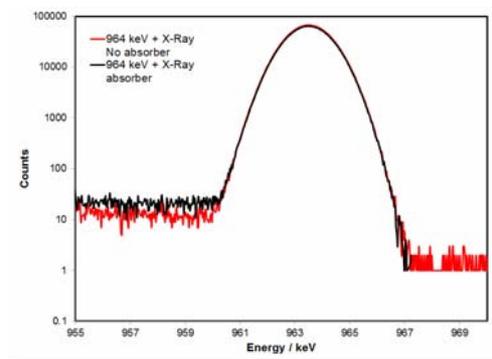


Fig. 5 – The shape of the peak at 964 keV of  $^{152}\text{Eu}$  simulated for the p-type detector in the presence of coincidence summing effects due to simultaneous emission of an X-Ray. Simulations made with PENELOPE. GEANT 3.21 simulations give similar results.

## 5. COINCIDENCE SUMMING CORRECTION FACTORS

Accurate values of the experimental coincidence summing correction factors (FC) [16] have been measured for the experimental cases considered above [9]. The values of FC were also obtained by simulation with GESPECOR, taking into account the detailed decay scheme of the nuclides [17]. In an initial set of computations the thickness (“nominal thickness”) of the dead layer which gives simulation results for the peak efficiency in accord with experimental values was used. The values of FC obtained in this case by simulation were in accord with all experimental values with the exception of the measurement with the p-type detector in the absence of the absorber. The computations were repeated for this case with different values of the thickness of the dead layer. In Fig. 6 the dependence of the correction factors on the ratio of the thickness used in the computation to the nominal value is presented.

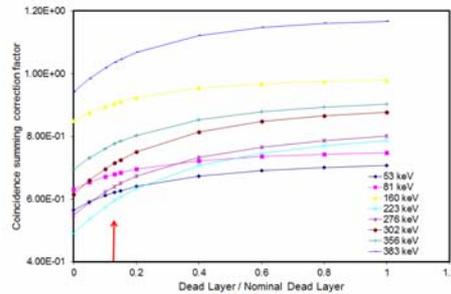


Fig. 6 – Coincidence summing correction factors as a function of the ratio of the thickness of the dead layer applied in the computation to the nominal value. P-type detector measurements without the absorber are considered. The arrow marks the value for which the simulated correction factors are in accord with the experimental values.

The results show that in the case of p-type detectors it is not possible to obtain by simulations both the peak efficiency and the coincidence summing correction factors due to low energy photons using a unique value of the thickness of the dead layer. The thickness of the dead layer that gives in the simulation correct values of the coincidence losses from the peaks should be significantly smaller than the nominal value. This behavior is due to the fact that a fraction of the charge produced in the dead layer can be collected, but not completely; then this event contributes to the total efficiency and coincidence losses effects, but not to the peak efficiency. In order to obtain correct results by simulation, the dead layer should be considered as composed from two domains, the nominal dead layer, from where the charge is incompletely collected, and a thinner domain, from where no charge contributes to detector signal. The nominal dead layer is useful for the evaluation of the peak efficiency, while the thinner domain for the evaluation of the total efficiency and of the coincidence losses from peaks. This idea is implemented in GESPECOR by the use of a reduction factor applied to the nominal thickness of the dead layer when total efficiency and coincidence losses from the peaks are evaluated; a more complex solution, proposed earlier, is more refined, but gives similar results [18]. The proposed procedures circumvent the need to describe the charge collection process in the simulation code, but the realistic solution would be to include this process in the simulation.

## 6. CONCLUSIONS

The dead layer of germanium detectors has a strong effect on the full energy peak efficiency and on the total efficiency. Monte Carlo simulations have been carried out to evidence this effect. The simulations produced both ideal spectra and realistic spectra, in which the experimental resolution was implemented. Two cases were considered, the emission of single photons and the coincident emission of two photons.

In addition to the effect on efficiency, in the case of p-type detectors and low energy photons, such as X-rays, in conjunction with coincidence summing, the dead layer produces specific effects on the peak shape and on the magnitude of coincidence summing corrections. Simulations with GEANT 3.21 and with PENELOPE cannot reproduce published experimental features. The difference between simulation and experiment can be due to partial charge collection from the volume of the dead layer. In order to obtain values of the coincidence summing correction factors in accord with experimental data in such cases, it is necessary to consider a complex structure of the dead layer. A simple solution of this problem is implemented in the GESPECOR software. However, the general solution would be inclusion of the charge collection process into the simulation codes.

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