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ABSTRACT

A Monte Carlo simulation has been developed using the Geant4 software to model the Compton suppression for a NaI detector and high-purity Germanium (HPGe) detector operating in anti-coincidence. Details of the implementation of detector geometries, energy resolution and suppression logic are described. The typical Compton suppression factor of 0.42 for a realistic detector configuration is reported here.

1. INTRODUCTION

Neutron activation analysis (NAA) is used to quantify the concentrations of around 60 different elements in a sample material [1]. It is both non-destructive of the sample and can reach sensitivities down to the parts-per-trillion. Often it is used in the design of novel detectors when searching for new physics occurring at energies on the order of 1 MeV. In this energy regime the background is dominated by natural radioactivity in the detector materials.

NAA involves a sample being placed in a neutron rich environment such as near the core of a nuclear reactor where the nuclei in the material absorb neutrons for some time. The various nuclei become unstable and undergo radioactive decay until stable. Following these decays “delayed” gamma rays are released which are of specific energies characteristic to the parent nuclide [2]. These are released with a half-life long enough that the material can be transported from the reactor to an HPGe detector to be analyzed.

The precision of these measurements is reduced in the lower energy region by the Compton continuums of each photopeak. The Compton continuum of a photopeak is the result of a photon interacting with an electron through Compton scattering and leaving the HPGe without depositing its full energy. The energy deposited is dependent on the angle of scattering and thus creates a continuous distribution of background before the photopeak (see FIG. 1) [3]. Its energy after the interaction is given by:

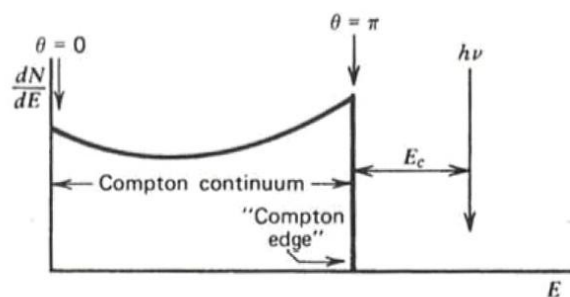


FIG. 1. Idealized Compton continuum, illustrating the relationship between the Compton edge and the photopeak. From Ref. [3].

$$E_{\gamma'} = \frac{E_{\gamma}}{1 + 2E_{\gamma}(1 - \cos \theta)} \quad (1)$$

where  $E_{\gamma}$  is the energy of the photon before the collision in MeV. In a head-on collision in which the photon is scattered opposite its original direction the equation is minimum:

$$E_c = \frac{E_{\gamma}}{1 + 4E_{\gamma}} \quad (2)$$

where  $E_{\gamma}$  has been replaced with  $E_c$  to represent the Compton energy (shown in FIG. 1). The detectable signal is produced by the recoiling electrons which, from conservation of energy, have an energy given by:

$$E_e = E_{\gamma} - E_{\gamma'} \quad (3)$$

Because the Compton photons scatter outside the HPGe crystal it is possible to remove their count in the histogram using a technique known

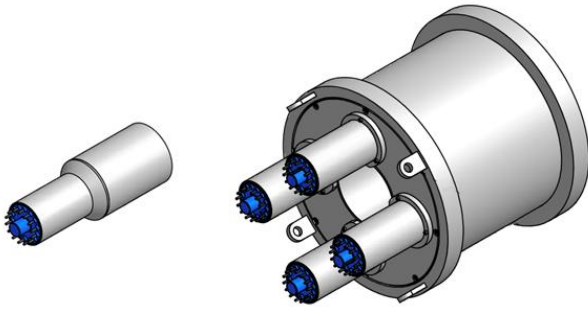


FIG. 2. Planned NaI shell detector apparatus. The HPGe crystal is placed within the hole in the shell (right) and then the NaI plug detector (left) to provide more coverage. The blue capped cylinders are PMTs. Image courtesy of Alpha Spectra, Inc.

as Compton suppression. The crystal is surrounded by an NaI detector shell. The planned NaI detector will also use a “plug detector” to plug the hole in the shell and provide more coverage (see FIG. 2). Counts measured by this shell can be linked to counts in the crystal based on the calibrated time between their coincidence. Once such a pair of counts has been identified it can be discarded. This simulation tests the effectiveness of different geometries and volumes of NaI.

## 2. METHODS

### 2.1. Operation of Geant4

The simulation was written using Geant4, a C++ package designed for Monte Carlo particle physics simulations. Geant4 has the benefits of having pre-built physics processes, particle types, and material types which can be implemented by defining them as part of the simulation. For example, in our simulation we define “low energy electromagnetism” and the simulation will calculate the proper interaction cross-sections for photons’ interaction with matter via the photoelectric effect, Compton scattering, or pair-production.

A run is defined as a full execution of the simulation with some given initial conditions. Each run is comprised of events, which are the emissions of individual gammas from the source in our simulation. Each event is then comprised of

individual steps that the particle takes as it passes through the material. The basic Geant4 simulation process is as follows:

1. The user defines the physics desired, the particles that will be simulated, the source of particles, the construction of the detector, and other initial conditions. (Note: each closed surface in the simulation is referred to as a “volume”).
2. A particle is generated with desired direction, energy, and other properties, at the particle source.
3. The distance along this direction to the end of the current object it is in is calculated (called a “step”).
4. This distance and the known cross-sections of the physical processes defined are used to determine the probabilities of interacting via those processes.
5. An interaction (or no interaction) is chosen randomly based on those probabilities.
6. The particle interacts, possibly generating secondary particles, losing energy, or exiting the current object.
7. Steps 3-6 are repeated for the primary and secondary particles until they have either exited the boundaries of the simulation or they have lost enough energy to not be tracked any longer (this completes one “event”).
8. The next particle is generated and steps 3-7 are repeated for it as well.
9. The process continues until all particles desired have been generated (called one “run”).
10. Track, particle, and energy deposition information from any stage of the simulation can be extracted then exported at the end of the execution of the simulation.

### 2.2. Modifications for our simulation

Our code extends this basic model to meet our specific needs:

- All particle categories except “short-lived” are defined as usable.
- Radiation transport, electro-magnetism, and decay processes are defined.
- The particle source was defined to be in the center of the NaI cylinder shell as a point source with random directions.
- For each step the energy deposition and length of the step are saved.
- For each event the total energy deposited and path length travelled in each volume is filled into a histogram for that volume.
- At the end of each run some calculations are performed on the collected data (RMS and average of energy deposited and path length, ratio of suppressed to unsuppressed continuum).

To test the effectiveness of different geometries of NaI we plan to rig the simulation to perform multiple runs with varying sizes and shapes of NaI and comparing the factor by which the continuum is suppressed. For now we have focused on implementing the basic functions of the simulation and improving its accuracy.

### 3. ADDED COMPONENTS

The following components have been added to the base code in this project:

- 3.1. Gaussian bin spreading
- 3.2. NaI geometry
- 3.3. Compton suppression mechanism
- 3.4. AutoCAD geometry

#### 3.1. Gaussian bin spreading

One inaccuracy of the simulation is that it fails to factor in fundamental sources of noise which produce the resolution (spreading) of the spectra of real gamma ray spectra. Because only the

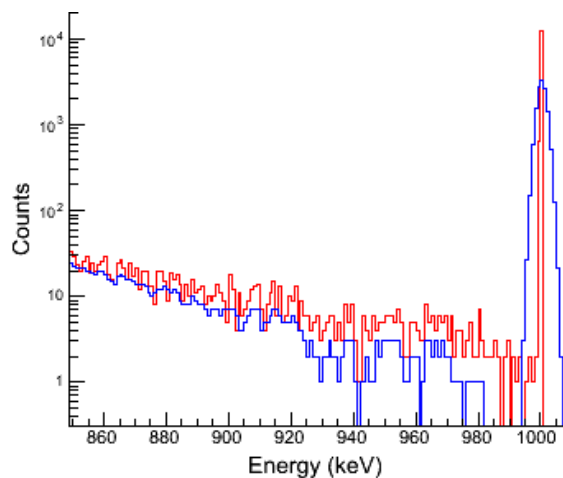


FIG. 3. Demonstration of histogram spreading near a photopeak. Red is pre-spread, blue post-spread.

amount of energy deposited through the physics is calculated—with no consideration of the operations of a real HPGe detector setup—Geant4 produces a delta function-like peak instead of the typical Gaussian peak one would expect. This does not impact the accuracy of the physics being simulated, but may impact the analysis afterwards if the histograms do not take such spreading into account.

To counteract this the histograms are manually spread after they are collected (see FIG. 3). The variance of a bin of a certain energy is given by

$$\sigma^2 = (\text{Resolution } \%)^2 \times \text{Energy} \quad (4)$$

where the resolution % is a scaling factor of that particular HPGe detector and is determined experimentally. Using this relationship, the program calculates the contributions from the Gaussian spreading of every bin on the first bin and totals that, and repeats this calculation for each bin. Effectively this is the same as spreading each bin separately then adding them together but is much simpler and not much slower.

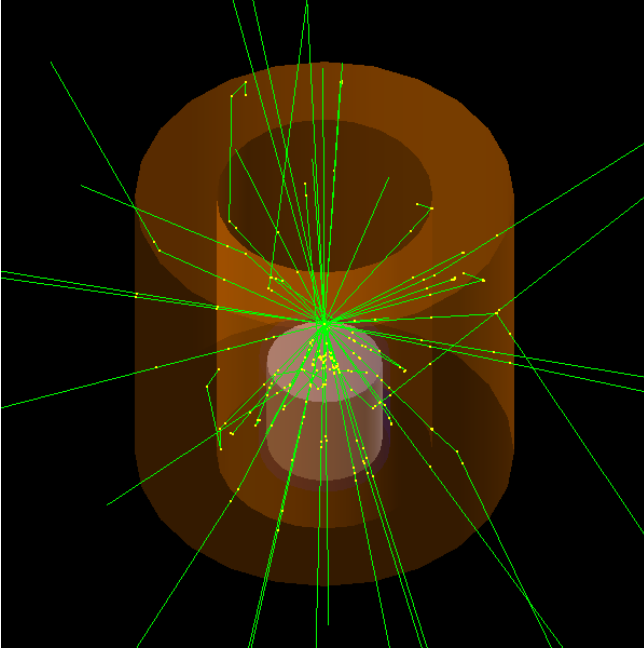


FIG. 4. Render of the simulation geometry with tracks of 50 primary particles shown. The NaI shell is orange; the HPGe crystal is the smaller grey cylinder within. Not visible is its housing.

### 3.2. NaI geometry

At this stage in the simulation we only included the minimum geometry to test the operation of the simulation, namely the NaI shell and the HPGe crystal with its housing (see FIG. 4). After the main analytical and operational components of the simulation are in place the remaining volumes will be introduced in order of importance (in particular the reflective material surrounding the NaI, the plug detector, and the lead shielding).

### 3.3. Compton suppression mechanism

Geant4 is capable of accurately simulating much of the actual process of Compton suppression, such as the calibration of the timing of the coincidence and the energy threshold needed to register a count in either detector.

The current incarnation of the suppression mechanism simply discards events that deposit energy in both the HPGe crystal and the NaI shell (see FIG. 5 for example). This works for rough comparisons of the effectiveness of different

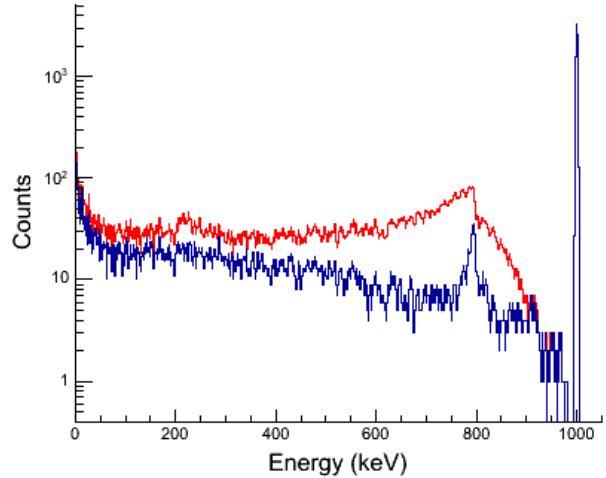


FIG. 5. Demonstration of Compton suppression on continuum of a 1 MeV photopeak. Red is unsuppressed and blue is the same spectrum with suppression enabled. Note that the photopeak is unaltered and so they overlap. Suppression factor of 0.42.

geometries but is only the first step in designing the suppression code.

The calculation of the suppression factor is straightforward. From the maximum of Eq. ( 3 ) the location of the Compton edge can be calculated based on the energy of photons used in the simulation [4]. Using this range the simulation adds the total counts from zero energy to the Compton edge in both the suppressed and unsuppressed histograms and takes the ratio of suppressed to unsuppressed counts.

### 3.4. AutoCAD geometries

While describing the geometry to Geant4 is easy for simple shapes such as cylinders and symmetrical setups, complex shapes become difficult to implement. For this reason the long-term goal is to incorporate more accurate geometries designed in AutoCAD. Unfortunately preparing a CAD drawing to be used by Geant4 is difficult, so for now the basic geometry suffices. Regardless, the NaI assembly has been drawn in anticipation of its future implementation (see FIG. 6).



FIG. 6. Render of CAD drawing of NaI detector assembly. Top is disassembled assembly to display hidden components.

#### 4. DISCUSSION

The immediate goals for the simulation are to improve the realism of the Compton suppression logic and add the remaining significant geometries. Subsequently the simulation will be prepared for comparison of varying sizes of NaI detectors. When the simulation is accurate enough and the design for the NaI detector is finalized we hope to use this simulation to aid in the process of NAA itself. Other practical applications of the simulation involve calculating the counting efficiency for different irradiated sample positions within the detector configuration and improving the overall sensitivity of NAA.

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- [1] R. J. Cashwell, University of Wisconsin College of Engineering, *Elements that can be detected with NAA*, <http://reactor.engr.wisc.edu/naa/element.htm> (Aug 24, 2012)
  - [2] K. S. Krane, *Introductory Nuclear Physics, 2<sup>nd</sup> ed.* (John Wiley & Sons, Inc., New York, NY, 1988).
  - [3] I. Rittersdorf, University of Michigan Department of Physics, Mar 20, 2007, *Gamma Ray Spectroscopy*, <http://www-personal.umich.edu/~ianrit/gammaspec.pdf> (Aug 23, 2012)
  - [4] University of Florida Department of Physics, Oct 31, 2011, *Gamma Ray Spectroscopy—Experiment GRS*, [http://www.phys.ufl.edu/courses/phy4803L/group\\_1/gamma\\_spec/gamspec.pdf](http://www.phys.ufl.edu/courses/phy4803L/group_1/gamma_spec/gamspec.pdf) (Mar 15, 2012)