HPGe/NaI Simulation
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Abstract

A simulation code was initialized for a HPGe detector surrounded by a NaI compton suppression detector interacting with gamma rays from 100keV to 10MeV. The simulation code was written from first principles, using C++ and ROOT and the goal was to optimize the NaI geometry for maximum compton suppression while maintaining a strong signal to noise. Preliminary results show better energy resolution of peaks beneath the Compton edge, but more analysis is necessary before conclusions can be reached.

1 Introduction

Gamma ray detection is useful in a number of different fields, including medicine, physics, astronomy. However, there is often difficulty in resolving the energies of gamma rays entering detectors because gamma rays often compton scatter within the detectors and then escape without being fully absorbed. In order to increase the resolution of gamma ray detectors, one can increase the qualitiy of these detectors or create setups that include multiple photon detectors for correlation of events within all the detectors. This allows for compton suppression and is necessary for better resolution of small peaks below the compton edge. For example, Figure 1 shows the improvement in energy resolution when a compton suppression system is put into place.

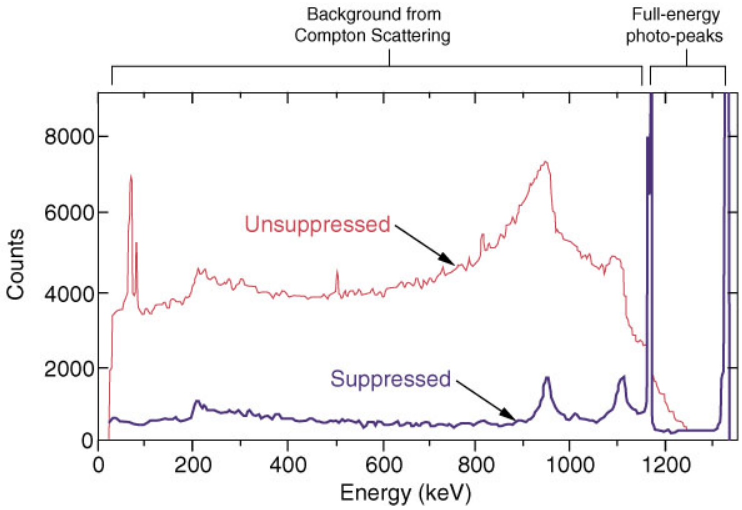

Figure 1: Sample Compton Suppression[Wikipedia]

An HPGe detector (High Purity Germanium detector) from an underground counting room in Saclay, France[1] will be surrounded by a NaI compton suppression detector of undetermined dimensions. Events with measurable photon energies in both detectors can be rejected from further analysis, decreasing the compton feature's amplitude. The geometry of the NaI detector determines how much suppression occurs; when the dimensions of the NaI detector increase the number of compton scattered photons detected increases. When these events are rejected from the analysis, this decreases the total signal but potentially increases the signal to noise ratio. Depending on the geometry of the compton suppression detector, a maximum total signal to noise can be reached.

2 Physics Background

There are many reasons to detect gamma ray photons: understanding nuclear activities within nuclear reactors, testing imaging techniques in nuclear medicine, treating cancer, understanding radioactive sources in terms of material properties, and studying gamma ray sources in the universe. Radioactive decay results from unstable atoms emitting ionizing particles to lose more energy and become more stable. There are three common types of decays: Alpha, beta and gamma. Alpha decay emerges from the interaction between the strong force and the electromagnetic force. Beta decay is mediated by the weak force; the ejected particles are electrons or positrons and electron anti-neutrinos or electron neutrinos. Gamma ray decay is produced by both nuclear and non-nuclear processes (non-nuclear examples include secondary gamma ray emission from astro objects) and alongside alpha and beta decays.

Gamma rays have high frequencies and therefore high energies. The energy range of gamma rays created as ionizing radiation from radioactive decays is from $10keV \rightarrow 10MeV$. When trying to detect gamma rays, the probability of interaction is proportional to thickness, density and absorption cross section of the detector material.

$$\frac{dN}{\mathrm{d}x} = -N\mu\mathrm{d}x \rightarrow \int \frac{N'}{N} = \int \mu\mathrm{d}x \rightarrow \ln(N) = -\mu x + A \rightarrow N = Ae^{-\mu x} \quad (1)$$

As shown in the equation series above, there is an exponential decrease of intensity with distance from incident surface. N is the number of photons, A is a coefficient that will be derived with each new intensity equation, x is the photon walk distance from the incident surface, μ is the absorption coefficient($\mu = n\sigma$, where is the absorption cross section and n is the number density of the material). Because intensity is proportional to the number of photons and to the probability of interaction, gamma rays are much more likely to interact closer to the incident surface, with less and less photons making further and further walk distances. The length of the average photon walk distance depends on the interacting material; in a vacuum, the average photon walk distance can be measured in kilometers while it is in centimeters within an HPGe detector. When the gamma ray's energy is greater than 1MeV, the mean free photon walk length is approximately the radiation length, so gamma ray detectors need thicknesses of at least a few radiation lengths to have good detection efficiency.

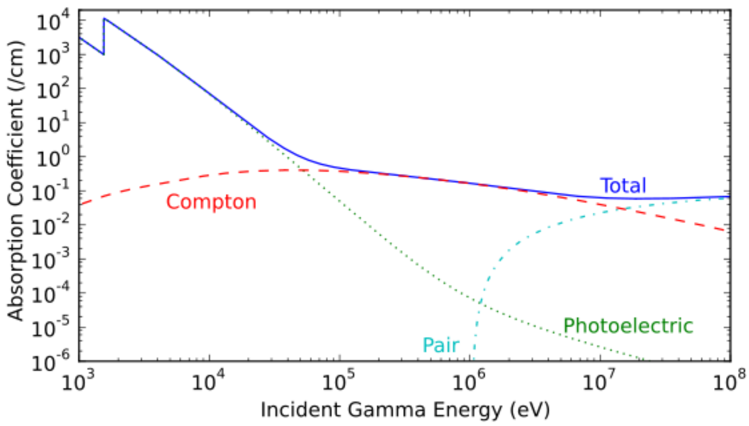

Figure 2: Material Attenuation Coefficients versus Gamma Ray Energy[Wikipedia]

Gamma rays as ionizing radiation from radioactive decay can interact with material in three different ways (as shown in Figure 2):

- Photoelectric effect: The gamma ray transfers all of its energy to an atomic electron, which is then ejected from the atom. The kinetic energy of the photoelectron(the ejected electron) is equal to the initial gamma ray's energy minus the electron's binding energy.

- Compton scattering: The gamma ray transfers enough energy to an atomic electron for ejection from its atom and a new photon scatters away in a different direction than initially. The probability of compton scattering is inversely proportional to the decrease in photon energy. Compton scattering is a type of inelastic scattering, which is an interaction process where the incident particle's kinetic energy is not conserved during the collision.

- Pair Production: This is possible when gamma ray energy is greater than or equal to 1.02MeV(rest mass energies for an electron plus a positron). The gamma ray interacts with the electric field of a nucleus and the gamma ray's energy is converted to an electron/positron pair. Any excess gamma ray energy becomes kinetic energy of the pair and recoil of emitting nucleus. The electrons and positrons from pair production often have enough energy to ionize other particles, continuing a chain of ionization as the particles move through a material.

Attenuation coefficients(the same as absorption coefficients) give an indication of the probability of a type of interaction occuring at certain energies. In Figure 2, the attenuation coefficients of the detector material are plotted against the incident photon energy in a log-log graph. In the lower range of initial photon energies, the predominant interaction type is the photoelectric effect which then exponentially decreases in probability as the photon energy increases. The probability of compton scattering interaction maintains semi-constant throughout the increase in photon energy. The pair production probability is zero until 1.02 MeV and then exponentially increases as photon energy increases.

When a gamma ray compton scatters off an electron, it transfers some of its energy to the electron and changes direction. Within a three-dimensional spherical coordinate system, this means that the theta and phi angles will change. While the new phi angle will be randomly distributed from $0 \rightarrow 2\pi$, the new theta will be dependent on the incident energy and new photon energies. This can be seen in the compton scattering formula: $\cos(\theta) = 1 - \frac{m_e c^2}{h}(\frac{1}{E'} - \frac{1}{E})$. M_e is the mass of the electron, h is the Planck constant, c is the speed of light and E/e' are the old/new energies of the photon. The Klein-Hishina formula is based on the compton scattering formula and gives the differential cross section for scattered photons from single free electrons, where the axes are oriented so that the original photon is travelling in the +z direction. The differential formulas are the following:

$$\frac{\mathrm{d}\sigma}{\cos(\theta)} = \frac{\pi\alpha^2}{m_e}\left(\frac{w'}{w}\right)^2\left(\frac{w'}{w} + \frac{w}{w'} - sin^2(\theta)\right) \tag{2}$$

$$w' = \frac{w}{1 + \dfrac{w}{m_e(1 - d(\cos(\theta)))}} \tag{3}$$

In Equation 2, α is the fine structure, M_e is the mass of the electron, and w is defined in Equation 3. Within the simulation code, only the photoelectric effect and compton scattering are coded in. Pair production has a high level of complexity due to the numerous ionizations that can occur from the created electrons and positrons. Since the energy range of the gamma rays entering the detector setup doesn't include a large range where pair production is possible, it is possible to realisically simulate gamma ray interactions without pair production.

3 Technical Background

3.1 Gamma Ray Detectors

The physics involved with both the NaI and HPGe detector is based on the band model of solids, or the splitting of orbitals with large collections of atoms. One atom has a discrete number of orbitals but when several identical atoms are combined into a molecule, the orbitals split due to the Pauli exclusion principle and produce molecular orbitals proportional to the number of atoms. When there is a large number of atoms together (such as in a solid), there are many orbitals with infinitetesimal differences between each other. With these infinitetesimal differences, it is simpler to consider the orbitals as a whole in continuous energy bands than discretely but there may be some energy intervals with no orbitals, no matter how many atoms, making band gaps. The band directly below a band gap is called the valence band and is the last set of bound electron orbitals. The band directly above a band gap is the conduction gap and electrons can move freely within the lattice of the solid.

Figure 3 visually describes the differences between the three types of solids: conductors, semiconductors and insulators. The Fermi level is the energy of the least tightly held electrons within a given solid at absolute zero. In conductors, the valence and conduction bands overlap and there is no band gap. In semiconductors, there is a small band gap and some excitation of electrons into the conduction band is possible. Insulators have a large band gap and it is very difficult to excite electrons into the conduction band due to the high amount of energy needed to free the electrons.

3.2 Scintillators

Scintillators are insulators but can be used in gamma ray detection to create luminescence (creation of photons) due to the high energies of the ionizing radiation. The ionizing radiation excites electrons from the valence band to the conduction band, creating electron hole pairs. These electron/hole pairs wander through the detector, exciting other electrons and producing more photons, until they reach a luminescence site. The scintillator is

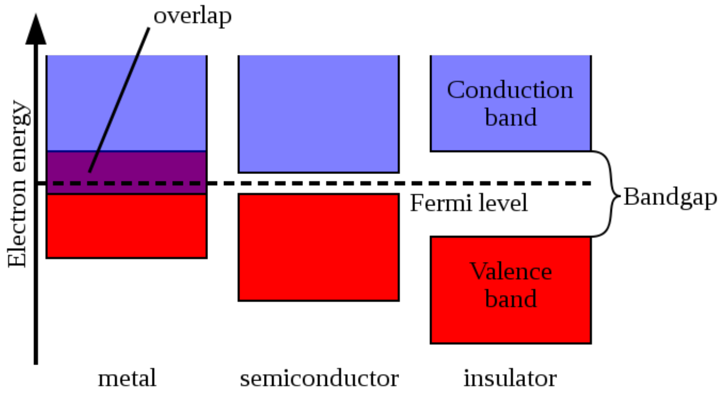

Figure 3: The Band Model of Solids[Wikipedia]

doped with some element that has orbitals in the band gap region of the scintillator, making luminescence sites. The wandering electron/hole pairs excite the dopants electrons into higher energy orbitals and then the dopants electrons will de-excite by emitting photons that will have energies that can escape the detector (due to the Stokes shift, the final emitted photon has less energy than the initial absorbed photon) because the dopants orbitals are within the band gap of the detector.

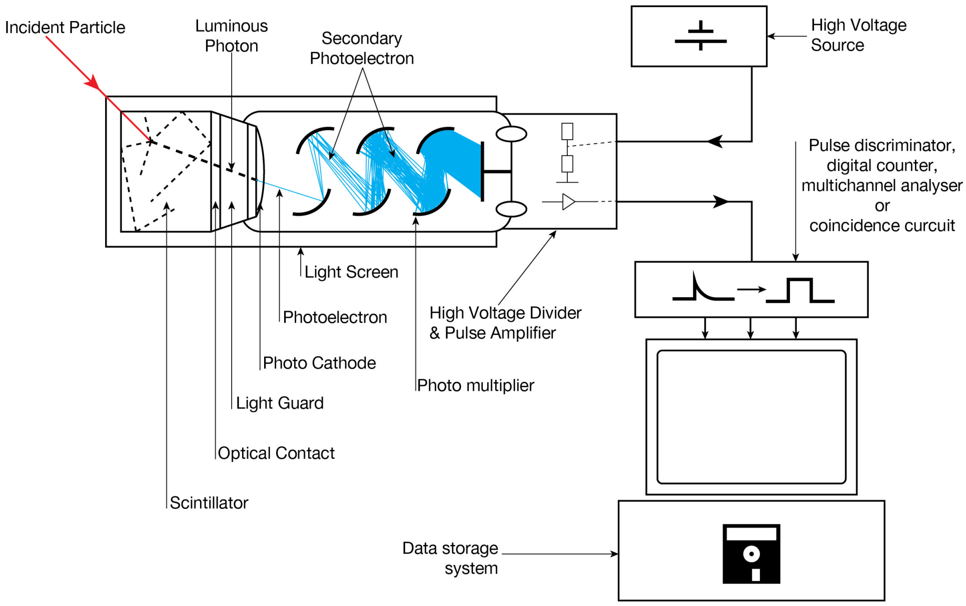

Figure 4: Method of Scintillation[Wikipedia]

Figure 4 visually describes the scintillation and amplification process. Photomultiplier tubes (PMTs) are utilized to multiply the current produced by the escaped photons by greater than 10^6. PMTs have a high internal gain (measure of the ability of a circuit to increase the power or amplitude of a signal), so only a few photons are needed for creating a measurable signal. A PMT is a vacuum tube usually made of glass or with a glass window with a photocathode at the entrance, an anode at the exit and dynodes inbetween. A photocathode is a thin layer of a compound that will release electrons when it absorbs visible or near visible photons. The dynodes are electrical conductors, as is the anode, and the negative potential will decrease in steps from the photocathode to the anode (ground potential), moving the current through the PMT. The electrons emitted from the photocathode are attracted to the first dynode and extract several electrons that go to the next dynode and make more electrons, etc.

Sodium Iodide (NaI, a scintillation material) is being used as the compton suppression detector within this setup. It can be produced in large crystals, giving good absorption efficiency, and is cheaper and easier to produce than semiconductor materials. However, the energy resolution of NaI compared to semiconductors is worse due to the secondary photon detection.

3.3 Semiconductors

Semiconductors have a simpler way of detecting gamma rays than scintillators. Ionizing radiation excites electrons into the conduction band, creating electron/hole pairs that are accelerated by an applied electric field out of the semiconductor into electrodes. A pulse is created within the electrodes that can be amplified and measured. The number of electron hole pairs is proportional to the ionizing radiation's transmitted energy. The amount of energy required to make these pairs is known and is independent of the ionizing radiation. Direct electron detection leads to better energy resolution and less error compilation than scintillators.

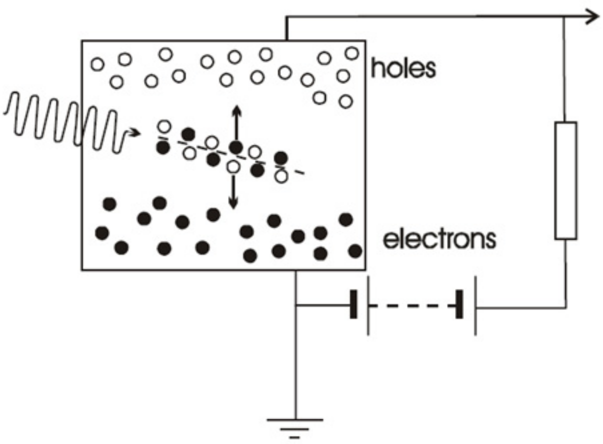

Figure 5: Gamma Ray Detection Using a Semiconductor[2]

Figure 5 demonstrates how gamma rays are detected within a semiconductor and the electron hole pairs are moved out of the detector. An HPGe detector is being used as the main gamma ray detector within the setup. The size of HPGe can be on the order of cm (unlike silicon) but needs to be high purity germanium or the material will not be a sufficient photon detector.

3.4 Physical Setup

The geometry created by the simulation code simply contains a HPGe detector surrounded by the NaI compton suppression detector with a photon source at some distance above the top cylinder surfaces of the detectors. For the moment, it is assumed that the empty space surrounding the detectors and photon source is vacuum filled. The detectors are cylinder shaped, heights and radii in order of cm, constant density throughout, and no dead layers included. The photon source can produce photons at discrete energies or from a continuous spectrum moving isotropically or incident to the top cylinder surfaces of the detectors. Figure 6 is a visual representation of the simple geometry setup.

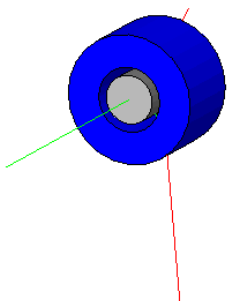

Figure 6: HPGe/NaI Gamma Ray Detection Setup

4 Code Setup

The simulation code for this gamma ray detection setup was created from first principles using C++ and ROOT and although this code was created for a specific detector setup, it can accomodate different detectors and materials. Three classes were created, as shown in Figure 7: master, geometry and photon.

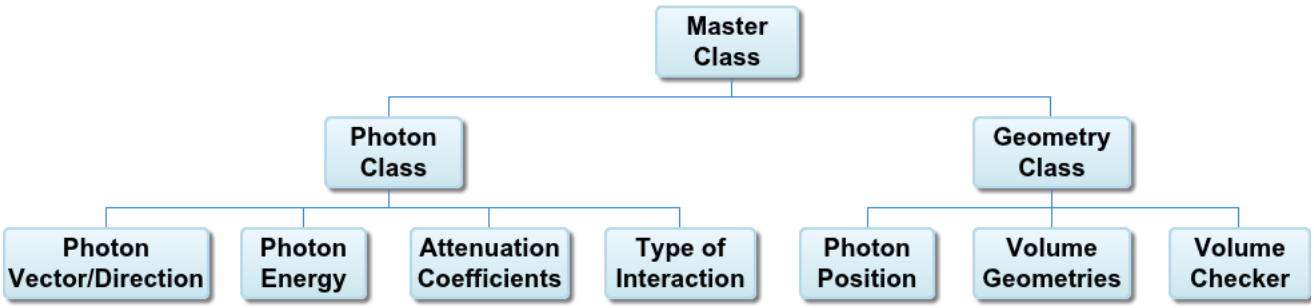

Figure 7: Simulation Code

The geometry class creates cylinder objects for the detectors, calculates the photon position within the total volume of the setup, and checks what volume the photon is in. The photon class maintains the photon energy, runs the material attentuation coefficient file reader and spline creator, and finds values for theta by the differential cross section, random phi, random photon length, and a random interaction finder. The master class manipulates the photon class, geometry class and a ROOT data tree for later analysis. It initializes geometry and photon objects, then walks the photon object through the setup, making changes in volumes, attenuation coefficients, energies, photon direction and distance for each successful photon event. The master class saves the position, deposited energy, volume number, type of interaction, photon event number and photon number for each successful photon event in a ROOT TTree branch. When a photon has been fully absorbed or escapes the entire geometry setup, the master class deletes the photon and geometry objects and saves the last photon event in a TTree branch.

5 Results and Discussion

The initial results from the simulation code can be seen in Figure 8, where the axes are counts versus amount of energy deposited in the HPGe detector. The blue curve is the unsuppressed analysis versus the suppressed analysis in red; the primary peak in the blue curve serves as the compton edge where suppression of this increases the energy deposition in the HPGe, as seen in the blue curve.

With the knowledge that the simulation code effectively simulate gamma ray interactions and compton suppression (see Figure 1 for comparison of compton suppressions), the physics involved within the code can be enhanced to better simulate gamma ray interactions. The following upgrades would be beneficial to the simulation code:

- Adding a dead layer on the HPGe detector that results from doping (photons that interact in this layer are never detected).
- Adding complexity to the NaI geometry, such as breaking up the cylinder into parts.
- Including pair production within the types of interactions gamma rays can undergo and formatting the code to correctly follow the resulting particles.
- Allowing the volume surrounding the detectors to be different gases, not just vacuum.

Once the simulation has been made sufficiently complex to realistically simulate gamma ray interaction within this detector setup, the best scintillator geometry (height, width) for best suppression needs to be found but not so much suppression that the signal to noise suffers.

6 Conclusion

A simulation code for a HPGe/NaI gamma ray detection setup has been created and verified. However, there are only initial results that using NaI as a compton suppression detector will be effective and the simulation

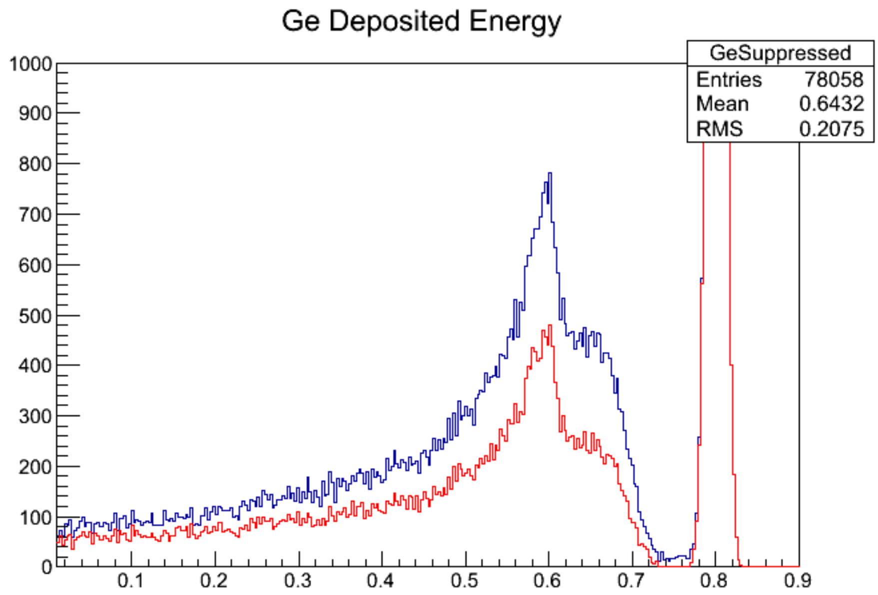

Figure 8: Initial Results of HPGe/NaI Simulation Code[Richard Ott]

code needs to become more complex before more simulations can be run. These complexities include adding dead layers, including pair production, changing the geometry of the NaI and adding flexibility to the material that can surround the detectors. Other complexities to take into account are that the HPGe is a p-type coaxial detector of 80% relative efficency and including the dopant to the NaI material properties. To conclude, it is possible to simulate gamma ray detectors from first principles and gain an understanding on the dependence of compton suppression on geometry.

7 Acknowledgements

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