Geometrical and Optical Improvements to GAGG Simulation

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This paper describes work done on geometrical and optical improvements to Geant4 simulations of Gadolinium Aluminium Gallium Garnet (GAGG) scintillator properties, in preparation for designing an array of such scintillators to be used for inbeam spectroscopy at the RIBF at RIKEN. In particular, this paper describes work done to include more varied geometries and optical measurement methods in order to simulate the widest range of potential crystal geometries, properties, and measurement photocathodes to determine an ideal method of photon delivery to a photocathode for conversion into a signal pulse.

I. INTRODUCTION

A. Scintillator Crystals, GAGG, and Inbeam Spectroscopy

For a given particle interaction with a detector, several potential pieces of information are relevant and can be gleaned from a signal pulse off of a detector, all of which can be gained to certain precision. This include (but are not limited to) position of the interaction in space, (which, depending on the design of the detector, may be determined by triangulation between various photocathodes, or may simply be known only to be within the volume of the detector) time of the interaction, (the precision of which is limited by the rate at which the detector responds to its incident particle) and energy deposited in the detector, the precision of which is determined by a characteristic energy response which depends on both material properties and geometric properties of the detector.

While many devices for measuring particle interactions exist, this paper describes a characterization of a particular scintillation material. The scintillation process is the process by which incident ionizing radiation (in this case, gamma rays) interacts with a material (possibly being absorbed in the process) and allows for some of its energy to be converted into visible photons. In the case of gamma rays, this allows for an extremely high energy photon (on the order of hundreds of keV) to be converted into tens of thousands of visible wavelength photons. Since gamma rays are extremely penetrative and statistical in their behavior and interactions, converting them into visible photons allows for them to contained in a particular material for counting.

The scintillation process relies on a crystal having a clear band gap between electron energy levels. If this is the case, an interaction between an atom in the crystal lattice and an incident gamma ray can have the effect of exciting an electron (or, in practice, many electrons) to a higher energy level. When it descends to ground state, it emits a photon whose energy is equal to the band gap energy the electron drops in its transition, in order to maintain conservation of energy. Since the band gap can be tailored to whatever energy difference is desired by introducing dopants into the material, this process allows for creating photons of any (within reason) energy desired. Figure 1 shows this process occurring.

Several current materials exist for these detectors. The current “top-of-the-line” material, High Purity Germanium, (HPGe) has certain downsides that make it a less-than-ideal choice for use at the RIBF. In addition to cost issues (both Germanium crystals and the supporting systems are extremely expensive to synthesize and maintain) Germanium crystals require a large support system, which corresponds to a high percentage of “dead space” (that is, space that is not detector) in the array. This results in loss of data as particles that could interact with detectors instead land in this support sys-
FIG. 1. The scintillation process. Incident radiation excites many electrons, which emit photons when the drop. In particular, HPGe corrodes on exposure to moisture in air, requiring protective casing, and is operational only at very low temperature, requiring coolant systems. GAGG, on the other hand, is operational at room temperature and in air - though it still requires a thin reflective shield to keep scintillation light in and ambient light out, this need not be a thick, airtight casing like HPGe requires.

Since GAGG systems require very little support material, and since much of the support material necessary scales with the size of the detector, (unlike, say, the coolant systems of an HPGe, which would be similar in size for any size crystal) GAGG detectors can be effectively miniaturized, allowing for high precision resolution even if the position measurement is limited to “event occurred within the size of the detector”. The main drawback is the lower energy resolution of GAGG crystals - energy resolution on the order of 5% at the main Caesium line[1], compared to less than 1% for Germanium[2].

In addition to the cost savings, however, the position resolution improvement is significant for use in an in beam facility. Since particles traveling down the beamlines of the RIBF will be moving relativistically, and the energies of interest in an interaction are the energies in the center-of-mass frame, knowing the angle off of the beamline is important to reconstructing the energy of the resultant photon in center-of-mass coordinates.

B. Monte Carlo Modeling

While “elementary” functions can be constructed for some (though certainly not all!) of the individual interactions incident particles undergo in the process of interacting with targets, a detector hit can consist of hundreds of thousands of such interactions. Rather than attempting to construct some analytical solution to relate the momentum of an incident particle with the probability of various response curves, such systems are best dealt with computationally. An additional difficulty, however, comes from the statistical and probabilistic nature of these particle interactions. While classically these solutions could be solved to arbitrary numerical precision by tracing each particle as it passes through space and detector with some arbitrarily small, but finite, time step, this is not possible for a quantized particle system. Instead, each simulation run is one possible outcome, and by simulating tens of thousands of runs, one can create probability distributions for all aspects of the detector’s response.

This is implemented through a software package developed by CERN, Geant4 (GEometry And Tracking, 4). Geant4, developed for modeling in-beam collisions and tracing the paths of the products of such events through detectors, handles all particle interactions with their mediums “under the hood” - the user simply designs a geometry, provides a set of material properties, defines the interactions of interest (in this case, primarily scintillation, scattering, absorption, and reflection) and provides a set of input
parameters, as well as defining a set of parameters of interest to be recorded. Geant4 then handles the backend of modeling all of the individual interactions and output particles, and outputs raw data files of the parameters of interest, which can then be analyzed in an analysis program such as ROOT. While this method can be extremely powerful, (and is often the only way certain system properties can be known) it can also require vast computational time to produce detailed or precise models of certain complex systems.

II. IMPLEMENTATION

Several properties are of interest in the output signal from a photocathode in order to determine energy of an incident gamma ray. These include the efficiency of the detector - that is, how probable it is that a certain incident gamma ray will deposit all of its energy in the crystal, the energy resolution of the detector - that is, how consistently a same energy deposited results in a same photon delivery to a photocathode, and the total photon delivery - the strength of the signal itself. Figure 2 displays how these characteristics would appear on a given energy spectrum.

Prior to this work, Wimmer Labs had only a very naive simulation method - a brick of a crystal attached to an equal sized brick of a photocathode, with no attempt to simulate the efficiency of the photocathode itself. This is shown in Figure 3. In practice, however, most photocathodes will be different sizes than their respective crystals. One aspect of my work consisted of implementing a way to model “tapering” of the detector in order for photocathodes of different sizes to better fit on detector crystals of different sizes. A demonstration of this new setup is shown in Figure 4. In particular, one goal in this project was to have as few properties as possible “hard-coded” in. Ideally, a user should be able to input any set of geometrical properties, and have a working simulation to that geometry.

A second part of my work consisted of modeling the statistical behavior of the photocathodes. Each model of photocathode has a characteristic response curve to energies of photons. The prior model did not take into account this effect, and so could produce results differing from experimental results if photon delivery varies by photon energy. This was dealt with simply by a basic “dice-rolling” Monte Carlo simulation: for an incident photon, the simulation would look up the probability of a photon of that energy being detected, and generate a random number between zero and one. If the number generated was lower than the probability of detection, the event would be simulated as “detected” and otherwise would be simulated as “missed”.

III. RESULTS AND FURTHER WORK

Blind simulation alone cannot provide all the necessary information to determine an ideal detector configuration. Simulation, rather, can only determine an ideal detector configuration given a certain set of material properties. Since GAGG is a new technology, many of its material properties are not yet well known or studied. Instead, the goal for current work should be to create a simulation that is as flexible as possible in its input parameters, so that when better information is available, all a user need do is tweak certain numbers or input files. Figure 5 shows a results spectrum for one possible set of input parameters, as an example of the sort of information that can be gleaned from such a simulation.

Several steps remain between these models and a full detector array. First will be simulating more possible interactions - this simulation models only direct, frontal beams. Additionally, this model will be condensed into a simple statistical model for pulse height - when modeling a full array, every photon interaction need not be modeled, and doing so will only drain computational time. Instead, the results of the smaller models can be plugged in as “black boxes” into the input of the larger models. Hopefully, however, this small-scale model will provide an effective stepping-stone to a large-scale model, and eventually a full implemented detector array.
FIG. 2. A spectrum for ten thousand runs. While this plot is constructed from a histogram of “number of photons detected per event” for ten thousand events, it can just as easily be thought of as a plot of a discrete probability distribution function (to arbitrary normalization) for probability of a certain number of photons being detected. From this plot one can see the efficiency of the detector (the integral of the peak compared to the total number of events), the energy resolution of the detector (the standard deviation of the fit gaussian on the peak) and the total photon delivery - the position of the peak on the x-axis. A high efficiency, narrow energy resolution, and high total photon delivery are all desired traits for an effective detector.

FIG. 3. A simple model. The purple box, close to the observer, represents the detector crystal itself, while the green, further away, represents the photocathode. This only works when detector and photocathode are the same size, which will rarely be the case in practical implementations.

FIG. 4. A model including tapering. Green and purple are flipped in space but have the same meanings. Now the crystal is tapered to fit onto a smaller photocathode.
FIG. 5. Simulation results, in the same vein as Figure 2 now for ten thousand runs on each of six different geometries - a 25mm by 25 mm by 100 mm crystal attached to a 15 mm by 15 mm photocathode, with 15 mm of the crystal tapered (dark blue), 30 mm (red), 45 mm (green), 60 mm (pink), 75 mm (cyan), and 90 mm (purple). In this case, we can see that in all cases increased tapering of the crystal for a constant sized photocathode improved photon delivery, but at the cost of significant efficiency losses and slight precision losses. While more detailed simulation on the region of interest would be necessary, it seems for this set of material properties, the 45mm tapering region provides significantly improved delivery with little loss in other aspects.