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GEANT4 Modeling of Ambient Temperature Perovskite Gamma-Ray Sensor †

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Abstract: Research efforts to develop high-efficiency ambient temperature photon sensors are ongoing due to the demand on measuring x-ray and gamma-ray radiation with high energy resolution. The inorganic wide-bandgap perovskites such as $CsPbBr_3$ are promising for large-volume crystal designs. This material has high mobility-lifetime product (10^{-2} cm^2 V^{-1}), low density of defects, and long-term stability for detection of photons and charge particles. The study of large-volume perovskite detectors is necessary, including development of computational models. The performance of a $CsPbBr_3$ gamma detector was studied using GEANT4 and ROOT toolkits. The Monte Carlo code GEANT4 utilizes geometry and materials data to model particle interactions with matter, event and track management, and visualization of results. The ROOT was used to process and analyze the gamma-ray energy distributions computed by GEANT4. The 8 cm^3 $CsPbBr_3$ crystal characteristics for the incident 662-keV gamma rays were the following: 1.1% energy resolution and 29.2% photo peak efficiency. The energy resolution of the perovskite sensor is comparable to that of a CZT sensor of a similar geometry; however, the larger volume perovskites can be synthesized.

Keywords: radiation sensor; gamma spectrometry; perovskite; ambient temperature

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1. Introduction

Development of ambient temperature radiation sensing technology is ongoing due to the demand on detecting x-ray and gamma-ray radiation with high energy resolution and sensitivity. Radiation sensor materials such as high purity germanium (HPGe), cadmium zinc telluride (CZT), thallium bromide, binary halide compounds, mercury (II) iodide have been studied for applications in security [1], aerial sensing of radiation [2,3], medicine [4], and scientific research [5] due to their properties such as high electron density, resistivity, and energy gap [6]. These materials have complicated crystal growth conditions such as precipitates in CZT crystals which can degrade detector performance due to electric defects that disturb photo-generated carriers hopping [7].

Inorganic perovskites such as $CsPbBr_3$ consist of high atomic number components without organic molecules. Due to such structure, it has a large gap between valence and conduction bands but lacking Van Der Waals gaps resulting in its great electrical and mechanical properties, and high mobility-lifetime product (10^{-2} cm^2 V^{-1}), low defect densities, and long-term stability for sensing photons and charge particles [6–8]. $CsPbBr_3$ perovskites are promising materials for large crystal designs with low defects.

While a stable crystallization method of $CsPbBr_3$ was reported with its properties, especially electrical and optical [7–9], the size control of single crystal growth is unstable. As a result, $CsPbBr_3$ crystals have a small volume. The study of large-volume perovskite sensors is necessary, including development of computational models. The performance of a gamma detector based on the $CsPbBr_3$ crystal was studied using GEANT4 toolkit to simulate the particle transport in matter.

2. Methods

2.1. GEANT4 Study of a Perovskite Sensor

The GEANT4 toolkit uses the Monte Carlo method:

$$f(x) = \sum_{i=1}^{n} N_i f_i(x) g_i(x), \quad (1)$$

where $N_i > 0$, $f_i\ (x)$ is normalized density functions on interval [x_1, x_2], $g_i\ (x)$ is rejection functions ($0 \le g_i\ (x) \le 1$), which is simulation statistical algorithms based on random sampling to calculate numerical results [10]. Figure 1 shows a modular structure of GEANT4 class categories to develop the desired computational model. Based on this process flow, GEANT4 can be used to configure a variety of simulation variables through the control of geometry and materials, particle interaction in matter, tracking management, digitization and hit management, event and track management, visualization framework, and user interface [11]. GEANT4 utilizes geometry and material data to model particle interactions with matter, event and track management, and visualization of computed tallies [12].

ROOT was utilized to process and analyze massive data calculated by GEANT4. The ROOT toolkit enables data processing and advanced statistical analysis. It uses information about a class of database; the name and title of a class, the size of an instance in bytes, its parent class(es), the names, types and description of its instance variables, the names and signatures of its member functions, a source code reference to the definition and implementation part of the class, and the address of the class object factory method used to create a new object [13]. The tree data structure is a main key factor of the system which allow each GEANT4 event information link to branches so that visualization process can be performed fast and effectively.

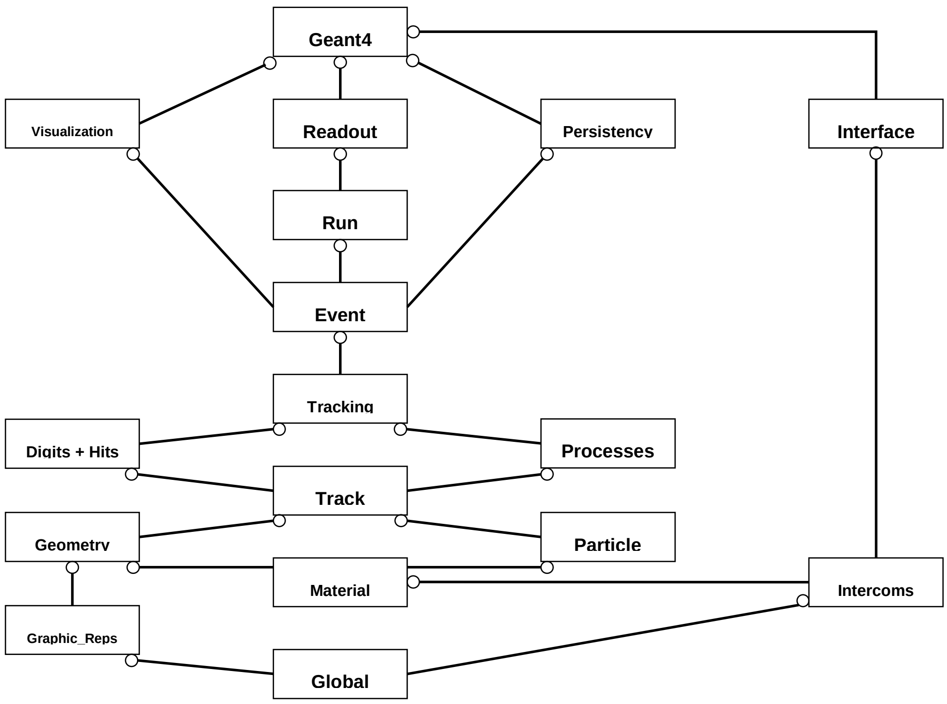

Figure 1. GEANT4 class categories diagram [5].

For the control of geometry and materials, the $CsPbBr_3$ perovskite structure was set up as ABX_3, where A = Cesium (Cs, atomic number 55, standard atomic weight 132.905 g/mole, density 1.93 g/cm^3), B = lead (Pb, atomic number 82, standard atomic weight 207.2

g/mole, density 11.34 g/cm³), and X = bromine (Br, atomic number 35, standard atomic weight 79.904 g/mole, density 3.1028 g/cm³).

The (2 × 2 × 2) cm³ $CsPbBr_3$ crystal was modeled with 4.42 g/cm³ density which represents a material of the 3.153 eV band gap and 1% energy resolution. Using the incident 662 keV gamma rays, photon and charged particle reactions and radiation transport in the volume of this perovskite sensor including particle traces was investigated.

3. Results and Discussion

Tracking management, digitization and hit management, event and track management were performed using a mono energetic distribution. Figure 2 shows the visualization of the simulation results.

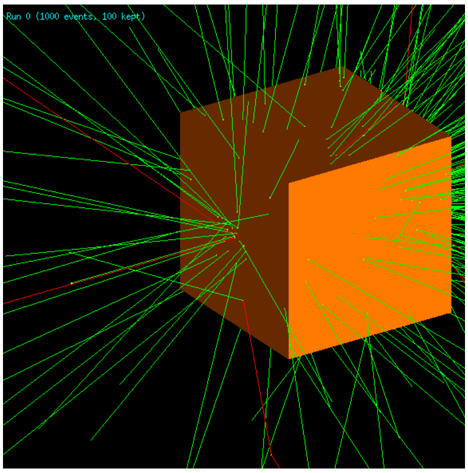

Figure 2. GEANT4 simulation: photon tracks in the perovskite crystal.

The GEANT4 simulation data were processed using ROOT, resulting in the gamma-ray spectrum of the perovskite detector at 662 keV (no Gaussian broadening was applied) shown in Figure. 3. The spectrum showed the full energy peak at 662 keV with the 7.07 keV full width at half maximum, and the Compton edge at 473 keV.

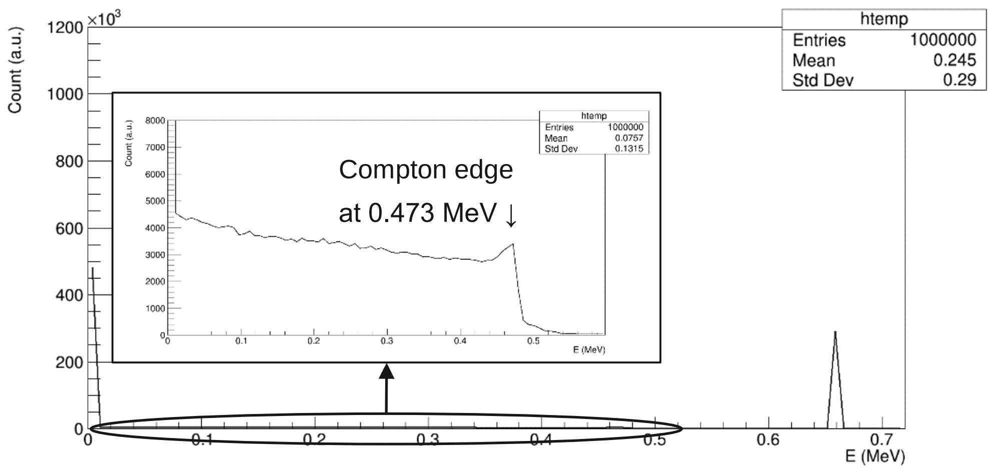

Figure 3. The $CsPbBr_3$ gamma-ray spectrum for the 662 keV incident photons.

4. Conclusions

Monte Carlo modeling of a perovskite gamma sensor was carried out using GEANT4. The 8 cm³ $CsPbBr_3$ crystal characteristics for 662 keV gamma rays were the following: 1.1% energy resolution and 29.2% photo peak efficiency. The energy resolution of perovskite detector is comparable to that of a CZT detector of a similar configuration [8]. This perovskite material is promising for the development of large-volume sensors to increase the gamma-ray detection efficiency.

Institutional Review Board Statement:

Informed Consent Statement:

Data Availability Statement:

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