# DETERMINING PROPERTIES OF THALLIUM BROMIDE RADIATION DETECTOR BY MONTE CARLO SIMULATION

### Ly Anh Tu, Nguyen Anh Duy and Cao Thi Hong Van

Department of Applied Physics, Faculty of Applied Science, Bach Khoa University VNU HCM, Ho Chi Minh City, Vietnam e-mail: lyanhtu1@gmail.com

#### Abstract

Thallium Bromide (TlBr) material has been emerging as one of the promising semiconductor materials with high spatial resolution, high efficient detection and good energy resolution (especially at 511 keV), based on recent progress with material purification and crystal growth and operation at room temperature. The studies about TlBr radiation detector have opened many prospects in producing electronic devices in the near future, for using as blue sensitive photodetectors, a real-time x-ray image sensor, a direct gamma-ray detector for nuclear medicine applications, especially for positron emission tomography (PET). The main purpose of this report is the application of Monte Carlo simulation to determine the properties of TlBr radiation detector beside predict the applications in the future.

## 1. Introduction

A semiconductor is the field of science and technology which has an extreme development. During decades, the semiconductor theories have been evolved in depth and the practical applications of semiconductor have been extended to a staggering degree. The study related to semiconductor crystals began to

Key words: Thallium Bromide radiation detector, Penelope, Monte Carlo simulation.

come from basic materials such as Ge and Si. These materials were used successfully in the detection and measurement of Gamma spectrum, mainly due to high energy resolution, the sensitive response of signal and small dimension. In addition, semiconductor detectors which are made from Ge or Si material are the most common type of X-ray spectroscopy and Gamma -ray. Detector Si recorded effectively for a low power (less than 20 keV). However, the disadvantage of detector Si was a low performance on recording Gamma-ray. Therefore, the attention began to focus more on detector Ge with higher performance record. Nevertheless, detector Ge also had the disadvantage that must be cooled by liquid Nitrogen to work optimally. Detector Si had high energy resolution that is also cooled by liquid Nitrogen. Hence, the need for research on other semiconductor material to fabricate detector can reliably operate at room temperature and the performance record is higher than Ge. Materials can help to fabricate detector which works at room temperature as TlBr, HgI<sub>2</sub>, CdTe,  $Cd_{1-x}$ ZnTe, PbI<sub>2</sub>, GaAs, InP, The development of detector operating at room temperature is especially necessary for a large number of practical applications. TlBr has emerged as one of the most promising materials because it has high Z number, high density, large band gap and based on the recent progress of clean material technology and crystal grown and operates at room temperature. A compact semiconductor detector operates at room temperature with high spatial resolution, high efficient detection and good energy resolution (especially at 511 keV) that will be the only advantage of TlBr more then LSO, BGO and CdTe/CZT which is the most common Gamma-ray detecting material in current Positron Emission Tomography applications.

### 2. Semiconductor material TlBr

**2.1 Thallium Bromide** TlBr has emerged as a special material because of its physical characteristics as large band gap (2.68 eV) and high density (7.5 g/cm<sup>3</sup>). TlBr crystal has the large atomic number (Tl: 81 and Br: 35) and high resistivity (>  $10^{10}\Omega.cm$ ). There are important factors for applications on the detector to reduce dimension and thickness.

Cadmium Zinc Telluride ( $Cd_{1-x}ZnTe$  or CZT) detector has high resolution and its band gap is 1.57 eV. That is enough to ensure for producing negligible heat leakage at room temperature. The atomic number of Cd(48) and Te(52) have a higher value compared to Ge(32), and the density of CZT is 6.2 g/cm<sup>3</sup> compared to 5.32 g/cm<sup>3</sup> of Ge [1]. The summary of the properties of CZT and TlBr is shown in Table 1.

By approximately  $10^{-3}$  cm<sup>2</sup>/V on  $\mu_e \tau_e$ , CZT detector has the best energy resolution just less than 1% with 662 keV Gamma-ray at room temperature. For comparison, Ge detector which has high purity has the resolution as 0.2% for same energy. Thus, any alternative CZT material must reach at least 1%

Material	Z	Density [g/cm <sup>3</sup> ]	Band gap [eV]	μ <sub>e</sub> [cm <sup>2</sup> /V.s]	$\tau_{e}[s]$
CZT	48,40,52	6.2	1.57	800-1300	(1-5) x 10 <sup>-6</sup>
TlBr	81,35	7.56	2.68	~50	~10-5

Table 1: Comparison on the properties of TlBr and CZT [1]

standard energy resolution. In contrast, TlBr crystal has  $\mu_e \tau_e$  as 10-4 cm<sup>2</sup>/V and energy resolution below 1% at 662 keV.



Figure 1: Linear Attenuation Coefficient on TlBr, CZT and Si [1]

#### 2.2 The surface characteristic of TlBr crystal

Radiation detector manufacturing technology includes cutting, polishing and engraving crystal surface, etc. The exposed electrode can affect the quality of the crystal surface and resistive contact. It is necessary to produce contact surface of the high-quality detector. For this reason, TlBr material should be processed. TlBr is a soft material the mechanical processing of the material is significant and material deformation is created in a variety of surfaces and structural defects as dislocation, drum, and other factors. Depending on processing technology, the depth of the surface layer can change faultiy from 10 m to 1 mm or even more. Hence, one of the specific objectives was the development of a surface processing technology, which allowed to solve some problems on the detector. Hardness testing and optical microscopy method are selected to control surface quality. The experiment applies TlBr crystal form of type A, L and S are produced according to Bridgman-Stockbarger method. The thickness of the sample is 2 mm and 5x5 mm2 square. The crystal is cut by a diamond blade. The sample surface after cutting is shown in figure 2a, which is visible cutting on each stain [2].

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Figure 2: TlBr crystal seen from optical microsope [2]

## 3. Monte Carlo simulation by PENELOPE

PENELOPE (Penetration and ENErgy Loss of Positrons and Electrons) uses FORTRAN77 code to perform simulation on the transmitted electron - photon of complex material systems include the number of areas is limited by the heterogeneity of the determinate surfaces. First, it was devised to simulate the energy transmitted and loss of positrons and electrons in the environment while the photon is added later. These interaction models are selected, and the data combined, enables simulation of electron transmittance, positrons and photons in the energy range from 100 eV to 1 GeV [3].

#### 3.1 Simulating detector and determinating performance

In the simulation of this paper, the geometry of detector includes Au layer 4 mm diameter, the middle layer TlBr 4x4 mm2 and Au layer ate the bottom 4 mm diameter. These layers locate parallel to Oxy plane and perpendicular to the axis Oz. The program Gview2D and Gview3D help to observe two or three dimensions and report errors in syntax definitions.



Figure 3: TlBr detector in Gview3D

After running program PENMAIN in PENELOPE by energy 662 keV, the result is shown in figure 4.



Figure 4: The graph corresponds to energy 662 keV

# 3.2 Determinating the efficiency of TlBr detector by different thicknesses

TlBr detector is considered by three different thicknesses as 0.8 mm, 1 mm and 2 mm in the range energy 0 - 800 keV. From each energy level, there is a change in PENMAIN.IN file. Then Command Prompt Window is opened to run PENMAIN.IN. The efficiency is calculated in each case.



Figure 5: The efficiency of TlBr detector on 0.8 mm, 1 mm, 2 mm thickness

The graph (figure 5) shows that when the photon energy becomes larger, the absorption efficiency decreases following the energy. The efficiency is high at 200 keV (83%). After that, it falls down at 800 keV (15%). TlBr crystal on 2 mm thickness has higher efficiency than 1 mm and 0.8 mm. This results from PENELOPE are close approximately the results in [4].





Figure 6: The efficiency of TlBr and CdZnTe detector

From the graph (figure 6), the efficiency is high in the range 100 - 200 keV. The efficiency of TlBr crystal is similar to CdZnTe crystal in the same range. In the range 1 - 3 MeV, the efficiency of TlBr crystal is almost higher than CdZnTe. It is also similar to the results in [4].

# 3.4 Determinating the efficiency of TlBr with Ohmic contact Au and Tl

The thickness is also 2 mm in this case. The efficiency at two contact materials Au and Tl is considered in the energy range 0 - 3 MeV. From the graph (figure 7), it can be seen that the efficiency of two materials is equivalent in 100 - 200 keV. The efficiency of contact material Au is higher than Tl from 1 MeV to 3 MeV.



Figure 7: The efficiency of TlBr with Ohmic contact Au and Tl

### 4. Results

By applying PENELOPE program based on Monte Carlo method, is has basically solved the problem of detector simulation. The efficiency of TlBr detector is calculated according to TlBr layer thickness and Ohmic contact as well as comparing to the efficiency of CdZnTe detector. TlBr detector has high efficiency from 100 keV to 200 keV. The efficiency of TlBr detector is equivalent to CdZnTe detector in same range energy. At 1 MeV energy onwards, the efficiency of TlBr detector is higher than CdZnTe detector.

## 5. Conclusion

In the simulation, calculating the performance of TlBr detector based on the thickness layer, the photon energy, and the Ohmic contact is a complex problem because of the interaction between photon and matter. By using PENELOPE program based on Monte Carlo method, this problem was basically solved.

The results from this simulation are very useful for manufacturing detector as well as predicting usability. However, they are only used for the reference purpose and need to compare with other results from many programs or methods and also with practical results. The simulation and the practical calculation also have many different conditions and errors. In the future, it is needed to contribute a professional program for calculating more accuracy.

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