Calculation of Atomic Parameters of Bismuth Germinate Detectors

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Abstract

In the present work, different methods were used to calculate the atomic cross-sections, electronic cross-sections, effective Z, effective electron density and mean free path for the $\text{Bi}_4\text{Ge}_3\text{O}_{12}$ gamma ray detector popularly known as BGO detector. The methods are Direct method using attenuation coefficients evaluated using WinXCom software, the others are Direct $Z_{\text{eff}}$ software, Auto$Z_{\text{eff}}$ software, XMuDat software and still another method used is Power law method. The results of first two methods i.e. Direct method and Direct $Z_{\text{eff}}$ software are in good agreement with each other. These results are also reproduced nicely by power law method. The $Z_{\text{eff}}$ predicted by Auto$Z_{\text{eff}}$ are too large compared with our predictions and XMuDat predicts too small value for $Z_{\text{eff}}$.

Key words: Attenuation coefficients, $Z_{\text{eff}}$, BGO Detector, Atomic cross-sections.

1. Introduction

Calculation of atomic cross-sections, electronic cross-sections, effective Z, effective electron densities, mean free path etc. are important in determining the penetration of gamma rays in various materials specially in $\gamma$-ray detectors. These parameters also help in choosing and designing various $\gamma$-ray detectors. These parameters are also important in other fields like radiation dosimeter, design of radiation shields etc. These atomic parameters has been calculated by various workers\textsuperscript{1-7} in different materials.

In case of gamma ray detectors, an alternative to NaI(Tl) scintillation detectors, Bismuth Germinate detectors $\text{Bi}_4\text{Ge}_3\text{O}_{12}$ (commonly known as BGO) are commercially available as crystals of various shapes and sizes. It has high density (~7.13 g/cm\textsuperscript{3}) and large atomic number of Bismuth (83). These properties make them

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highly probable for photo electric effect compared to other available scintillators. Also its chemical, mechanical and non-hygroscopic nature makes BGO easy to handle, use and store.

BGO is an example of a pure inorganic scintillator that does not require the presence of trace activators (like Tl in NaI detectors). In BGO luminescence is associated with an optical transition of the Bi$^{3+}$ ion. There is relatively large shift between the optical absorption and emission spectra of the Bi$^{3+}$ states. Therefore there is relatively little self absorption of its light in the scintillator itself and crystal remains almost transparent over large dimensions.

However, one major drawback of BGO is that the light yield of it is about 10 to 20 % as compared to NaI(Tl) detector. In spite of this fact BGO detectors are very widely used in many fields like particle physics, aerospace, nuclear medicine, geology exploration etc. BGO arrays are most popular for gamma ray spectroscopy where space is limited and are used in association with semiconductor detectors in anti Compton suppression mode. These days they are widely used in positron emission tomography because of their timing characteristics.

In these $\gamma$-ray spectroscopic studies, precise response functions of BGO are required. In order to calculate the response functions, the precise mass attenuation coefficients, electron densities effective atomic number of the detector as a function of energy of incident radiations are required. However, the experimental data for these parameters are scarce for $\gamma$-rays. Therefore, in the present work it was decided to calculate these parameters from ab-inito and also evaluate these parameters with various theoretical codes available.

To the best of our knowledge, no such calculations are available in literature. We could find one such work$^8$, where effective Z of BGO detector has been experimentally evaluated at only 5.1 MeV incident gamma ray energy.

2. Theory:

The effective atomic number and other related parameters can be calculated in number of ways. The methods used in the present work are described below:

2.1 Direct Method:

In this method$^9$ $\gamma$-ray beam while passing through a given material gets attenuated. Intensity (I) of the attenuated beam is connected to the intensity ($I_0$) of unattenuated beam while passing through a material of thickness x cm.is given by the Lambert – Beers law

$$I = I_0 e^{-\mu x}$$

$\mu$ is known as linear attenuation coefficient as its units are cm$^{-1}$. Mass attenuation coefficient $\mu_m$ is given by

$$\mu_m = \frac{\mu}{\rho}$$

(1)

If the material through $\gamma$ - ray is passing is a composite material, then total $\mu_m$ will be

$$\mu_m = \sum_i W_i \frac{\mu_i}{\rho}$$

(2)

Here $W_i$ is the weight fraction if the $i^{th}$ element.

For composite materials, the weight fraction is given by

$$W_i = \frac{n_i A_i}{\sum_i n_i A_i}$$

with the condition $\sum_i W_i = 1$

where $A_i$ is the atomic weight of the $i^{th}$ element and $n_i$ is the number of formula units. For example, in Bi$_4$Ge$_3$O$_{12}$, $n_i$ for Bi is 4, for Ge it is 3 and for O it is 12.

Mass attenuation coefficients $\mu_m$ for a given material and energy have been calculated using the
WinXCom software\(^{10}\).

The values of mass attenuation coefficients have been used to calculate the total atomic cross-section \(\sigma_t\) using the relation\(^{11}\)
\[
\sigma_t = \frac{\mu M}{N_A}
\]
(3)

Where \(M\) is the atomic mass of the material and \(N_A\) is Avagadro’s number.

Total electronic cross-section \(\sigma_e\) for a material is given by\(^{12}\)
\[
\sigma_e = \frac{1}{N_A} \sum_i f_i A_i (\mu \mu_m) \frac{Z_i}{Z_{eff}}
\]
(4)

where \(f_i\) is the fractional abundance of the element \(i\) with respect to the number of atoms such that \(\sum_i f_i = 1\)

\(Z_{eff}\) is the ratio of total atomic cross-section \(\sigma_t\) and total electronic cross-section \(\sigma_e\) and is evaluated using the relation
\[
Z_{eff} = \frac{\sigma_t}{\sigma_e}
\]
(5)

Number of electrons per unit mass or effective electron number or electron density can be determined using the relation\(^{12,13}\),
\[
N_e = \frac{\mu_m}{\sigma_e}
\]
(6)

Finally, the average distance between two successive interactions or photon mean free path is given by
\[
\lambda = \frac{1}{\mu}
\]
(7)

2.2 Direct \(Z_{eff}\) software:

The software Direct \(Z_{eff}\) was developed by Adam and Tanfer\(^{14}\) for calculating effective atomic numbers, effective electron densities, mass attenuation coefficients etc. between the energy range 1 keV to 100 GeV. In the present investigations, this software has been used to compare our theoretical results for electron densities and effective atomic number as a function of incident gamma rays for BGO detector.

2.3 Power Law:

There is another oversimplified way to evaluate \(Z_{eff}\). This formulism is known as Power Law and is of the form\(^{15}\)
\[
Z_{eff} = \sqrt[m]{\prod f_i Z_i^m}
\]
(8)

As discussed, \(f_i\) is the fractional abundance of the element \(i\) with respect to the number of atoms such that \(\sum_i f_i = 1\). Various workers\(^{16,17}\) used a value of 2.94 for the exponent \(m\) in eq (8).

2.4 XMuDat software:

This software developed by Nowotny\(^{18}\) is capable to produce a single value of \(Z_{eff}\) for compounds. It
uses the following formula for the calculation of $Z_{\text{eff}}$

$$Z_{\text{eff}} = \left( \sum_i \alpha_i Z_i^{m-1} \right)^{1/(m-1)}$$

where $\alpha_i$ is the fractional number of electrons of the $i$th element and $m$ is a constant between 3 and 5. Its value is normally set equal to 3.6 for materials with $Z_{\text{eff}} < 6$ and about 4.1 for compounds with $Z_{\text{eff}} > 6^{19}$.

2.5 AutoZ\text{eff} software:

In AutoZ\text{eff} software$^{20}$ $Z_{\text{eff}}$ is determined by considering the co-relation between atomic cross-section and atomic number. In this software a matrix of cross-sections is constructed for atomic numbers varying between 1 to 100 and energies between 10 keV to 1 GeV. The cross-sections for polyelemental materials were calculated via linear additivity. These cross-section values were than compared with the cross-section matrix as a function of $Z$ and at each energy effective atomic numbers were extracted by interpolation of $Z$ values between adjacent cross-sectional data.

3. Results and discussion

Variation of total atomic cross-section, electronic cross-section, effective $Z$, effective electron density and mean free path as calculated by Direct method are shown in figs (1), (2), (3), (4) and (5) respectively. These values are evaluated according to the equations (3), (4), (5), (6) and (7) respectively.

For comparison, effective $Z$ and effective electron density as calculated using Direct $Z_{\text{eff}}$ software are also shown in Figs (6) and (7) respectively.

As is evident from figs (3) and (6) effective $Z$ calculated as per relations are nicely reproduced by Direct-$Z_{\text{eff}}$ software and similar conclusion can be drawn for effective electron density as is evident from figs (4) and (7). At different energies, $Z_{\text{eff}}$ was also evaluated using software AutoZ\text{eff}. The results are shown in fig. 8. In table 1, we display the values of effective $Z$ calculated by three methods, viz., Direct method, Direct $Z_{\text{eff}}$ software and AutoZ\text{eff} software at some energies. As is evident from the table, the effective atomic number $Z_{\text{eff}}$ calculated by Direct method and Direct $Z_{\text{eff}}$ software are in very good agreement in the entire energy range of 1 MeV to 50 MeV.

| Energy (MeV) | Direct method | Direct $Z_{\text{eff}}$ software | Auto $Z_{\text{eff}}$ software |
|-------------|---------------|---------------------------------|-----------------------------|
| 1           | 32.13         | 32.20                           | 34.07                       |
| 2           | 31.03         | 31.10                           | 31.88                       |
| 3           | 32.80         | 32.84                           | 32.98                       |
| 5           | 36.69         | 36.60                           | 34.60                       |
| 10          | 43.28         | 43.25                           | 36.29                       |
| 20          | 49.00         | 48.95                           | 37.27                       |
| 40          | 52.34         | 52.37                           | 37.85                       |
| 50          | 53.01         | 53.04                           | 37.93                       |

The $Z_{\text{eff}}$ calculated by AutoZ\text{eff} software is also in good agreement with the Direct and Direct $Z_{\text{eff}}$ software predictions up to 5 MeV. At higher energies its predictions under estimate the value of $Z_{\text{eff}}$.

Calculations by power law method reproduces the $Z_{\text{eff}}$ values around 20 MeV with $m = 2.94$. For higher
energies ~ 50 MeV, the value of m around 3.1 gives the better results and for lower energies, the value of m around 1.3 reproduces the results nicely.

Software XMuDat predicts the $Z_{\text{eff}}$ for BGO detector as 73.

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Fig 5: Variation of mean free path as a function of energy of gamma rays by Direct method.
Fig 6: Variation of $Z_{eff}$ as a function of energy of gamma rays as calculated with Direct-$Z_{eff}$ software.
Fig 7: Variation of effective electron density as a function of energy of gamma rays as calculated with Direct-$Z_{eff}$ software.
Fig 8: Variation of $Z_{eff}$ as a function of energy of gamma rays as calculated with Auto-$Z_{eff}$ software.
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