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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_{eff} software, Auto Z_{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_{eff} software are in good agreement with each other. These results are also reproduced nicely by power law method. The Z_{eff} predicted by Auto Z_{eff} are too large compared with our predictions and *XMudat* predicts too small value for Z_{eff} .

Key words: Attenuation coefficients, Z_{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 γ -ray detectors. These parameters also help in choosing and designing various γ -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 workers¹⁻⁷ 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 ($\sim 7.13 \text{ g/cm}^3$) and large atomic number of Bismuth (83). These properties make them

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 γ -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 γ -rays. Therefore, in the present work it was decided to calculate these parameters from ab-initio 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 work⁸, 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 method⁹ γ -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

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

μ is known as linear attenuation coefficient as its units are cm^{-1} . Mass attenuation coefficient μ_m is given by

$$\mu_m = \frac{\mu}{\rho} \quad (1)$$

If the material through γ - ray is passing is a composite material, then total μ_m will be⁹

$$\mu_m = \sum_i w_i \frac{\mu_i}{\rho} \quad (2)$$

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

For composite materials, the weight fraction is given by

$$w_i = \frac{n_i A_i}{\sum_i n_i A_i} \quad \text{with the condition} \quad \sum_i w_i = 1$$

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

Mass attenuation coefficients μ_m for a given material and energy have been calculated using the

WinXCom software¹⁰.

The values of mass attenuation coefficients have been used to calculate the total atomic cross-section σ_t using the relation¹¹

$$\sigma_t = \frac{\mu_m M}{N_A} \quad (3)$$

Where M is the atomic mass of the material and N_A is Avagadro's number.

Total electronic cross-section σ_e for a material is given by¹²

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} (\mu \mu_m)_i = \frac{\sigma_t}{Z_{eff}} \quad (4)$$

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 σ_t and total electronic cross-section σ_e and is evaluated using the relation

$$Z_{eff} = \frac{\sigma_t}{\sigma_e} \quad (5)$$

Number of electrons per unit mass or effective electron number or electron density can be determined using the relation^{12,13}.

$$N_e = \frac{\mu_m}{\sigma_e} \quad (6)$$

Finally, the average distance between two successive interactions or photon mean free path is given by

$$\lambda = \frac{1}{\mu} \quad (7)$$

2.2 Direct Z_{eff} software:

The software Direct Z_{eff} was developed by Adam and Tanfer¹⁴ 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 form¹⁵

$$Z_{eff} = \sqrt[m]{f_i Z_i^m} \quad (8)$$

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 Nowotny¹⁸ is capable to produce a single value of Z_{eff} for compounds. It

uses the following formula for the calculation of Z_{eff}

$$Z_{Eff} = (\sum_i \alpha_i Z_i^{m-1})^{\frac{1}{m-1}}$$

where α_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 $Z_{eff} < 6$ and about 4.1 for compounds with $Z_{eff} > 6$ ¹⁹.

2.5 Auto Z_{eff} software:

In Auto Z_{eff} software²⁰ Z_{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 then 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_{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_{eff}* software and similar conclusion can be drawn for effective electron density as is evident from figs (4) and (7). At different energies, Z_{eff} was also evaluated using software Auto Z_{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_{eff} software and Auto Z_{eff} software at some energies. As is evident from the table, the effective atomic number Z_{eff} calculated by Direct method and Direct Z_{eff} software are in very good agreement in the entire energy range of 1 MeV to 50 MeV.

Table 1: Effective Z calculated by Direct method, Direct Z_{eff} and Auto Z_{eff} software

Energy (MeV)	Direct method	Direct Z_{eff} software	Auto Z_{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_{eff} calculated by Auto Z_{eff} software is also in good agreement with the Direct and Direct Z_{eff} software predictions up to 5 MeV. At higher energies its predictions under estimate the value of Z_{eff} .

Calculations by power law method reproduces the Z_{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_{eff} for BGO detector as 73.

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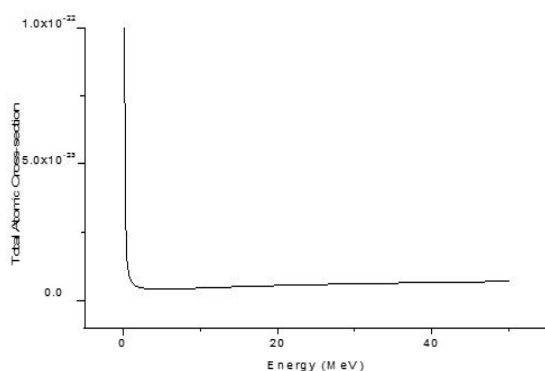


Fig 1: Variation of total atomic cross-section as a function of energy of gamma rays by Direct method.

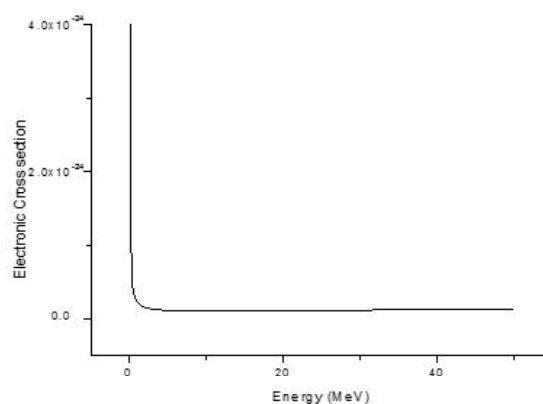


Fig 2: Variation of electronic cross-section as a function of energy of gamma rays by Direct method.

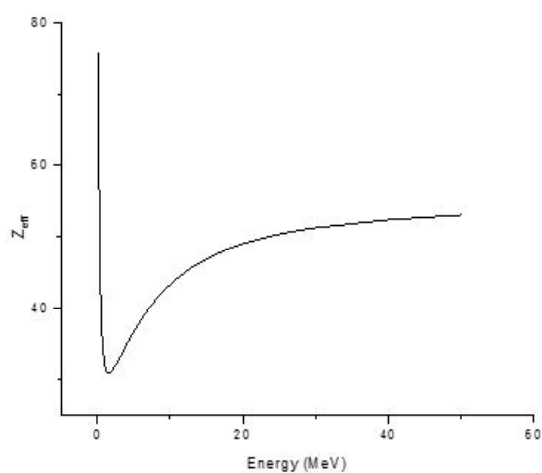


Fig 3: Variation of effective Z as a function of energy of gamma rays by Direct method.

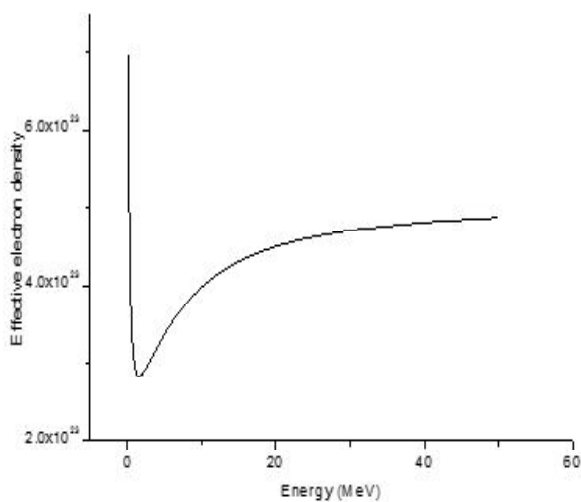


Fig 4: Variation of effective electron density as a function of energy of gamma rays by Direct method.

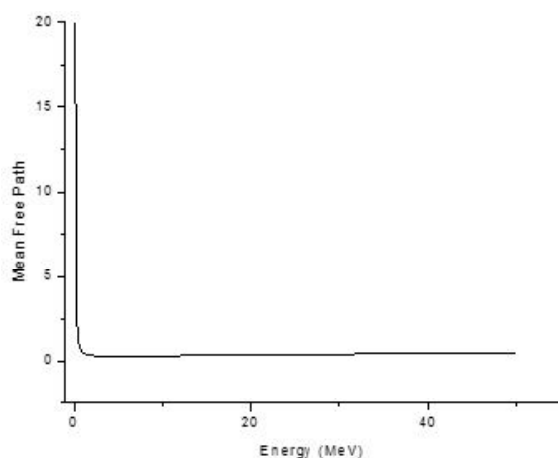


Fig 5: Variation of mean free path as a function of energy of gamma rays by Direct method.

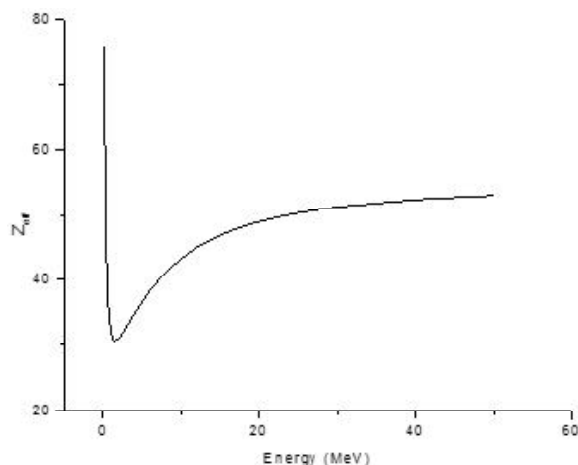


Fig 6: Variation of Z_{eff} as a function of energy of gamma rays as calculated with *Direct- Z_{eff}* software.

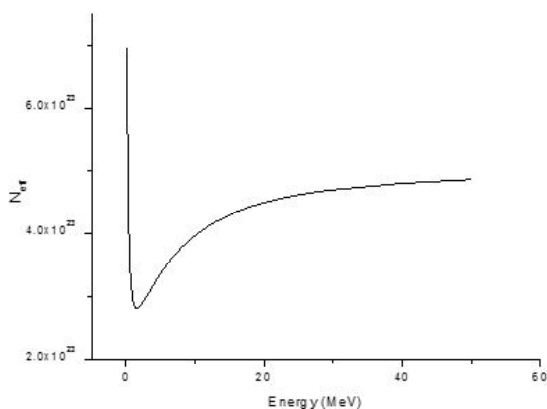


Fig 7: Variation of effective electron density as a function of energy of gamma rays as calculated with *Direct- Z_{eff}* software.

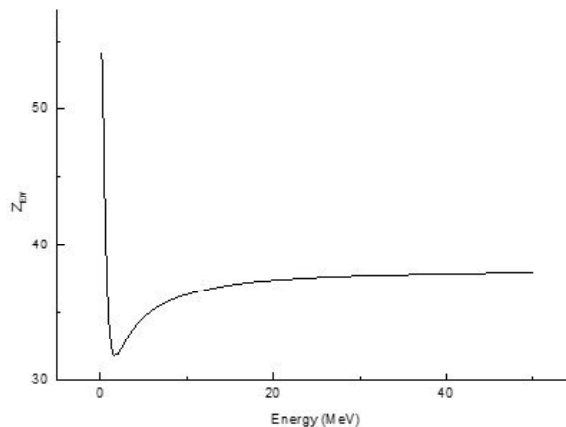


Fig 8: Variation of Z_{eff} as a function of energy of gamma rays as calculated with *Auto- Z_{eff}* software.

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