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A SEMI-EMPIRICAL MODEL FOR THE GAMMA-RAY RESPONSE FUNCTION OF GERMANIUM DETECTORS BASED ON FUNDAMENTAL INTERACTION MECHANISMS

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A model for describing the response function of large volume gamma-ray detectors over the range of incident gamma ray energies between 1.0 and 6.5 MeV has been developed and applied to a 39% high purity germanium detector. Functional forms for describing the various features of the response function are based either on empirical functions or on the shape of exact analytical expressions for the interaction mechanisms as in the case of multiple Compton scattering of the primary and the annihilation photons. These functions are combined and fit by an appropriate linear–nonlinear least squares method to measured single energy photon spectra. The model parameters so obtained are then fit to simple functions of the incident gamma-ray energies to form the complete response function of the detector. Validity of the model is demonstrated by synthesizing a ^{49}Ca spectrum using the response function and comparing it to the equivalent measured spectrum.

1. Introduction

Generation of spectral response functions of radiation detectors is a problem of generic interest in spectroscopy applications involving both modeling of measurement systems in order to predict the spectral response of the system and unfolding or analysis of measured spectra to yield the source spectrum that is incident on the detector. A typical case of the former application is reported by Gardner and Doster [1], in which they combined a Monte Carlo predicted X-ray fluorescence source energy spectrum with an analytical response function of their Si(Li) detector to synthesize an accurate predicted spectrum of austenitic stainless steel. Use of a detector response matrix to unfold measured spectra has been reported by many investigators including Ingersoll and Wehring [2], who used an experimentally generated response matrix to unfold NE-213 gamma-ray spectra.

Response functions can be generated by one of three different methods: one method is to measure the pulse height spectra resulting from a large number of monoenergetic sources and to form a response matrix as a function of pulse height and source energy by suitable interpolation of the measured spectra. Another way is to model the energy deposition within the detector resulting from all of the major mechanisms by the use of Monte Carlo simulation. The third method is to fit analytical functions that describe the various features of measured spectra from single energy sources, obtain the best (least-squares) estimates of the parameters in the fitting functions, and then obtain (again by least-squares) these parameters as a function of source energy. All of these methods have inherent advantages and disadvantages. The first and the third methods are more direct than the second method, but they require the availability of either a large or small number of monoenergetic sources covering the range of interest for the source energy. The Monte Carlo method requires a good understanding of the geometry and dimensions of the detector which are not easily specified for certain types of detectors such as Ge detectors. On the other hand, the Monte Carlo method gives the user a great deal more insight into the physics of spectrometry than the other two methods which are based on experimental data.

The Monte Carlo approach to the study of the response of Ge detectors has been used and reported by a large number of authors [3–10]. Wainio and Knoll [3] developed a Monte Carlo program for relatively small Ge detectors in which they followed the gamma-ray interactions and the secondary electrons formed from these interactions and compared the results to a measured ^{60}Co spectrum which showed that the

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relative shapes of the Compton continua were in agreement. Meixner [4] formulated a simplified Monte Carlo program for Ge detectors using assumptions such as neglecting the insensitive regions of the detector and using isotropic scattering in the laboratory system. The results showed good agreement with measurements as far as the relative shapes of the features were concerned. Seltzer [5] has reported a thorough study of the response of intrinsic Ge detectors to photons with energy less than about 300 keV. Based on Monte Carlo simulated spectra, he formulated empirical analytical expressions for the various spectral features including the Ge X-ray escape, the Compton continuum for single scatter corrected empirically to include multiple scatter contribution, the backscatter continuum due to the backing material, and the full energy peak. The generated response matrix was used to unfold the measured spectrum from a tungsten-anode X-ray generator. Various other authors have used Monte Carlo codes to generate Ge response functions resulting from extended sources [6,7], to study the effects of detector cladding and shielding [8], to investigate the response of Ge detectors to high energy beta- and gamma-rays [9], and to determine the effect of multiple interactions on pulse shapes from coaxial Ge detectors [10].

In this paper, we present the response function of a 39% high purity germanium detector. Our use of the response function is in generating gamma-ray spectra from Monte Carlo models of neutron capture gamma-ray analysis systems for bulk media. For this application, the best way to include the detector response function is as an analytical expression and we have therefore chosen the third method (namely, fitting analytical functions to experimental spectra from single energy photons) mentioned earlier to generate the response function. Various investigators have used a similar approach to fit the full energy peak region of the spectrum. Prominent among these are the papers by McNelles and Campbell [11], Jorch and Campbell [12], and by Campbell and Jorch [13], in which they examined single peak fitting by using additive functions and by using convolution to account for the low-energy tailing which is observed in Ge and Si(Li) detectors. A number of publications have studied the effects of using many different types of peak fitting functions on the analysis of high resolution gamma-ray spectra [14–19].

All of the fitting programs referenced above are concerned only with the Gaussian peak and its associated tail and background continuum. However, for the generation of synthesized spectra, the complete spectral range of the response function must be considered. For high energy gamma-rays, this involves fitting the Compton continuum, the annihilation photon escape peaks and their Compton continuum features, the full energy peak and the incomplete charge collection tail, and the background continuum. Gardner and Doster [1] have developed such a complete response function for a Si(Li) detector. In the present paper we follow the same general principles for numerical fitting of the Ge spectra, but the functions that describe some of the features are quite different.

2. Spectral features and models

The energy range of interest in this paper for gamma-ray spectra is from about 1 MeV to some high energy limit dictated by the highest gamma-ray energy for which spectra could be collected. The lower limit of 1 MeV is due to the fact that below this energy, the measured spectra generally contain features that are either highly system dependent or do not result directly from the incident photon.

Within this energy range, the spectral features that have to be modeled are (i) the full energy peak, (ii) the single escape peak, (iii) the double escape peak, (iv) the incomplete charge collection (exponentially shaped) tail on the left side of the full energy peak, (v) the uniform incomplete charge collection from zero to the full energy, (vi) the Compton continuum including the multiple scatter region, and (vii) the Compton scattering of one of the annihilation photons before its escape which contributes to a continuum in the region between the two escape peaks.

For the case of an incident photon of energy E_0 MeV, the functions described in sects. 2.1–2.9 are used to describe the various spectral features.

2.1. Full energy peak

A Gaussian distribution with variance B_1^2 and a normalization parameter A_1 is used to describe the full

energy peak excluding the tail on the left side:

$$f_1(E_0, E) = \left(\frac{A_1}{\sqrt{2\pi}\,B_1}\right) \exp\left\{-\frac{(E-E_0)^2}{2B_1^2}\right\}. \tag{1}$$

2.2. Single escape peak

A Gaussian distribution with peak at $E_0 - 0.511$ MeV, variance B_2^2 and normalization parameter A_2 is used:

$$f_2(E_0, E) = \left(\frac{A_2}{\sqrt{2\pi}\,B_2}\right) \exp\left\{-\frac{[E-(E_0-0.511)]^2}{2B_2^2}\right\}. \tag{2}$$

2.3. Double escape peak

This function is similar to the one for the single escape peak except that the peak location is at $E_0 - 1.022$ MeV:

$$f_3(E_0, E) = \left(\frac{A_3}{\sqrt{2\pi}\,B_3}\right) \exp\left\{-\frac{[E-(E_0-1.022)]^2}{2B_3^2}\right\}. \tag{3}$$

2.4. Exponential tail on the low energy side of the full energy peak

The functional form used is the convolution of an exponential function with a Gaussian function. The resulting function is given by

$$f_4(E) = A_4 \exp\left\{\frac{(E-E_0)}{\sqrt{2}\,\pi B_1 B_4}\right\} \operatorname{erfc}\left\{\left[\frac{(E-E_0)}{\sqrt{2}\,B_1}\right] + \left[\frac{1}{2B_4}\right]\right\}. \tag{4}$$

This function has the same form as the corresponding expression that is used for the short term exponential tail in the computer code Gauss VII [18].

2.5. Flat continuum

A constant function

$$\begin{aligned} F(E') &= a, \qquad E' < E_0, \\ &= 0, \qquad E' > E_0, \end{aligned} \tag{5}$$

when folded with a Gaussian function gives an expression of the form

$$f_5(E_0, E) = A_5 \operatorname{erfc}\left\{\frac{(E-E_0)}{\sqrt{2}\,B_1}\right\}. \tag{6}$$

Such a function was used by Doster and Gardner [1] in the X-ray response function for a Si(Li) detector and it is observed that a similar function is also needed for Ge detectors.

2.6. Single scatter Compton continuum

The expression for the energy deposited in a single Compton scatter is well documented in textbooks [20]. In order to account for the roll-off at the Compton edge that is observed in experimental spectra, we terminate the electron energy function with a complimentary error function. The modified single scatter function is given by

$$\left.\begin{aligned} f_6(E_0, E) &= A_6\left[\left(\frac{E_0}{E'}\right)+\left(\frac{E'}{E_0}\right)-1+\cos^2\theta\right]\operatorname{erfc}\left[\frac{(E-B_5)}{\sqrt{2}\,B_6}\right], \qquad E \leqslant E_c \\ f_6(E_0, E) &= 0, \qquad E > E_c, \end{aligned}\right\} \tag{7}$$

where $E' = E_0 - E$ and is equal to the photon energy,

$$\cos\theta = 1 + \left(\frac{m_0c^2}{E_0}\right) - \left(\frac{m_0c^2}{E'}\right),$$

and

$$E_c = E_0 \Big/ \left[1 + \frac{m_0c^2}{2E_0}\right].$$

2.7. Multiple scatter Compton continuum

The single Compton scatter function does not adequately fit measured Compton continuum regions in gamma-ray spectra. Moreover, the region between the Compton edge and the full energy peak contains contributions from multiply scattered gamma-rays. For these reasons, we have derived expressions for the energy deposition due to two and three Compton scatters. The derivations assume that the spatial distributions of once-scattered and of twice-scattered photons within the detector are uniform. The derivations are long and tedious and are available from the authors.

The energy deposition function, f_7, for double Compton scattering is given by the following set of equations:

$$\left.\begin{aligned} f_7(E_0, E) &= 0, \qquad \alpha'' > \alpha, \\ f_7(E_0, E) &= A_7\int_{\alpha''}^{\alpha} H(\alpha, \alpha')H(\alpha', \alpha'')\,\mathrm{d}\alpha', \qquad \alpha/(1+2\alpha) < \alpha'' < \alpha, \\ f_7(E_0, E) &= A_7\int_{\alpha/(1+2\alpha)}^{\alpha''/(1-2\alpha'')} H(\alpha, \alpha')H(\alpha', \alpha'')\,\mathrm{d}\alpha', \qquad \alpha/(1+4\alpha) < \alpha'' < \alpha/(1+2\alpha), \\ f_7(E_0, E) &= 0, \qquad 0 < \alpha'' < \alpha/(1+4\alpha), \end{aligned}\right\} \tag{8}$$

where

$$H(\alpha, \alpha') = \alpha'/\alpha^3 + (1/\alpha + 2/\alpha^2 - 2/\alpha^3)(1/\alpha') + 1/\alpha^2\alpha'^2 + 2/\alpha^3 + 1/\alpha^4,$$

and

$$\alpha = E_0/(m_0c^2), \qquad \alpha' = E'/(m_0c^2), \qquad \alpha'' = E''/(m_0c^2), \qquad E'' = E_0 - E.$$

The energy deposition function, f_8, for triple Compton scattering is given by the following set of

equations:

$$\left.\begin{aligned}
&f_8(E_0, E) = 0, \qquad \alpha'' > \alpha,\\
&f_8(E_0, E) = A_8 \int_{\alpha''}^{\alpha} \int_{\alpha''}^{\beta} H(\alpha, \beta)\, H(\beta, \gamma)\, H(\gamma, \alpha'')\, \mathrm{d}\gamma\, \mathrm{d}\beta, \qquad \alpha/(1+2\alpha) < \alpha'' < \alpha,\\
&f_8(E_0, E) = A_8 \left[\int_{\alpha/(1+2\alpha)}^{\alpha''/(1-2\alpha'')} \int_{\alpha}^{\beta} H(\alpha, \beta)\, H(\beta, \gamma)\, H(\gamma, \alpha'')\, \mathrm{d}\gamma\, \mathrm{d}\beta \right.\\
&\quad \left. + \int_{\alpha''/(1-2\alpha'')}^{\alpha} \int_{\beta/(1+2\beta)}^{\alpha''/(1-2\alpha'')} H(\alpha, \beta)\, H(\beta, \gamma)\, H(\gamma, \alpha'')\, \mathrm{d}\gamma\, \mathrm{d}\beta \right],\\
&\text{for } \alpha/(1+4\alpha) < \alpha'' < \alpha/(1+2\alpha),\\
&f_8(E_0, E) = A_8 \int_{\alpha/(1+2\alpha)}^{\alpha''/(1-4\alpha'')} \int_{\beta/(1+2\beta)}^{\alpha''/(1-2\alpha'')} H(\alpha, \beta)\, H(\beta, \gamma)\, H(\gamma, \alpha'')\, \mathrm{d}\gamma\, \mathrm{d}\beta,\\
&\text{for } \alpha/(1+6\alpha) < \alpha'' < \alpha/(1+4\alpha),\\
&f_8(E_0, E) = 0, \qquad 0 < \alpha'' < \alpha/(1+6\alpha).
\end{aligned}\right\} \tag{9}$$

All of the integrations in equation sets (8) and (9) can be performed analytically.

2.8. Compton continuum of annihilation photon

Between the two escape peaks, there is a feature that resembles a Compton continuum. This appears to be caused by Compton interaction of an annihilation photon before escaping from the detector. For simplicity, we have chosen to fit this feature by a single Compton scatter model similar to eq. (7), i.e.,

$$\left.\begin{aligned}
&f_9(E_0, E) = A_9 \left[\left(\frac{E_1}{E_1'} \right) + \left(\frac{E_1'}{E_1} \right) - 1 + \cos^2\theta_1 \right] \operatorname{erfc}\left[\frac{(E_2 - B_7)}{\sqrt{2}\, B_8} \right], \qquad E_2 < E_{C1},\\
&f_9(E_0, E) = 0, \qquad E_2 > E_{C1},
\end{aligned}\right\} \tag{10}$$

where

$$E_1 = 0.511 \text{ MeV}, \qquad E_2 = E - (E_0 - 1.022), \qquad E_1' = E_1 - E_2,$$

$$\cos\theta_1 = 1 + \left(\frac{m_0 c^2}{E_1} \right) - \left(\frac{m_0 c^2}{E_1'} \right), \qquad E_{C1} = E_1 \Big/ \left[1 + \left(\frac{m_0 c^2}{2E_1} \right) \right] = \tfrac{2}{3} E_1.$$

2.9. Multiple scattering of annihilation photon between the annihilation photon Compton edge and the single escape peak

This region is fitted simply by another complimentary error function similar to that in eq. (6):

$$f_{10}(E_0, E) = A_{10} \operatorname{erfc}\left[\frac{(E_2 - B_9)}{\sqrt{2}\, B_{10}} \right]. \tag{11}$$

The combination of the functions described in sects. 2.1–2.9 forms the response function of the detector. It contains 10 parameters (B_1–B_{10}) that appear in nonlinear functions of energy and 10 linear parameters (A_1–A_{10}). These model parameters have to be estimated from standard spectra of gamma-rays at known photon energies and the parameter values are then fitted to simple polynomial functions of photon energy.

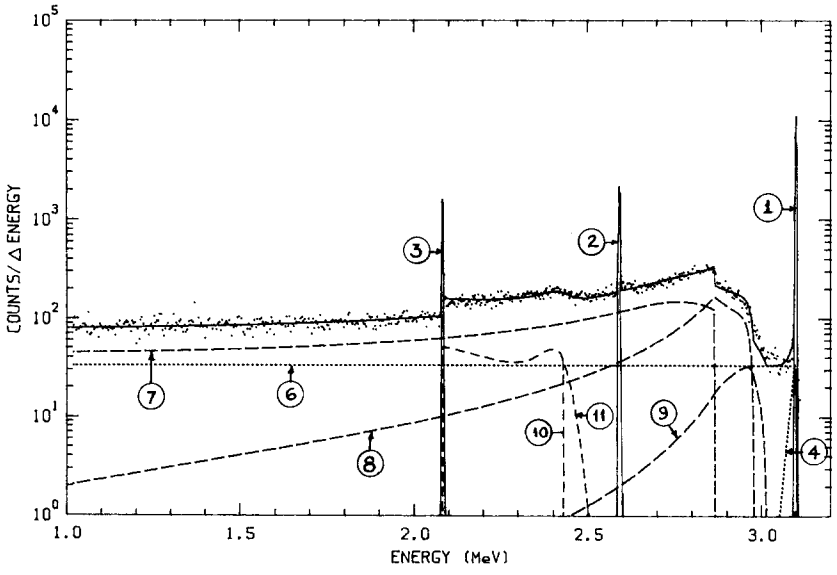

Fig. 1. ^{37}S 3.1033 MeV gamma-ray spectrum, measured (···), fitted spectrum (———), and its components. The number labels for the components refer to the corresponding equation numbers in sect. 2.

3. Determination of model parameters

The response function parameters are estimated for each source energy by a least squares fit of the response function to experimental standard spectra taken on a specific detector at known source photon energies. The detector was a 39% intrinsic germanium detector. Most of the gamma-ray sources in the high energy range have more than one energy, making it difficult to do parameter searching on their spectra. We have used the gamma-ray sources given in table 1 to obtain standard spectra.

The sources were prepared by irradiation of Al, Na, S, and H_2O in the N.C. State University Research Reactor and their spectra were recorded using standard spectroscopy instrumentation including a 2048-channel pulse height analyzer. Particular attention was given to accumulating the spectra at low enough counting rates to avoid the problems of resolution loss, pulse pile-up, and gain shift.

A linear–nonlinear least squares fitting program based on the Marquardt algorithm [21] was used to fit the experimental spectra to the response function model and to estimate the model parameter values. This program, called CURCON, is a modification of the nonlinear least squares fitting routine provided by Bevington [22]. The parameters A_1–A_{10} are determined by linear regression based on the reduced chi-square function and the parameters B_1–B_{10} are determined by the Marquardt technique which uses a combination of a gradient search and parabolic interpolation. The response function for each photon energy was expressed as a probability distribution function by normalizing its integral over the complete range to unity.

Figs. 1–4 show the experimental spectra and the model fits for all of the isotopic sources listed in table

Table 1
Gamma-ray sources used in estimating the response function parameters

Sources	Energy of photons (MeV)
^{28}Al	1.778770
^{24}Na	2.754142
^{37}S	3.1033
^{16}N	6.129170

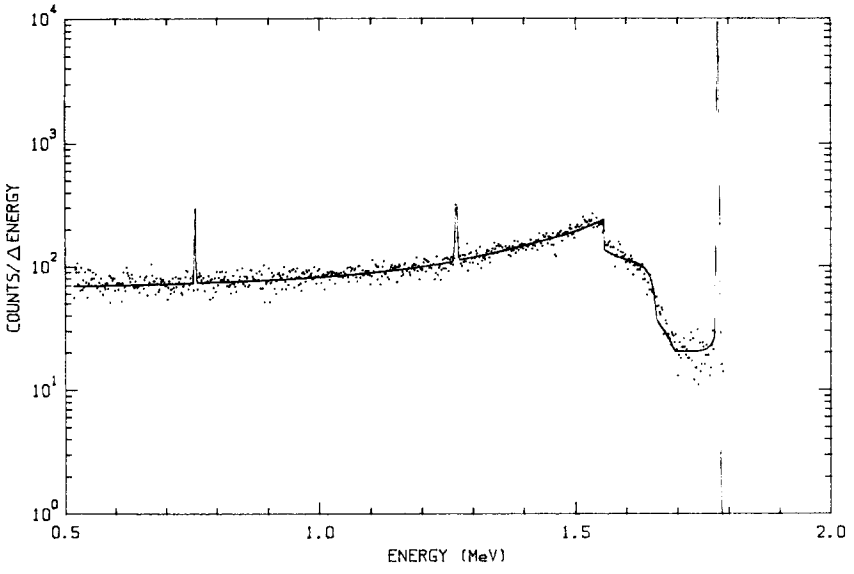

Fig. 2. ^{28}Al 1.7787 MeV gamma-ray spectrum, measured and fitted spectra.

1. The fits are generally excellent for energies greater than 0.5 MeV. Fig. 1 also shows the contribution of the fitting function for each of the features as discussed in sect. 2.

The model parameters B_1–B_6 are shown in figs. 5 and 6 as a function of photon energy E_0. All of the parameters are smoothly varying functions of energy so that they can be fit by simple functions of photon energy. The polynomial expressions for all of the parameters are given in table 2.

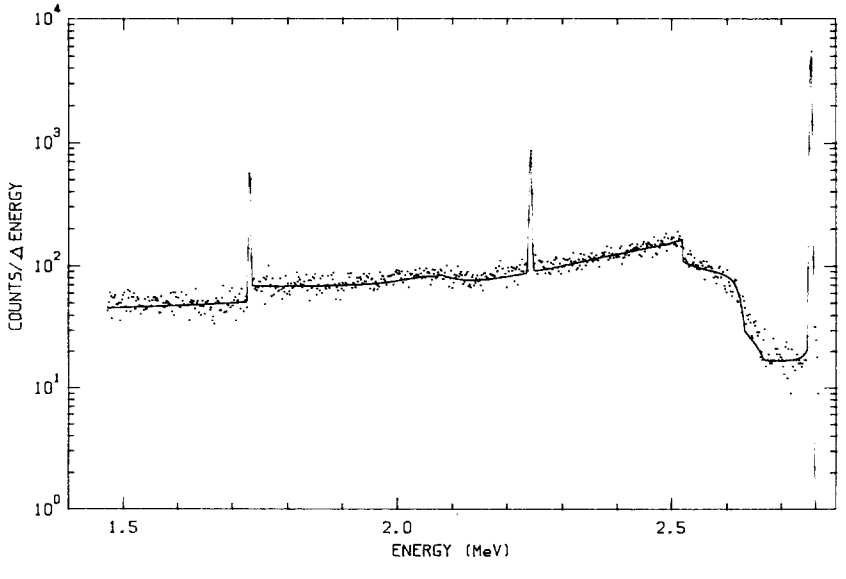

Fig. 3. ^{24}Na 2.754142 MeV gamma-ray spectrum, measured and fitted spectra.

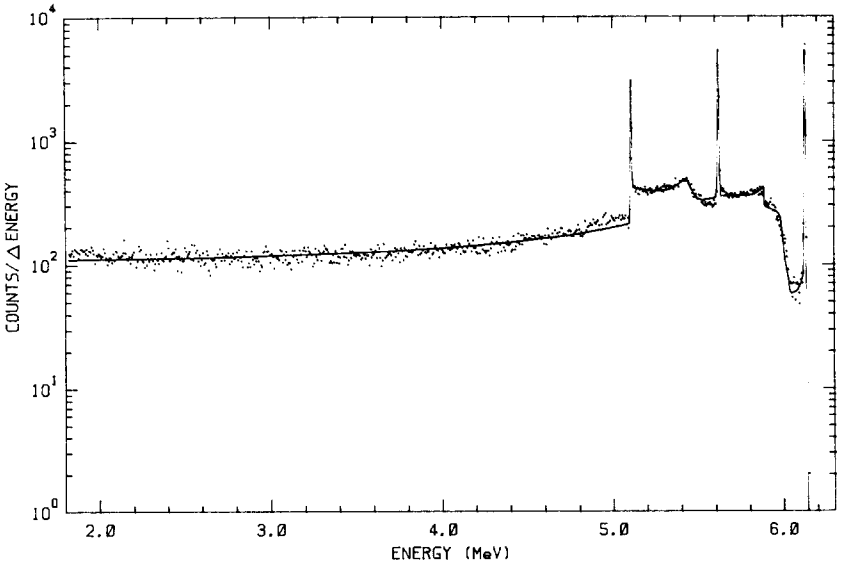

Fig. 4. ^{16}N 6.12917 MeV gamma-ray spectrum, measured and fitted spectra.

4. The response function and its verification

The response function in the approximate photon energy range 1–6.5 MeV for the particular detector we have used is given by

$$R(E_0, E) = \sum_{i=1}^{10} f_i(E_0, E), \tag{13}$$

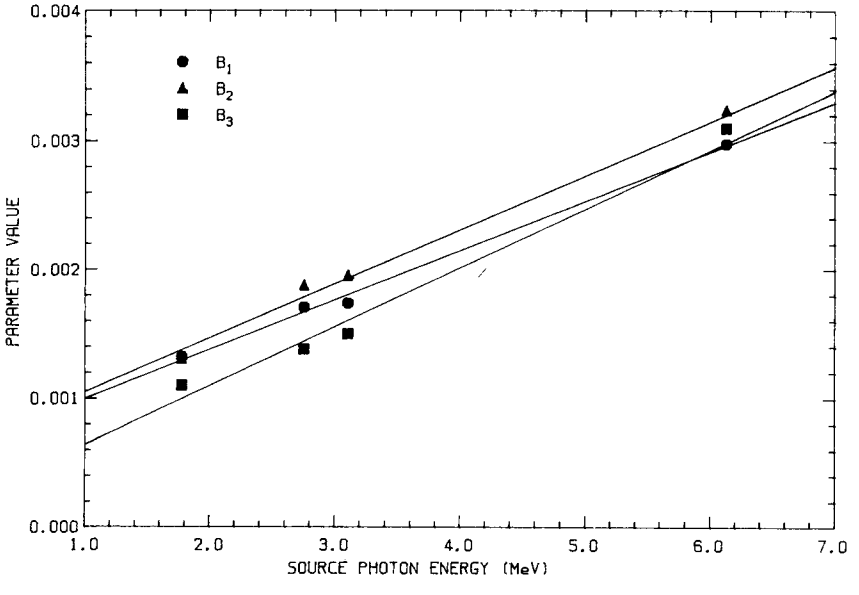

Fig. 5. Various nonlinear parameters in the Ge detector response function.

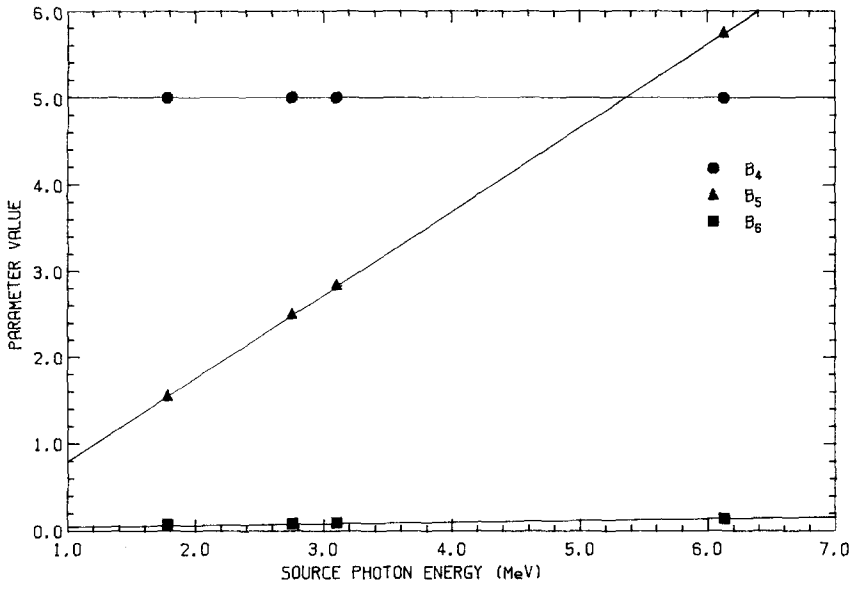

Fig. 6. Additional nonlinear parameters in the Ge detector response function.

where the $f_i(E_0, E)$ are given in sect. 2 for $i = 1, 2 \ldots 10$.

The response function of the germanium detector must be verified by generating the spectrum for an isotope that emits multiple photons and comparing it to its experimental spectrum. We have chosen ^{49}Ca for this purpose since it emits monoenergetic gamma rays of two different energies. Fig. 7 shows the model prediction and the experimental spectrum. The agreement is good in all regions beyond about 0.6 MeV.

Table 2
Fitted functions for the response function parameters

Parameter	Fitted function of energy, E
A_1	$-0.937680+0.203032\times10^{1}\ E_0^{-0.2}-0.892372\ E_0^{-0.4}$
A_2	$-0.102569\times10^{-1}+0.107664\ \sqrt{E_0}-0.205109\times10^{-1}\ E_0$
A_3	$-0.635789\times10^{-1}+0.688801\times10^{-1}\ \sqrt{E_0}-0.141398\times10^{-1}\ E_0$
A_4	$0.154572\times10^{-1}+0.390365\times10^{-2}\ E_0$
A_5	$-0.110826\times10^{-1}+0.911437\times10^{-1}/\sqrt{E_0}$
A_6	$0.721355\times10^{-2}+0.185895/E_0^2$
A_7	$-0.775913\times10^{1}+0.204322\times10^{2}\ E_0^{0.1}-0.124189\times10^{2}\ E_0^{0.2}$
A_8	$-0.343254\times10^{-2}+0.213600\times10^{-1}\ E_0-0.882892\times10^{-3}\ E_0^2$
A_9	$-0.733405\times10^{-1}+0.815994\times10^{-1}\ \sqrt{E_0}-0.134590\times10^{-1}\ E_0$
A_{10}	$-0.248304+0.307059\ \sqrt{E_0}-0.680431\times10^{-1}\ E_0$
B_1	$0.624674\times10^{-3}+0.380308\times10^{-3}\ E_0$
B_2	$0.649538\times10^{-3}+0.414838\times10^{-3}\ E_0$
B_3	$0.188524\times10^{-3}+0.455144\times10^{-3}\ E_0$
B_4	5.0
B_5	$-0.156849+0.965065\ E_0$
B_6	$0.443463\times10^{-1}+0.169773\times10^{-1}\ E_0$
B_7	0.3406689
B_8	0.30288849×10^{-1}
B_9	0.35122882
B_{10}	0.31844873×10^{-1}

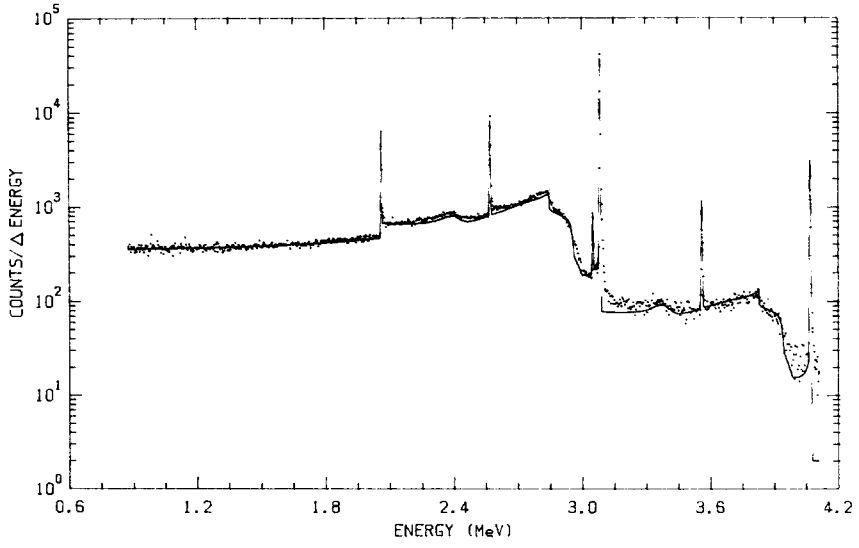

Fig. 7. ^{49}Ca 3.0844 MeV and 4.0719 MeV gamma-ray spectrum, measured and generated using Ge detector response function.

5. Discussion and summary

In this paper, a systematic method of determining the energy spectrum response function of germanium detectors for high energy gamma-rays is presented. The mathematical form of the response function can be generally applied to any large volume germanium detector. The parameter values are specific to a particular detector and the approach does not require any prior knowledge or assumptions regarding the shape or dimensions of the detector active volume.

The response function of a 39% intrinsic germanium detector is presented in the form of an analytical function of photon energy and the spectral energy variable. It contains ten different features, each described by a mathematical expression that extends over its entire range. Five of these ten features are Compton scattering distributions and are described by theoretical expressions, thus minimizing the number of model parameters to be estimated. To the knowledge of the authors, expressions for energy deposition from double and triple Compton scattering have not been reported before in the literature on radiation detectors.

The response function contains ten nonlinear parameters which appear in the mathematical functions which describe the various features. These functions are then combined as a linear sum using ten linear parameters. Of the nonlinear parameters (B_1–B_{10}) B_4, B_7, B_8, B_9 and B_{10} are independent of the source energy as shown in table 2. B_7, B_8, B_9 and B_{10} which appear in the representation of the Compton distributions for the annihilation photon are constants because their values are nearly the same as the values of B_5 and B_6 when those parameters are evaluated at 0.511 MeV, indicating self consistency in the response function parameters.

The response function is benchmarked against an experimental spectrum obtained for ^{49}Ca. As evident from fig. 7 the agreement is excellent. Using the response function it should be possible to synthesize the spectrum which is to be expected for any given source energy distribution with energies between 1 and 6.5 MeV. We expect one major use of this to be in capture gamma-ray spectroscopy using small samples exposed to neutron beams where synthesized spectra may be used to test detection limits of individual elements inside a sample matrix.

Our primary use of the response function of the Ge detector is in capture gamma-ray analysis of bulk samples. We can now take a measured spectrum containing a large number of full energy peaks, synthesize the unscattered gamma-ray spectrum corresponding to all of the photon energies and photon yields and subtract it from the measured spectrum to obtain the scattered photon spectrum. The scattered photon

spectrum may contain information about the bulk sample that may not be evident from the measured spectrum alone. Research along these lines is presently underway. We are also able to combine our Monte Carlo programs for simulating on-line capture gamma-ray analyzers [23,24] with the response function model to generate spectra for the purpose of system design optimization and for calibration.

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