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Nuclear Instruments and Methods in Physics Research B 213 (2004) 100–104

NIM B
Beam Interactions with Materials & Atoms

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A new Monte Carlo assisted approach to detector response functions

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Abstract

The physical mechanisms that describe the components of NaI, Ge and Si(Li) detector responses have been investigated using Monte Carlo simulation. The mechanisms described focus on the shape of the Compton edge, the magnitude of the flat continuum, and the shape of the exponential tails features. These features are not accurately predicted by previous Monte Carlo simulations. Probable interaction mechanisms for each detector response component are given based on this Monte Carlo simulation.

Keywords: Detector response; Monte Carlo; Spectrometry

1. Introduction

Detector response functions (drfs) are becoming more and more useful in radiation detection for spectrometry purposes. Specifically, Monte Carlo models used to predict incident photon spectra are applied in conjunction with the detector response function to translate photon spectra incident on the detector to a pulse-height spectrum. The detector response function is defined as the pulse-height distribution for an incident monoenergetic γ- or X-ray usually denoted $R(E', E)$ where E' is the pulse-height energy and E is the incident γ- or X-ray energy. The drf is a probability distribution function (pdf) which has the properties that it is always larger than or equal to zero over its entire range and integrates over all E' to unity.

In principle, one could use Monte Carlo simulation entirely to produce drfs if all of the pertinent detector characteristics were known *exactly*. However, there are many features of interest that cannot be determined and cannot be simulated. Features like the detector imperfections within the crystal, which significantly affect the flat continuum, are impossible to determine. The same is true for determining the standard deviation of the Gaussian detector resolution and the extent and shape of the exponential tails. Generating these

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doi:10.1016/S0168-583X(03)01540-4

characteristics by Monte Carlo is not a practical solution. Instead, Monte Carlo simulation can be used to determine the extent of the full energy peak, the Compton continuua and the annihilation photon and X-ray escape peaks. We propose to use Monte Carlo simulation to obtain these features and then augment these results with separate simple programs that are used to match a limited number of experimental single-energy spectral data for the three features: (1) Gaussian standard deviation of the full energy peak (and entire spectrum), (2) exponential tail(s) and (3) flat continuua. These effects must be included to obtain the final pulse-height spectra. Since they are presently not in the existing general purpose codes like MCNP [9], it is important to be able to implement them after and outside of a normal Monte Carlo simulation.

2. Summary of previous work

There are three basic approaches to obtaining detector response functions. They are identified as [1]:

- *Experimental*. Where one obtains the response in matrix form from a large number of measured monoenergetic spectra and interpolates for other energies. These are more appropriately described as library spectra because they include the effects of interactions in the shielding or source.
- *Monte Carlo*. Where one generates response functions by simulation for a large number of monoenergetic spectra and interpolates for other energies. This approach minimizes the amount of experimental work required and gives valuable insight into the actual processes that take place within the detector, but additionally requires very careful analysis and description of the problem for sufficient accuracy. Monte Carlo simulation appeared potentially useful for producing the entire spectra [2,3,10] but did not calculate the features that are specific to each detector (even when detectors are essentially identical in shape and size).
- *Semi-empirical*. Where one determines an analytic model for separable detector features and uses least-squares fits to a smaller number of single energy results and then generalizes these results with energy to provide a continuous model. This approach utilizes general physical mechanisms that lead to the simple shapes of the various features. However, this method does not give much insight into the physical processes that take place inside of the detector. A series of papers [1,7,8] outlined the semi-empirical approach that has been adopted as a standard method for constructing detector response functions.

For other work not included in this paper, see [6].

Most of the experimental digital library data was obtained from Heath [4,5] for a number of single γ-ray energies. These data were very carefully taken under standard conditions and represent the best benchmarked data available. It is reasoned that if we can simulate these standard spectra accurately then we should be able to simulate the detector response functions just as accurately by simply removing the surrounding material from the Monte Carlo simulation.

3. Components of the detector response function

A Monte Carlo code, CEARDRF [6], has been developed at NCSU to simulate the response of a bare Si(Li), Ge, or NaI detector crystal to a monoenergetic γ-ray point source. The unique feature of this code is that the individual components of the detector response function are specifically tallied and produced separately. Distributions of any physical mechanism can be produced directly from the simulation. The spectra generated by the Monte Carlo code, CEARDRF, was compared with the results from the general purpose code MCNP version 4B2 [6,9].

Using the specific-purpose code, CEARDRF, the individual components can be produced with their true shape limited only by the description of the physics in the simulation. The components are shown in Fig. 1 convolved with a Gaussian of the appropriate resolution. The features present are:

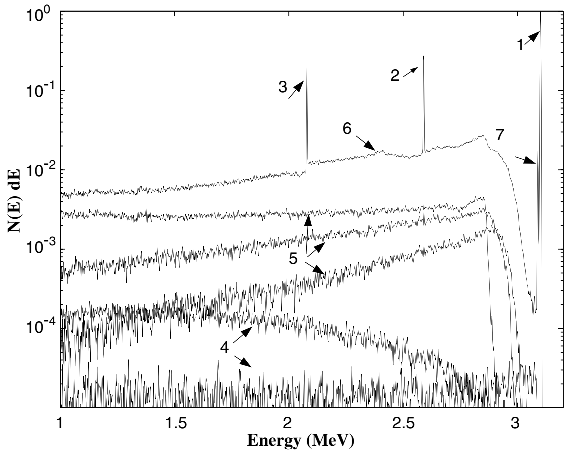

Fig. 1. Physical mechanisms of detector response.

(1) the full energy Gaussian peak, (2) a single Gaussian escape peak due to annihilation photons, (3) a double Gaussian escape peak due to annihilation photons, (4) a flat continuum that ranges from zero to the full energy peak, but is comprised from two physical features, (5) a Doppler broadened Compton scattering continuum broken into first, second and third Compton scatters from zero to the full energy peak, (6) a Compton scattering continuum between the first and second escape peaks due to the Compton scattering of one of the annihilation photons and (7) X-ray escape peaks from detector component elements such as Ge, Si and I.

One of the first distinctions is the shape of the flat continuum. The flat continuum was previously considered to be a single feature but is actually comprised of two different mechanisms that give a flat distribution when combined. In lower energy spectra, a second distinct feature is the shape of the Compton edge. The Compton edge as predicted by previous Monte Carlo simulation produced a very sharp change in slope indicating a 180° Compton scatter event. Including the low-energy Doppler effect on the energy of the incident photon produces a shape that matches the experimentally observed shape of the Compton edge. The dominant contribution to the shape of the Compton edge is from the first and second Compton scatters.

3.1. Exponential tails

The exponential tail behavior to the left of the photopeak has been well established for semiconductor detectors [11–13]. Using CEARDRF, the components of the photopeak are broken into two contributions. The first includes the energy due to photoelectron deposition varying from zero to the incident energy less the binding energy. The second contribution includes energy deposited from Auger electrons, satellite X-rays and the Lα fluorescence X-rays. Examination of these components reveals that the low-energy tail can be explained by incomplete charge carrier collection by diffusion towards the surface of the detector crystal, insensitive regions in the frontal layers of the crystal and by partial energy loss of secondary radiation. The insensitive layer was defined to be the range of the photoelectron and is not constant. This is an important separation of the effect of local properties on the detector response from the bulk properties of the detector crystal. Fig. 2 shows the typical shape of the combined effect on the photopeak shape generated when particles are forced to interact within the frontal region of the detector. This shows the contribution of the low-energy loss

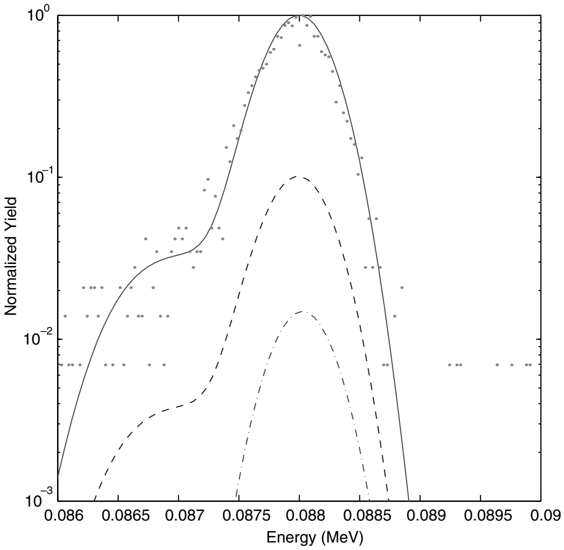

Fig. 2. Exponential tail components for Si(Li) #1 Cd-109: experiment (··); Auger component (––) and photoelectron component (– ·).

mechanisms on the shape of the photopeak. Interestingly, this shape resembles the combined short-term and long-term exponential peak shapes used with the semi-empirical approach to detector response functions [1,14].

Previously, the magnitude of this contribution has been at least one order of magnitude off. We adapt the general shape developed for incomplete charge collection developed by Goto [12] as a pseudo electron density modification. The model given by Goto is based on a one-dimensional electron carrier density model for silicon and looks like: $f(z) = 1 - (1 - R)\exp(-Cz)$, where R controls the rate change in density. The shape is an exponential that quickly reaches saturation.

3.2. Flat continuum losses

Electron losses to the sides of the detector create a flat continuum component to the detector response. While Monte Carlo simulation includes electron losses, it underpredicts the magnitude of the loss when comparing with experimental spectra. The difference in magnitude was attributed to an increased loss within the range of the photoelectron. More recent studies indicate that the entire photon spectrum contributes to the shape of the flat continuum.

The components that describe the flat continuum have been subdivided into a Compton electron and photoelectron contribution. A proposed solution was to increase the electron leakage artificially by increasing the electron range thus simulating charge loss due to imperfections or electron channeling effects. This could be included in the Monte Carlo simulation by modifying the density of the material for the electron when an electron is created. Sood [6] demonstrates the effect of including a pseudo electron density modification for a HPGe detector at 0.662 MeV. An alternative to this is to reduce the photopeak by a specified fraction and distribute it to the rest of the spectrum. This offers the advantage of a convolution approach after the basic Monte Carlo simulation that is particular to a specific detector. A constant value for a specific detector applied to the photopeak appears sufficient to regenerate the distribution.

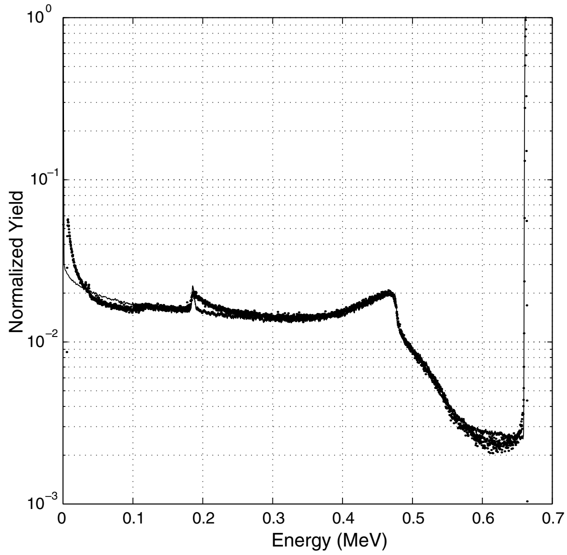

Fig. 3. Results for HPGe #1, Cs-137: experiment (··); Monte Carlo assisted simulation (–).

4. Detector response function validation

Fig. 3 shows the comparison of experimental data and calculated response. The calculated response represents the combination of the MCNP generated spectra including Doppler broadening with the convolution of the flat continuum and Gaussian resolution and the addition of the photopeak shape.

5. Summary and conclusions

There are several features of the detector response function that have required improvement. The ideas presented here effect the fundamental components of detector response. Through the use of Monte Carlo simulation, the shape of the fundamental physical mechanisms that produced the detector response have been described.

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