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by Rahadi Wirawan

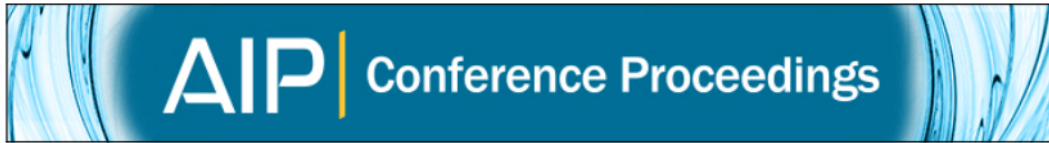
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Simulation of Energy Absorption Spectrum in NaI Crystal Detector for Multiple Gamma Energy Using Monte Carlo Method

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Abstract. The spectrum of gamma energy absorption in the NaI crystal (scintillation detector) is the interaction result of gamma photon with NaI crystal, and it's associated with the photon gamma energy incoming to the detector. Through a simulation approach, we can perform an early observation of gamma energy absorption spectrum in a scintillator crystal detector (NaI) before the experiment conducted. In this paper, we present a simulation model result of gamma energy absorption spectrum for energy 100-700 keV (i.e. 297 keV, 400 keV and 662 keV). This simulation developed based on the concept of photon beam point source distribution and photon cross section interaction with the Monte Carlo method. Our computational code has been successfully predicting the multiple energy peaks absorption spectrum, which derived from multiple photon energy sources.

Keywords: absorption, gamma energy, Monte Carlo method, NaI, scintillation detector.
PACS: 07.85.Nc

INTRODUCTION

Sodium iodide (NaI) crystal especially with thallium as an activator NaI(Tl), ones of the most inorganic scintillator that widely used for the detection of ionizing radiations, especially gamma rays [1].

Detection system of gamma rays in NaI(Tl) based on a scintillation process that releasing the photon in the UV or visible-light range, when an excited electron in the scintillator returns to its ground state. The scintillation process depends on the energy deposition or energy absorption in scintillator material. Through the simulation approach, gamma energy absorption spectrum in NaI(Tl) crystal can be modeled.

Monte Carlo method is a numerical solution of interaction problems between objects with other objects or to the environment based on the relationship between them. It has been established as an appropriate method for modeling a large variety of physical situations and useful for predicting the experiment result based on the theory [2, 3]. The characteristic of Monte Carlo simulation is using the random number and random variables [3].

In this paper, we present a simulation model of gamma energy absorption spectrum in NaI scintillation crystal detector. The simulation program constructed using a Monte Carlo method based on the probability of gamma interaction process.

The simulation can be used to predict the multiple energy peaks spectrum detected which generated from multiple monoenergetic gamma rays which known.

THEORETICAL BACKGROUND

The spectrum of gamma energy recorded from a radiation source depends on the type of radiation detector used and the mechanism of interaction by which the radiation energy is deposited in the detector. In the case of gamma rays photons, the energy transferred to detector primarily in photoelectric, Compton scattering, or pair production interactions [4]. The contribution of the photon gamma interactions that occur in the material are described by the linear attenuation coefficient of material. The total attenuation coefficient is a combination of all the interactions that occur in the material written by the equation

$$\mu(E) = \mu_{PE}(E) + \mu_{CS}(E) + \mu_{PP}(E)$$
$$= \frac{\rho N_A}{A}\left(\tau(E) + \sigma(E) + \kappa(E)\right) \qquad (1)$$

where $\tau(E), \sigma(E), \kappa(E)$ are the cross section of photoelectric interactions, Compton scattering and pair production, respectively.

FIGURE 1 show that three dominant interaction of gamma ray with the matter. The interaction take place depends on the initial gamma-ray energy and the atomic number (Z) of material absorber. The photoelectric and Compton effects are the interaction types take place for initial gamma-ray energies less than 1 MeV.
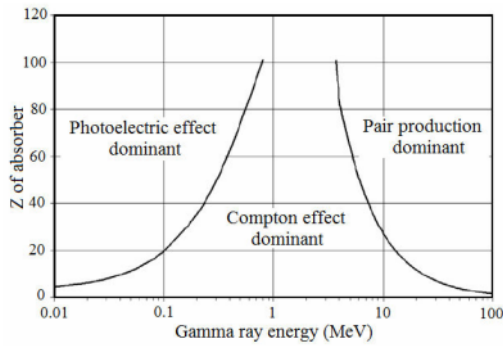
FIGURE 1. Three major types of gamma-ray interaction [1].

As mentioned before that a photon may interact through the photoelectric, Compton scattering or pair production processes. The interaction coefficient represents the compound process, and can expressed by equation

$$\mu(E) = \sum_i \mu_i(E) \qquad (2)$$

Thus, the fractional probability for i interaction is:

$$P_i = \frac{\mu_i(E)}{\mu(E)} \qquad (3)$$

In other words, the kind of interaction based on the relative attenuation coefficients at the location point of interaction, not on how the particle arrived at that point.

Computational Model

The computational program based on the probability distribution function of photon interaction.

$$f(s)\, ds = \mu \exp(-\mu s)\, ds \qquad (4)$$

where μ is the interaction coefficient. Using the inverse function method, the mean free path of photon is expressed as

$$s = -\frac{1}{\mu_{total}}\ln(\xi) \qquad (5)$$

where, ξ is a random quantity with uniform distribution between 0 and 1.

In the emitting gamma rays from the isotropic point source model what we used, the orientation of photon emission based random distribution of polar and azimuthal angles as shown in FIGURE 2. With the solid angle $d\Omega = sin\theta d\theta d\phi$, the probability distribution function for θ and ϕ are $P(\theta) = \frac{1}{2} sin\theta$ with normalized over $(0,\pi)$ and $P(\phi) = 1/2\pi$ with normalized over $(0,2\pi)$. The polar and azimuthal angle was sampled by the equation

$$\theta = \cos^{-1}\left(1 - 2\xi_1\right) \qquad (6a)$$
$$\phi = 2\pi \xi_2 \qquad (6b)$$

where ξ_1 and ξ_2 are the uniform random between 0 and 1.
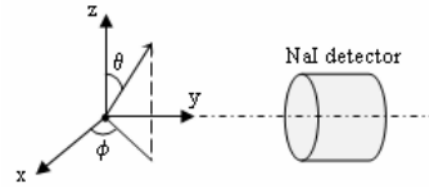
FIGURE 2. Coordinate system of photon generate

The initial direction of gamma photons is given by the equation as

$$u_0 = \sin\theta\cos\phi \,; v_0 = \sin\theta\sin\phi \,; w_0 = \cos\theta \quad (7)$$

In addition, the interaction point (x, y, z) of a gamma photon in NaI detector material is calculated by using the formula:

$$x = x_0 + u_0 s$$
$$y = y_0 + v_0 s$$
$$z = z_0 + w_0 s \qquad (8)$$

where $(x_0,\ y_0,\ z_0)$ is the initial position in front of surface detector, s is photon mean free path and initial photon direction (u_0, v_0, w_0).

Photon interaction in material distinguished into two main events: photon scattering or photon absorption. In addition, for gamma energies between 100 keV and 700 keV the dominant interaction are photoelectric effect and Compton scattering. The cross section scattering interaction is determinate by the *Klein-Nishina* formula [5]

$$\sigma_C = Z2\pi r_e^2 \left\{ \frac{1+\varepsilon}{\varepsilon^2} \left[\frac{2(1+\varepsilon)}{1+2\varepsilon} - \frac{\ln(1+2\varepsilon)}{\varepsilon} \right] + \frac{\ln(1+2\varepsilon)}{2\varepsilon} - \frac{1+3\varepsilon}{(1+2\varepsilon)^2} \right\} \quad (9)$$

with r_e is classical electron radius (2.82 fm) and $\varepsilon = h\nu/m_o c^2$. The linear attenuation coefficient of Compton scattering:

$$\mu_{CS}(E) = \frac{\rho N_A}{A} \sigma(E) \quad (10)$$

Once the photon interacts, the scattered photon can have a different energy (E') and direction angles (Θ, Φ) relative to the initial directions. The scattered photon energy is:

$$E' = \frac{E}{1 + \frac{h\nu}{0.511 MeV}(1 - \cos\Theta)} \quad (11)$$

Angular deflection of photon direction due to scattered interaction shows in FIGURE 3.
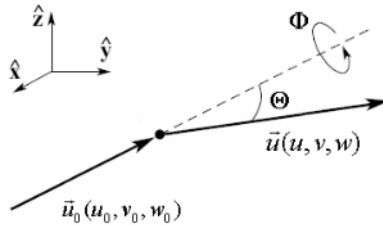

FIGURE 3. Photon deflection direction in single-scattering event.[5]

After scattering interaction, photon direction change by the equation [3, 6]:

$$u = u_0 \cos\Theta + \sin\Theta(w_0 \cos\Phi \cos\phi - \sin\Phi \sin\phi)$$
$$v = v_0 \cos\Theta + \sin\Theta(w_0 \cos\Phi \sin\phi + \sin\Phi \cos\phi)$$
$$w = w_0 \cos\Theta - \sin\Theta \sin\theta \cos\Phi \quad (12)$$

The total linear attenuation coefficient of NaI crystal scintillation detector between 100 and 700 keV is given by the formula:

$$\mu(E) = 5.18\left(\frac{E}{100keV}\right)^{-2.85} + 0.539\left(\frac{E}{100keV}\right)^{-0.450} cm^{-1} \quad (13)$$

where photon energy E in units keV [7].

Based on the fractional probability for interaction, the interaction type is decided by the interaction rejection method. The interaction type is chosen randomly based on the critical value or scattering attenuation ratio to total coefficient attenuation.

$$ratio = \frac{\mu_{CS}(E)}{\mu(E)} \quad (14)$$

If the random number generate (random) ≤ ratio, the photon is scattered. In the other hand, if (random) > ratio, photon interaction is classified as absorption process.

In this work, simulating photon with the Monte Carlo method includes three main processes which are described through the flowchart below:
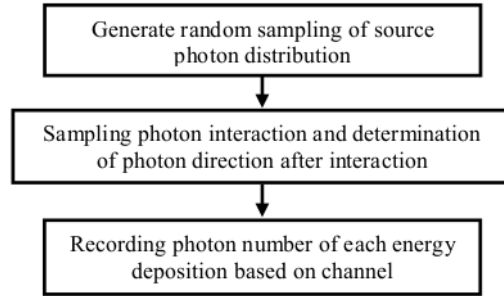
Generate random sampling of source photon distribution

Sampling photon interaction and determination of photon direction after interaction

Recording photon number of each energy deposition based on channel

FIGURE 4. Three process Monte Carlo method.

RESULT AND DISCUSSION

In this work, we have used the Monte Carlo methods to obtain absorption spectra of gamma ray in NaI crystal detectors for single or multiple gamma energy sources. FIGURE 5 shows the simulation result of energy absorption spectrum of monoenergetic gamma rays 662 keV. From the simulation result, the backscatter peak energy can be identification in energy channel 185 keV. The backscatter peak is the peak energy spectrum of scattered gamma ray after 180-degree scattering angles. Moreover, for Compton edge take place in the energy 477 keV.

The energy absorption spectrums result from simulation (FIGURE 5) have the same trend with its done by Tawara which using EGS4 simulation

program. At the edge of spectrum, indicates the full-energy peak (photoelectric peak) of gamma energies source [8].
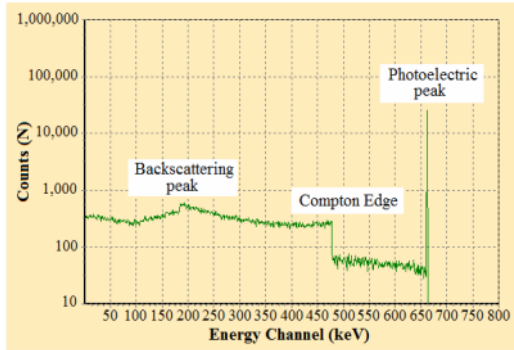

FIGURE 5. Energy absorption spectrum simulation of monoenergetic 662 keV, with NaI crystal (2 cm radius, 2 cm thickness), 1 cm source-detector distance of central axis NaI crystal detector.

Backscattering peaks for several energy sources that identified from simulation curve result has not significantly different with determinate by Compton scattered energy formula and the experimental data from Sabharwal [9] as shown in TABLE 1.

TABLE 1. Backscattering energy (keV).

Energy (keV)	Simulation	Theory	Experiment
279	134	133.37	133.3
320	143	142.07	142.1
511	171	170.33	170.3
620	185	184.35	184.3

Geometric efficiency of the NaI crystal detector is determined based on the ratio of photon that detect on the detector surface to photon emission from a gamma ray source. FIGURE 6 shows the geometric efficiency based on source vertical position from detector axis.
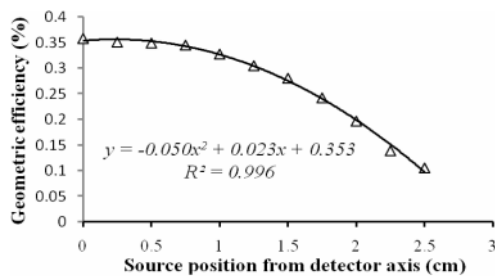

FIGURE 6. Geometric efficiency from simulation result of NaI crystal detector (radius 2 cm and 2 cm thickness, 1 cm source-detector distances).

The polynomial fitting curve of geometric efficiency data gives a relation between geometric efficiency (y) and source position (x) in the form

$$y = -0.050x^2 + 0.023x + 0.353 \qquad (15)$$

FIGURE 7 and 8 show the simulation result for the energy absorption spectrum of two and three gamma rays source with energy peaks of 297 keV, 400 keV and 662 keV.
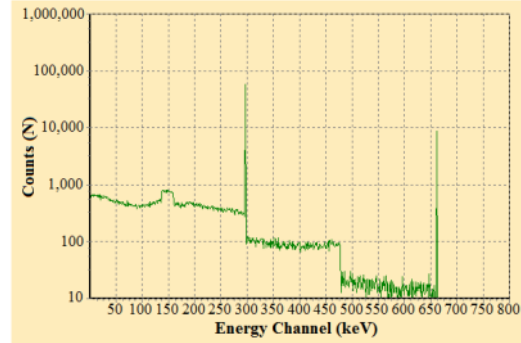

FIGURE 7. Energy absorption spectrum simulation of 297 keV and 662 keV with NaI crystal (2 cm radius, 4 cm thickness), and 1 cm source-detector distance of central axis NaI crystal detector.
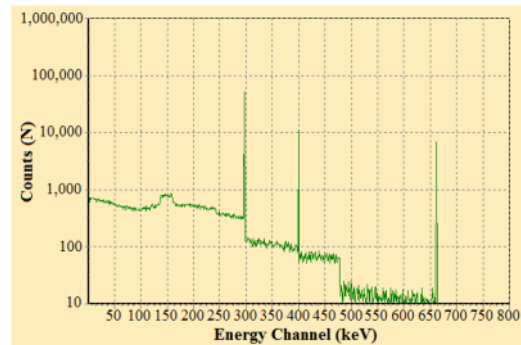

FIGURE 8. Energy absorption spectrum simulation of 297 keV, 400 keV and 662 keV with NaI crystal (2 cm radius, 4 cm thickness), and 1 cm source-detector distance of central axis NaI crystal detector.

The each peaks of photon energy in FIGURE 7-8 shows the gamma energies of photon source. The presence of gamma photon energies below the Compton edge of the 662 keV energy peak (high energy sampled in simulation) changing the length of Compton continuum.

CONCLUSIONS

The computational program has been successfully to simulate the multiple energy peaks absorption spectrum, which derived from multiple photon energies sources by the Monte Carlo method approach. The present work can be used to predicting the position of energy peak, Compton peak and backscattering peaks in the energy distribution spectrum that detected by the scintillation NaI(Tl) crystal detector.

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B19