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GESS-A Code for Verification of Shielding Integrity by Monte Carlo Method

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=**Abstract**=

GESS-a computer code for simulation of energy spectra for gamma-ray in NaI(Tl) scintillator has been developed. The Monte Carlo method was employed to simulate physical behaviours of particle transport in a medium.

In the processes of simulation, all the interaction processes such as Rayleigh and Compton scattering, photoelectric effect and pair production were considered. The resulting electron slowing down spectrum was also considered with the CSDA model.

For the purpose of verification of the code, a measurement gamma spectrum for incident gamma energy of 1.33 MeV was performed. The measured values appeared to be slightly higher than the theoretically calculated values.

1. Introduction

The non-destructive inspection method with NaI(Tl) scintillation detector have been employed to detect deficiencies in heavy shields. Although considerable experimental data are now available for detection of deficiencies in shield, theoretical calculations have become an increasingly important method for supplementing the data in photopeak regions where the scattered photons appear dominantly as the shield becomes thicker. Therefore, as a way of solution to problems of the above method a computer program based on Monte Carlo calculations which can predict the gamma energy spectrum in NaI(Tl) crystal was developed in this study.

In order to simplify the calculation of the deep penetration of gamma-rays, the configuration of the shields was considered as a infinite slab. And then the gamma spectrum was calculated for the case of isotropic incidence of 1.33 MeV photons located off the inner surface of the shield.

As physical processes that gamma rays undergo, only Compton and Rayleigh scattering were considered in shield region, and in detector region all the types of interaction were taken into consideration. The bremsstrahlung radiation spectrum was determined on the basis of the data calculated by Zerby and Moran using the CSDA model for electron degradation precesses and the bremsstrahlung cross sections given by Born approximation. The particles generated from a collision were traced through the crystal until they have escaped or been absorbed by the crystal.

A general description for the Monte Carlo

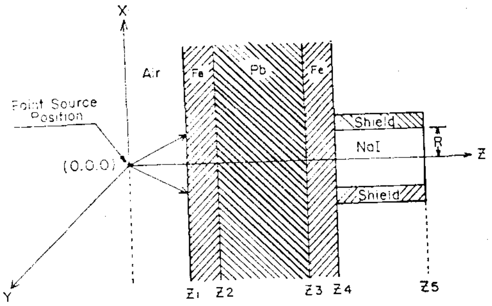

Fig. 1. Diagram showing source, shield and detector geometries.

code, GESS, is given in next three sections. Some variance reduction techniques[1] were employed for efficient simulation.

Comparisons of theoretical calculations with experimental gamma spectrun from NaI(Tl) crystal are presented.

2. Geometrical Model and Source Parameters

The geometrical model considered in this study is shown in Fig. 1.

The initial isotropic point source was transformed into the circular disk source uniformly distributed with radius on the shield plane. For sources uniformly distributed on a disk, the probability density function (pdf) describing the distribution of source points as a function of radius is given by

$$\mathrm{P}(r)\,\mathrm{d}r=\frac{Z_1}{1-u}\cdot\frac{r\mathrm{d}r}{(Z_1^2+r^2)^{3/2}} \tag{1}$$

with

$$u=\frac{Z_1}{\sqrt{Z_1^2+R^2}}$$

From Eq. (1) we can get the cumulative distribution function (cdf). Here a random number n used to select a value P(r) can be used to select a random sample of r;

$$r=Z_1\sqrt{\left[\frac{1}{1-n(1-u)}\right]^2-1} \tag{2}$$

Considering the rectangular coordinate, we can get the initial coordinates and the initial direction cosines of the source particles at its incident point on the shield surface.

3. Particle Transport in Shield Region

A. Determination of the Path Length and the Collision Parameter

The path lengths and collision parameters have been determined on the basis of the total and the individual cross section. It is necessary to the nuclide involved in the interaction and the interaction type.

For this determination both the total and the individual interaction cross section must be available for each nuclide over energy range of interest. Photon cross sections for shield material were taken from values given by Hubbell[2]. Then the cross sections for any given energy were taken from values obtained by cubic spline interpolation[3].

If the total cross section is σ_T, then path lengths, d, between interaction sites are determined from

$$d=-\frac{1}{N\sigma_T}\ln n \tag{3}$$

where n is a random number between 0 and 1 and N is the atomic density.

Let the cumulative fractional interaction cross section for Rayleigh scattering, photoelectric effect and Compton scattering, respectively, be defined by

$$\mathbf{r}_1=\frac{\sigma_R}{\sigma_T},\quad \mathbf{r}_2=\frac{\sigma_R+\sigma_p}{\sigma_T}$$

$$\mathbf{r}_3=\frac{\sigma_R+\sigma_p+\sigma_c}{PT} \tag{4}$$

where σ_R, σ_p and σ_c are the cross section for Rayleigh scattering, photoelectric effect and Compton scattering, respectively. Then the type of interaction was determined by selecting a random number n; if $o<n<r_1$, the interaction is Rayleigh scattering, photoelectric effect if $r_1<n<r_2$, or Compton scattering if $r_2<n<r_3$ or pair production if $r_3<n<1$. Because n is uniformly distributed on the unit interval, each type of interaction is sampled with probability r_1, r_2, r_3.

B. Determination of Parameters after Collision

As the energy absorption in the shield region is not important, Rayleigh and Compton scattering were only considered in the shield region. Each photon history is terminated when either the processes which it undergo are absorption events or the energy of the photon falls below 1.28 MeV.

Consider the case where the photons undergo Rayleigh scattering. Then the angular distribution of scattered photons was determined on the basis of a formula given by Franz[4]. His formula describing the differential cross section $d\sigma$ as a function of scattering angle Θ is given by

$$d\sigma(u) \propto e^{-\frac{u}{\pi}}\ du \tag{5}$$

with

$$u = KZ^{-\frac{1}{3}}\ (\mathrm{E/mc^2})\ \ \sin\left(\frac{\Theta}{2}\right) \tag{6}$$

where K is a normalization constant, N is the atomic number, E is the energy of the photon and mc^2 is the rest energy of the electron.

By selecting a random number one obtains:

$$u = -\pi \ln n \tag{7}$$

By equating Eq. (7) to Eq. (6) we can obtain the scattering angles. And the azimuthal angle is sampled from a uniform distribution between 0 and 2π.

For Compton scattering, it is usually more convinient to use the wavelength in Compton units instead of the energy variable.

The increase in the wavelength associated with a Compton scattering event can be expressed as the scattering angle. Therefore, it is necessary to know the angle of Compton scattering and the new value of the wavelength.

The most commonly used procedure for obtaining these quantities is based on the Klein-Nishina probability density function. Of the various methods for sampling from the Klein-Nishina pdf, Kahn method[5] based on the composition rejection technique was employed here.

Having determined the energy and direction of the scattered photon, the energy of the recoil electron is simply the photon energy difference before and after the collision, and its scattering angle is determined from the conservation laws. The azimuthal angles of the photon and the electron were sampled from the uniform distribution.

4. Particle Transport in Detector Region

A. Determination of Initial Coordinates

When a photon escapes the shield region, it is necessary to know whether the photon hit the detector before its slowing down below the cut-off energy or not. First, consider the case where the photon exits through the side wall of the detector. Then the intersection length can be given by simultaneously solving the equation for the right circular surface of the cylindrical detector and the equation for the straight line of the photon path.

$$R^2 = X_R^2 + Y_R^2 \tag{8 a}$$

$$X_R = x + lu \tag{8 b}$$

$$Y_R = y + lv \tag{8 c}$$

$$Z_R = z + lw \tag{8 d}$$

where (X_R, Y_R, Z_R) are the coordinates of the photon exit point at the surface of the detector, (x, y, z) are the coordinates of the present interaction site, (u, v, w) are the direction cosines of the photon, l and R are the intersection length and the radius of the detector, respectively.

If the photon exits from the side of the detector, the one root is positive and the other is negative. A check for this is done by calculating Z_R and comparing it with the equations of the end-planes of the detector. Thus, Z_R equals to $z+lw$. If Z_R is within the horizontal boundaries of the detector, then the coordinates of the present interaction site (x, y, z) are selected as the initial coordinates of the photon inside the detector.

Second, condsider the case where the photon enters through the front of the detector. If z is within the horizontal boundaries of the detector, and $(x^2+y^2)<R^2$, then (x, y, z) are the initial coordinates of the photon.

B. Determination of Path Length and Collision Parameter

The cross sections given by Plechatay and Terral[6] were used. In order to obtain the corss sections for any given energy, the total cross section σ_T is fitted to a polynomial as a function of energy as follows.

$$\sigma_T(E)=\exp\left[\sum_{k=1}^{4} B(j,k)\,(lnE)^{k-1}\right] \text{ barns} \tag{9}$$

where E is in keV, j defines the energy interval and the coefficients $B(j,k)$ are obtained from least square fits of the cross sections. The path lengths of the photon in the detector medium are calculated by the same sampling method as in the shield medium.

The partial-to-total cross section ratio is fitted to a polynomial as follows.

$$\frac{\sigma_i(E)}{\sigma_T(E)}=\exp\left[\sum_{k=1}^{4} A(i, j, k)\ ln(E)^{k-1}\right] \tag{10}$$

where i specifies the event considered ($i=1$ refers to photoelectric effect, $i=2$ to Compton scattering, $i=3$ to pair production). The coefficients $A(i, j, k)$ are obtained by the same method as the $B(j, k)$.

C. Determination of Parameters after Collision

All the type of interactions such as Rayleigh scattering, photoelectric effect, Compton scattering and pair production were considered in the detector region.

Consider the case where the photon undergoes photoelectric interaction. Then the kinetic energy transfered to a single electron by the photon of energy E is given by

$$T=E-W \tag{11}$$

where T is the kinetic energy of the electron and W is the shell binding energy herein taken as the K-shell binding energy for iodine, i.e., 33.16 keV. The probability for the excited iodine atom to emit Auger electrons is 17%. In other cases fluorescent radiation[7] is emitted isotropically with an energy given by the difference between the K and L shells, i.e., 28 keV.

For the photon undergoes pair production in the coulomb field of a nucleus, the energy balance is given by

$$T_+ + T_- = E-2\,mc^2 \tag{12}$$

wherer T_+ and T_- are the kinetic energy of positron and electron, respectively.

Positrons and electrons are assumed to be emitted at a mean polar angle given by Bethe and Askin[8] Also their azimuthal angles are assumed to be uniformly distributed, 180° apart.

D. Slowing Down of Charged Particles

The process of slowing down of charged particles involves very large numbers of interactions with relatively small energy loss per collision, in constract to the slowing down of gamma ray, which undergo rather few but large energy loss interations. Because of the large number of interactions it is too time consuming in the calculations to treat electron and positron slowing down by the Monte Carlo method. Mean range and energy loss mechanism of charged particles, therefore, were considered here.

The approximate theory[9] of Wilson for electron slowing down was used to determine the mean path length and energy loss of the charged particles. Based on his theory, the mean distance traveled by an electron (or positron) with kinetic energ T, in radiation length is given by

$$d=d_o \ln 2\, ln\left(1+\frac{T}{E_c \ln 2}\right) \qquad (13)$$

where d_o is a radiation length and E_c is the so-called critical energy at which the radiation and collision energy loss become nearly comparable. In this study the values of E_c and d_o were taken from the article by Bethe and Ashkin[8].

If the mean distance, d, takes the particle outside the crystal, the energy carried away is computed by solving Eq. (13) for T, where d is taken as the distance traveled outside the crystal, designated as d'. Then the energy carried away from the crystal, T_p, is given by

$$T_p=E_c \ln 2\,(e^{d'/d_o \ln 2}-1) \qquad (14)$$

so that $(T-T_p)$ is absorbed by the crystal.

In our calculation the slowing down of electrons and that of positrons were treated identically.

Two 511 keV annihilation photons of 180° apart are assumed to orginate at the end of the positron path. Then they are tracked like primary gamma rays. If the positron escapes from the crystal, no annihilation photons are created inside the crystal. In this case, an amount of (T_p+2mc^2) was considered of energy carried away outside the crystal.

The Wilson slowing down theory includes excitation and ionization losses and radiation losses in the field of the nucleus, that is, bremsstrahlung. In our computer program it was assumed that all ionization and excitation energy lossess are completely absorbed by the crystal, whereas bremsstrahlung photons are treated as primary gamma-rays.

E. Simulation of Bremsstrahlung

In order to simulated the emission of bremsstrahlung radiation, the number of photons emitted, their energy and their angular distribution have to be evaluated.

By defining $K(E_0, k)\,dk$ to be the total number of photons in the energy interval $(k, k+dk)$ produced by an electron with initial energy E_0, $K(E_0, k)$ is given by

$$K(E_0, k)=\int_{k+1}^{g}\frac{\Sigma_j \Phi_j^{a}(E, k)}{\Sigma_j\left(-\frac{dE}{dx}\right)_j}\,dE + \int_{g}^{E_0}\frac{\Sigma_j \Phi_j^{bb}(E, k)}{\Sigma_j\left(-\frac{dE}{dx}\right)_j}\,dE \qquad (15)$$

where, $\left(-\frac{dE}{dx}\right)$ is the stopping power and the index j refers to the j-th element of the NaI. $\Phi^a(E, k)$ and $\Phi^b(E, k)$ are Born approximation cross section[10,11] taking into account and taking no account of electron screening effect respectively. The number of photons emitted in the energy interval (k_{min}, E_0-1) by an electron of initial energy E_0 is defined by

$$N(E_0, k) = \int_{min}^{E_0-1} K(E_0, k)\,dk \qquad (16)$$

Equation (16) was numerically integrated for $k_{min}=5\times10^{-3}(E_0-1)$. The data obtained were then fitted by the least square method to get $N(T_0, k_{min}) = 0.1837+3.014\times10^{-4}T_0-3.328\times10^{-9}\ T_0^2$ (17)

$T_0=(E_0-1).\ mc^2$ keV.

Bremsstrahlung photon has a relative eneryg distribution independent of electron energy E_0[11]. Therefore, in order to determine the energy of bremsstrahlung photon the normalized curve for 2 MeV electron was chosen as a universal curve. The probability distribution function, $f(x)$, is given by

$$f(x) = \frac{K\{(T_0=2\,\text{MeV},\ x(E_0-1))\}}{N(2\,\text{MeV},\ k_{min})} \qquad (18)$$

where $x=k(E_0-1)$ is defined in (0.005, 1).

The cumulative distribution function can be written by

$$n=\int_{0.005}^{x} f(x')\,dx' \qquad (19)$$

Solution of Eq. (19) gives the photon energy, $k=x(E_0-1)$, a function of a random number n. The results were fitted to give the expression below;

$$K=10Ek(n)\ (E_0-1) \qquad (20)$$

where $Ek(n)$ is a constant expressed as a function of random number n. The angular distribution of bremsstrahlung photons was assumed to be isotropic distribution.

5. Results and Discussion

The computer program yields the gamma energy loss spectrum in the form of histogram of the number of gamma rays experiencing an energy loss in a given energy interval, that is, the energy range is divided into intervals by a set of energy points E_0, E_1, E_2......E_T, where $E_0=1.28$ MeV, $E_T=1.33$ MeV. The lower bound, 1.28 MeV, is arbitrary and the energy intervals selected were of equal size. Calculated gamma energy loss spectrum is shown in Fig. 2, which is resulted from a 10^5 samples of source particles.

The energy loss spectrum is compensated for in an auxiliary calculation[12,13] which can produce the broadened spectrum from the

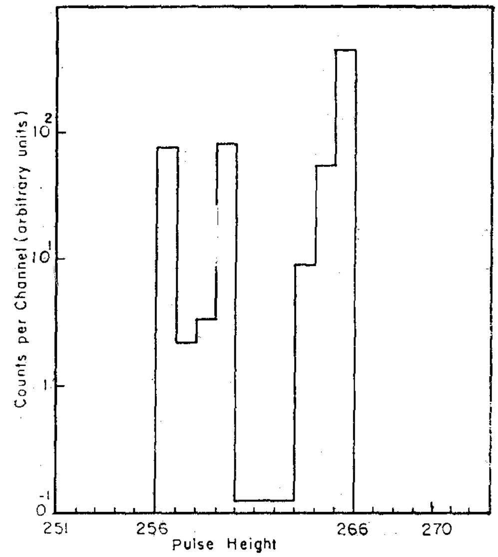

Fig. 2. Calculated gamma spectrum in the total absorption

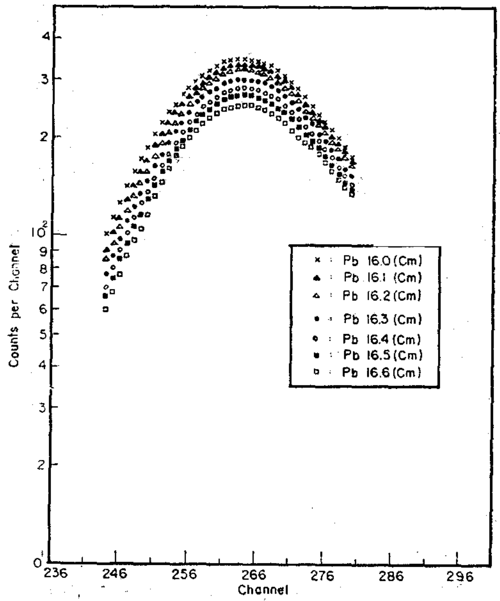

Fig. 3. Pulse-height spectrum smeared with a Gaussian function.

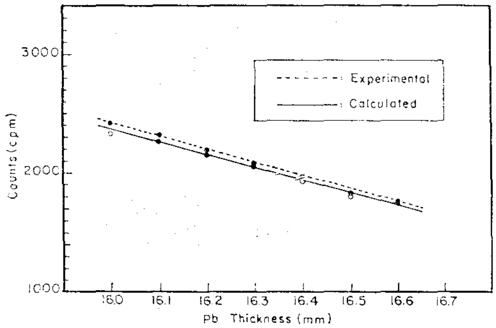

Fig. 4. Comparison of calculated with experimental results.

histogram by performing the integral

$$R(E')=\int_{1.28}^{E_0}\frac{1}{(2\pi\alpha E)^{1/2}}\exp\left[\frac{-(E-E')^2}{2\alpha E}\right]I(E)\,dE \qquad (21)$$

where the constant α is chosen empirically to give a selected percent half-width at the maximum energy.

The broadened spectra in variations with thickness(16.0, 16.1, 16.2, 16.3, 16.4, 16.5 and 16.6 cm) of lead are shown in Fig. 3. Under the same conditions, for comparison of the calculational results with experimental results, the areas under peaks lying from 256 channel to 266 channel were calculated. The results are shown in Fig. 4. The calculated curve on the whole agrees with the experimental curve, but the former appears slightly lower than the latter.

This is mainly due to discrepancy of cross section used. And also the diffence is presumably due to scattering of photons from the photomultiplier, and from surrounding materials interacting in the crystal. Such effects are not considered in the Monte Carlo calculation.

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몬테칼로 방법에 의한 차폐체 건전성 검증코드 개발

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=요　약=

본 연구에서는 NaI 검출기에서 감마스펙트럼 시뮤레이션 코드인 GESS를 개발하였다. 감마선에 의한 모든 상호작용이 시뮤레이션 과정에서 고려되었으며, 생성된 하전입자의 스펙트럼은 CSDA 모델에 기반을 두어 계산하였다. 매질내에서 입자 수송에 대한 해석수단으로는 몬테칼로 방법을 적용하였다.

코드의 검증을 위하여 1.33 MeV의 입사 감마선에 대한 스펙트럼이 본 연구에서 개발된 코드에 의해 계산되었으며, 계산된 스펙트럼은 대체적으로 실험에서 얻은 스펙트럼과 거의 동일한 분포를 나타내고 있다.