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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
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CALCULATED RESPONSE OF A 5.5 × 5.5 cm HIGH-PURITY Ge DETECTOR TO GAMMA RAYS WITH ENERGIES UP TO 20 MeV*

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Monte Carlo calculations have been done of the energy and angular response of a 5.5 × 5.5 cm, high-purity Ge detector, for gamma rays incident with energies from 0.1 to 20 MeV. Results are given for the absolute probabilities of total energy absorption and of single and double annihilation escape, which relate the areas of the peaks in the measured pulse-height distribution to the intensities of incident gamma-ray lines.

Keywords: detection efficiency; escape peaks; gamma rays; Ge detectors; response function; total absorption peak.

1. Introduction

Because of their good energy resolution, high-purity Ge detectors are preferred in many applications of gamma-ray spectroscopy. A 5.5 × 5.5 cm cylindrical detector, among the largest of such detectors which are presently available with good energy resolution, has been selected in the design of the Gamma-Ray Remote Sensing Spectrometer to be flown on NASA's Mars Observer Mission, scheduled for 1990. This experiment will measure from orbit the gamma-ray line emission induced in the Martian surface by incident cosmic rays, solar protons, and secondary neutrons, as well as that due to the presence of natural radioactivity. Measurement of these line emissions will provide the basis for the elemental analysis and geochemical mapping of the Martian surface.

The conversion of the measured pulse-height distributions to the actual gamma-ray line fluxes incident on the detector requires knowledge of the detector response as a function of the incident photon energy, particularly the absolute probabilities of the delta-function features in the absorbed energy spectrum (i.e., the total-absorption and the single- and double-annihilation-escape peaks) which largely determine the multi-peaked pulse-height signature of an incident gamma ray. The work reported here was done to provide this information. Using a fully coupled photon/electron Monte Carlo code used in an earlier study [1][1] of 3"×3" NaI detectors, calculations were done for gamma rays incident on the Ge detector with energies from 0.1 to

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*This work was carried out with support from the Department of Energy (Office of Health and Environmental Research).

[1]Numbers in brackets indicate the literature references at the end of the paper.

20 MeV. Calculations for various angles of incidence confirmed the anticipated result that, by appropriate scaling, the angular dependence of the response function can be effectively eliminated. The main results are given in a table of scaled total-absorption, single-annihilation-escape and double-annihilation-escape probabilities _vs_ energy, along with a table giving the energy and angular dependence of the detection efficiency which is used as the scaling parameter.

2. Method of Calculation

For a monoenergetic, monodirectional photon beam, the spectrum of energy absorbed in the detector, $D(E;E_0,\theta_0)$, can be written as the sum of a continuum, $C(E;E_0,\theta_0)$, and a line spectrum:

$$\begin{aligned} D(E;E_0,\theta_0) = {} & C(E;E_0,\theta_0) \\ & + P_0(E_0,\theta_0)\ \delta(E - E_0) \\ & + P_1(E_0,\theta_0)\ \delta(E - E_0 + mc^2) \\ & + P_2(E_0,\theta_0)\ \delta(E - E_0 + 2\ mc^2) \\ & + P_3(E_0,\theta_0)\ \delta(E - E_K)\ , \end{aligned} \qquad (1)$$

where E_0 is the energy of the incident photon, θ_0 is its angle with respect to the axis of the cylindrical detector, E is the energy absorbed in the detector, δ is the delta function, and mc^2 is the electron rest mass. P_0 is the probability that the entire energy of the incident photon is deposited in the detector, and can be interpreted as the area under the total-absorption peak. P_1 and P_2 are the probabilities that all of the incident energy is deposited with the exception of the amounts mc^2 and $2\ mc^2$, respectively, which are carried out of the detector by one or two unscattered annihilation quanta. P_1 and P_2 are then the areas under the single- and double-escape peaks, respectively. P_3 is the probability that the all of the incident energy is deposited except that carried away by unscattered Ge K x rays (with a weighted average energy E_K). Because P_3 is relatively unimportant for photon energies above 0.1 MeV, it will be ignored in the remainder of this report.

The detection efficiency, $\eta(E_0,\theta_0)$, is the probability that the incident photon will have at least one interaction in the detector leading to the deposition of energy, and is thus equal to $\int_0^{E_0} D(E;E_0,\theta_0)\ dE$. However, the evaluation of the detection efficiency can be accomplished independently through the solution of the geometrical problem, without knowledge of the absorbed-energy spectrum (see, e.g., ref. [2]). For example, for the case of a monoenergetic photon beam incident along the axis of a right-circular cylinder, the detection efficiency is simply

$$\eta(E_0,0°) = 1 - \exp[-\mu(E_0)z]\ , \qquad (2)$$

where μ is the photon attenuation coefficient and z is the height of the detector.

The Monte Carlo calculations of the absorbed-energy spectra were carried out using the ETRAN code [3]. The Monte Carlo model treats in rather full detail the processes involved in the production and transport of all components of the photon-electron cascade initiated by the incident gamma rays. Compton scattering, photoelectric absorption and pair production are taken into account in tracing the histories of the primary gamma rays as well as of secondary photons (bremsstrahlung, annihilation quanta, fluorescence x rays). The methods used to simulate the trajectories of electrons and positrons that are set in motion in photon interactions (electron-positron pairs, Compton electrons, photoelectrons, Auger electrons) take into account elastic and inelastic angular deflections, energy loss (including fluctuations) due to atomic excitation and ionization (knock-on production) and to bremsstrahlung production, and the production of characteristic x-rays and Auger electrons in K-shell ionization events. Positrons are treated as electrons, except for the emission of two annihilation quanta when the positron stops in the target.

The pertinent distributions, cross sections, and related data used in the calculation of electron transport are discussed in some detail elsewhere [1,4-10]. Data on photon interaction cross sections were taken from the compilations of Hubbell [11]; some auxiliary atomic data used for Ge can be found in ref [12].

The detector was assumed to be a right-circular cylinder, 5.5 cm high and 5.5 cm diameter, of uniformly distributed Ge (density of 5.323 g/cm^3). No surrounding material, such as mechanical and thermal encapsulation or a charged-particle anti-coincidence mantle, was taken into account. The distribution of such material is not yet accurately known. Moreover, it should be adequate to correct for the effect of such material on the bare-detector peak probabilities by means of a simple attenuation factor, thereby avoiding the introduction of any extrinsic angular dependence.

A broad, monoenergetic, monodirectional beam of photons was assumed incident on the endface and/or sides of the detector at an angle θ_0 with respect to the detector axis. The histories of the incident gamma rays and all generations of secondary photons and electrons were followed until they either escaped from the detector or reached a cut-off energy of 1 keV. Electron histories were also terminated within the detector if their energy fell below 10% of the incident photon energy, provided the shortest distance to any boundary was greater than the residual electron range. This greatly speeded up the calculations, at the expense of the neglect of only a small amount of low-energy bremsstrahlung. For each cascade from a sample of 20,000 incident gamma rays, the energy deposited E was scored as the difference between the incident energy E_0 and the energy carried out of the detector by escaping electrons, positrons or photons. Dividing the scores by the incident number provided estimates of the spectrum of absorbed energy, normalized to one incident gamma ray.

3. Results

Preliminary to analyzing the Monte Carlo results, detection efficiencies were calculated using the analytical/numerical methods developed by Trombka et al [2]. Table 1 gives the detection efficiency as a function of θ_0 for monodirectional gamma rays incident with energies from 0.1 to 20 MeV. Table 1 also includes the detection efficiency for an isotropic flux of gamma rays, and gives as a function of θ_0 the projected area of the detector by which an incident flux should be multiplied to determine the count rate. The results in Table 1 indicate that for this detector the detection efficiency at any energy or angle is greater than about 40%, and the maximum variation with angle at a given energy is typically about a factor of 1.5.

The photon attenuation coefficient, also given in Table 1, is close to its minimum value at 5 MeV. Judging that at this energy the incident photon can perhaps best probe the shape of the detector, 5 MeV was chosen to study the angular variations of the peak probabilities, P_0, P_1 and P_2, in the absorbed-energy spectrum. The results are shown in Table 2 which gives the calculated values of the scaled peak probabilities P_i/η, and estimates of their standard deviation, for angles of incidence θ_0 from 0 to 90°. The standard deviation of the individual values of P_i is

$$\sigma(P_i) = [P_i(1-P_i)/N]^{1/2} \quad , \qquad (3)$$

with N=20000. No discernable trends with θ_0 are evident in the P_i values, and — with the exception of the anomalously low value for P_1 at 15° (judged a statistical fluke) — the scatter in the values is consistent with their standard deviations. In the earlier similar study [1] for a 3"x3" NaI detector (also a cylinder whose height equals its diameter), no significant angular dependence for the scaled peak probabilities P_i/η was found for gamma-ray energies of 0.661, 6.13 and 12.0 MeV. Therefore, the angular dependence of the peak probabilities can to a good approximation be accounted for through the use of the appropriate values of the detection efficiencies. Table 2 also gives values of the detection efficiency from the Monte Carlo calculations[2]. The good agreement with the corresponding values from Table 1 provides a useful check on the Monte Carlo sampling procedures.

For incident gamma-ray energies of 20, 10, 2, 1.6, 1, 0.5, 0.2 and 0.1 MeV, Monte Carlo calculations were done for θ_0 = 0 and 90°. After finding agreement generally within statistical limits between the values of P_i/η for the two incident angles, the average of the two results was adopted for each energy. The scaled peak probabilities were smoothed as a function of energy by means of a least-squares cubic-spline algorithm [13], and interpolated to intermediate energies. The results are shown in Fig. 1 and listed in Table 3. Combined estimated uncertainties (due to statistical fluctuations, averaging over incident angles, and smoothing), are less than ~ 2% for P_i greater than 0.2 and grow to ~ 5% for P_i = 0.02 and ~ 10% for P_i = 0.005.

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[2]The statistical errors associated with the values of the detector efficiencies from the Monte Carlo calculations can be estimated using Eq (2) with η_{MC} in place of P_i.

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Table 1. Detection efficiencies $\eta(E_0,\theta_0)$ for a cylindrical 5.5 × 5.5 cm high-purity Ge detector. Results, for broad beams of gamma rays incident with energies E_0 (attenuation coefficients μ), are given as a function of θ_0, the angle of incidence with respect to the detector axis. Detection efficiencies are given in the last column for the case of an isotropic incident flux. Entries at the bottom give, for each incident angle, the projected area of the detector by which an incident gamma-ray flux should be multiplied to determine the count rate.

E_0 (MeV)	μ (cm^2/g)	θ_0=0°	15°	30°	45°	60°	75°	90°	iso
20.0	0.0353	0.644	0.519	0.458	0.435	0.441	0.474	0.543	0.466
15.0	0.0334	0.624	0.502	0.442	0.420	0.425	0.457	0.524	0.449
10.0	0.0316	0.603	0.484	0.426	0.404	0.409	0.440	0.505	0.432
8.0	0.0310	0.597	0.478	0.421	0.399	0.404	0.435	0.499	0.427
6.0	0.0311	0.597	0.479	0.421	0.399	0.405	0.435	0.499	0.428
5.0	0.0316	0.603	0.484	0.426	0.404	0.409	0.440	0.505	0.432
4.0	0.0327	0.616	0.495	0.436	0.414	0.419	0.451	0.517	0.443
3.0	0.0352	0.643	0.518	0.457	0.434	0.440	0.473	0.542	0.465
2.0	0.0407	0.696	0.565	0.500	0.476	0.483	0.519	0.592	0.509
1.5	0.0463	0.742	0.606	0.539	0.514	0.522	0.560	0.637	0.549
1.0	0.0567	0.810	0.669	0.599	0.574	0.583	0.624	0.706	0.612
0.8	0.0633	0.843	0.702	0.631	0.606	0.616	0.659	0.743	0.645
0.6	0.0729	0.882	0.741	0.671	0.646	0.657	0.701	0.786	0.686
0.5	0.0797	0.903	0.764	0.695	0.670	0.682	0.727	0.812	0.711
0.4	0.0896	0.927	0.792	0.725	0.701	0.714	0.758	0.843	0.742
0.3	0.107	0.956	0.829	0.765	0.744	0.757	0.801	0.883	0.784
0.2	0.152	0.988	0.885	0.833	0.817	0.829	0.869	0.941	0.852
0.15	0.224	0.999	0.925	0.887	0.876	0.887	0.919	0.975	0.904
0.1	0.502	1.000	0.967	0.950	0.945	0.951	0.968	0.995	0.959
Projected Detector Area (cm^2)		23.76	30.78	35.70	38.19	38.08	35.37	30.25	35.64

Table 2. Scaled peak probabilities P_0, P_1 and P_2, and the detection efficiency η_{MC} from the Monte Carlo calculations for broad beams of 5-MeV gamma rays incident at an angle θ_0 with respect to the detector axis. Numbers in parentheses indicate the estimated statistical uncertainty in the last significant figures.

θ_0	η_{MC}	P_0/η	P_1/η	P_2/η
0°	0.603	0.0847(26)	0.0551(21)	0.0370(17)
15°	0.482	0.0858(29)	0.0433(21)	0.0408(20)
30°	0.424	0.0844(31)	0.0539(25)	0.0398(21)
45°	0.403	0.0810(31)	0.0560(26)	0.0392(22)
60°	0.405	0.0889(33)	0.0567(26)	0.0389(22)
75°	0.438	0.0854(31)	0.0577(25)	0.0374(20)
90°	0.506	0.0807(28)	0.0545(23)	0.0385(19)

Table 3. Calculated values of the peak probabilities for total absorption, P_0, single-annihilation escape, P_1, and double-annihilation escape, P_2, for the 5.5 × 5.5 cm Ge detector irradiated by broad beams of gamma rays incident with energy E_0. The results have been scaled by the detection efficiency to remove dependence on the angle of incidence.

E_0(MeV)	P_0/η	E_0(MeV)	P_0/η	P_1/η	P_2/η
0.1	0.964	1.2	0.248	0.000709	0.000644
0.15	0.898	1.5	0.220	0.00253	0.00206
0.2	0.791	2.0	0.187	0.00868	0.00661
0.3	0.592	3.0	0.142	0.0267	0.0199
0.4	0.478	4.0	0.109	0.0431	0.0316
0.5	0.411	5.0	0.0836	0.0539	0.0388
0.6	0.367	6.0	0.0648	0.0598	0.0419
0.8	0.310	8.0	0.0398	0.0611	0.0403
1.0	0.274	10.0	0.0255	0.0540	0.0341
		15.0	0.00971	0.0290	0.0181
		20.0	0.00434	0.0122	0.00853

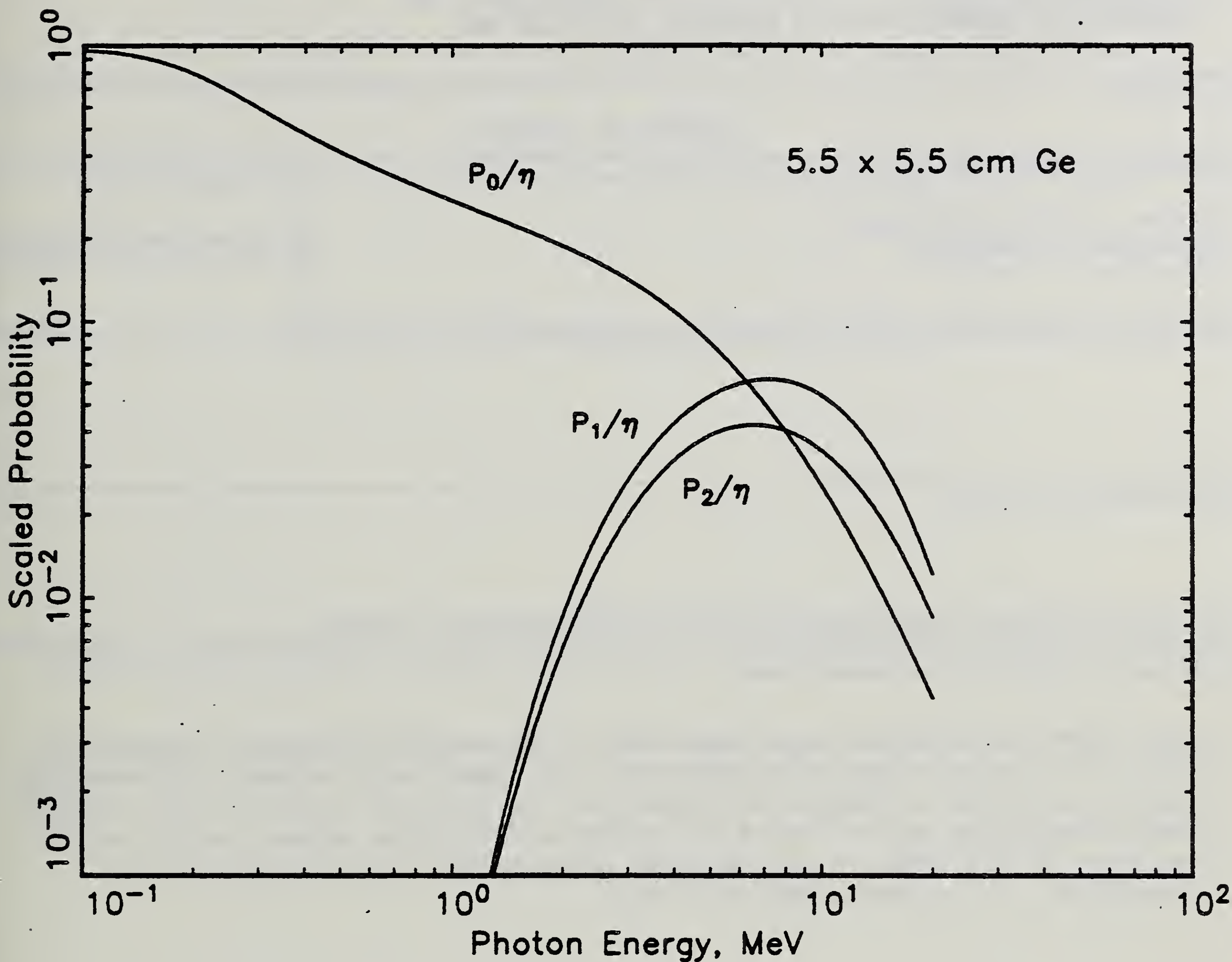

Figure 1. Peak probabilities for total absorption, P_0, single-annihilation escape, P_1, and double-annihilation escape, P_2, for the 5.5 × 5.5 cm Ge detector irradiated by broad beams of gamma rays incident with energy E_0. The results have been scaled by the detection efficiency η to remove dependence on the angle of incidence.

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Stephen M. Seltzer

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Monte Carlo calculations have been done of the energy and angular response of a 5.5 × 5.5 cm, high-purity Ge detector, for gamma rays incident with energies from 0.1 to 20 MeV. Results are given for the absolute probabilities of total energy absorption and of single and double annihilation escape, which relate the areas of the peaks in the measured pulse-height distribution to the intensities of incident gamma-ray lines.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

detection efficiency; escape peaks; gamma rays; Ge detectors; response function; total absorption peak

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