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**Modification to the Klein-Nishina Cross Section for
Ge Electrons at High Statistics Limit**

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Abstract

Modification factors for the Klein-Nishina cross-sections for gamma-ray with energies between 50 keV and 250 keV incident on Ge electrons have been obtained at the high statistics limit. In this limit, the Ge electrons can then be treated as they are obtained from the self-consistent augmented plane wave calculations, without considering the orientation of crystal lattice with respect to incident photons. The kinematics corrections (i.e. outgoing momenta), on the other hand, have to be taken into account on an event by event basis. Even so, the computing time has been reduced dramatically since the relativistic calculation of the modifications to the Klein-Nishina cross sections is the most tedious one. The modification factors are almost linear with respect to incident photon energy in the interesting energy range with respect to a given photon outgoing angle.

In our study of Monte Carlo simulation of the HPGe (high-purity germanium) gamma-ray spectra of Pu standards¹⁾ we have noticed that the Monte Carlo Code MCNP²⁾ does not properly taking into account bound electron momenta in matter in either kinematics or cross sections. In fact, by using the Khan³⁾ method (for gamma-ray energies below 1.5 MeV) and the Koberlinger⁴⁾ method (for gamma-ray energy above 1.5 MeV) for sampling of the Klein-Nishina cross section, the MCNP actually assumes that the electrons in the material are free and at rest. In most of the cases, taking into account such subtle effects from photons scattering of bound electrons is not necessary for a reasonable reproduction of a gamma-ray spectrum. However, we are concerned that in some cases, these effects might be significant, when an important gamma-ray line occurred just at the Compton edge of a strong gamma-ray line.

The study of the Compton profile for photon incident on electrons in matter has long been an interesting^{5,6)} topic both theoretically and experimentally. Because of differences in electron momenta distributions among materials, the Compton profile not only changes with respect to the energy of photons but also with the scatterers; therefore, the measured experimental data are always subtle. How to properly simulated the Compton profile using results obtained from experiments can always be a challenging task. For example, Felstenier et al.⁷⁾ trying to obtain the Ge Compton profile by integrating the measured form factor for a monoenergetic gamma-ray. The results are in decent agreement with the measured Compton profile for the monoenergetic gamma-ray. However, we are concerned about the availability of the measured form factor for various

materials and for different gamma-ray energies as well as the non-relativistic approaches used in the calculation.

We are trying to take into account the effect from bound electrons in Ge from another point of view. Basically, we are using the theoretically calculated electron momentum distributions instead of using the measured form factors so that we do not have to rely on the availability of the measured form factors. We are also taking into account relativistic corrections in both photon-electron kinematics and cross sections. In this report we summarized results from our study at the high statistics limit in which the orientation of the crystal is irrelevant.

HPGe Gamma-ray spectrum for a monoenergetic photon source

Figure 1 shows a spectrum taken from a HPGe detector with a ^{109}Cd source (which is a monoenergetic 88-keV gamma-ray emitter). The photo-peak (E_γ), Compton edge (E_c), Compton profile, and multiple (2 or more) Compton scattering regions are labeled. The shape at the region from $E_\gamma E_c$ to E_γ also depends (apart from the ballistic effect, trappings, etc.) on the Compton profile because of energy conservation. In general, the Compton edge represents the maximum recoil electron energy when the incident gamma-ray scatters backwards. For a reasonable Ge detector the peak-to-Compton ratio (ratio of the peak height at the photo peak and the Compton edge) is about 100:1, and the peak-to-double Compton ratio is roughly about several thousand to one. We have only taken into account the effect from a single Compton scattering in our study.

Kinematics for Photon-electron scattering and the Klein-Nishina cross sections

Figure 2 shows a general kinematics of the Compton effects, the incident photon (with momentum k_i and polarization ϵ_i) interacts with an electron (with four-momentum p_i and spin α_i), and the outgoing photon (k_f , ϵ_f) and outgoing electron (p_f , α_f). If the incident photon define the z-axis (i.e. outgoing photon in the positive x-z plane), the four momenta $k_f(0)$, $k_f(1)$, $k_f(2)$, $k_f(3)$ for the outgoing photon are (in $\hbar = c = 1$ unit):

$$\begin{aligned} k_f(0) &= [p_i(0)+k_i(0)]^2 - m^2 - p_i(1)^2 - p_i(2)^2 - [p_i(3)+k_i(0)]^2 \\ &\quad / \{2(p_i(0)+k_i(0))2[p_i(1)\sin\theta + [p_i(3)+k_i(0)]\cos\theta\} \\ k_f(1) &= k_f(0)\sin\theta \\ k_f(2) &= 0 \\ k_f(3) &= k_f(0)\cos\theta \end{aligned}$$

where θ is the angle in the laboratory for the outgoing photon and m is the mass of the electron. From momentum conservation we have $p_f = p_i + k_i + k_f$.

The lowest⁸⁾ order (e^2) of the Compton effect has only direct and exchange terms. The transition matrix, T_{fi} , is

$$T_{fi} = -e^2 \bar{u}(p_f, \alpha_f) \{ \epsilon_f [1 / (p_i - k_i - m)] \epsilon_i + \epsilon_i [1 / (p_i - k_f - m)] \epsilon_f \} u(p_i, \alpha_i)$$

where $\bar{u}$ is $u^\dagger \gamma_0$, and u is the Dirac spinor, γ is the Dirac matrix, and e is the charge of electron.

Therefore, the scattering cross section for photons on unpolarized electrons is

$$d\sigma/d\Omega = \alpha^2/2 \sum_{\alpha_f, \alpha_i} |T_{fi} / e^2|^2 (k_f/k_i)^2$$

where α is the fine structure constant.

For unpolarized photons scatter on rest electrons, the cross section reduced to the Klein-Nishina cross section:

$$d\sigma/d\Omega = (\alpha^2/4) m^2 (k_f/k_i)^2 [(k_f/k_i + k_i/k_f - \sin^2\theta)]$$

where m is the mass of the electron.

The MCNP uses the Klein-Nishina cross section for the Compton scattering.

Figure 3 and 4 show differences between free electrons and bound Ge K-shell electrons in both the kinematics and scattering cross sections, only two extremes are plotted. We have chosen to use K-shell electrons in Ge to demonstrate the effect, for other shells (i.e. L, M, etc.) these effects are smaller. These figures demonstrate the effects due to the finite momentum distributions of the bound electrons. For this particular case, the electron momenta could produce up to 5% differences in both scattering kinematics and cross sections.

Electron Wave Functions in Ge

Around 1930s, by applying hydrogen-like wave functions to bound electrons, Wentzel⁹⁾ and Bloch¹⁰⁾ already realized that the Compton scattering from the bound electrons results in both broadening of the Compton line and asymmetrical shape of the line. Results from their calculations show that the calculated Compton effects are in satisfactory agreement with the measurements.

Instead of using the hydrogen-like wave function, we have taken a step further, using the Augmented Plane Wave functions^{11,12)} to describe the electron momentum

distributions in Ge. In this formalism, the electron momentum distribution $\rho(p)$ is given by

$$\rho(p) = N \sum_{n,k,G} \left| \int_{\text{unitcell}} e^{-ip \cdot r} \Psi_{n,k}(r) d^3r \right|^2 \delta_{p,k+G}$$

where k is a vector in the first Brillouin zone and in the n -th band and the corresponding wave function is $\Psi_{n,k}(r)$. G is the reciprocal lattice vectors, N is the normalization constant, and δ is the Kronecker delta. Details of calculating the wave functions can be found in Ref. 12.

High statistics limit

At the high statistics limit, in which the orientation of the crystal is irrelevant the modified photon electron cross section can be written as a simple form factor multiplied to the Klein-Nishina cross section,

$$d\sigma/d\Omega = S(E_\gamma, \theta) (d\sigma/d\Omega)_{K-N}$$

The form factors $S(E_\gamma, \theta)$ at the energy region of our interest are shown in Figure 5. We have obtained these form factors by applying relativistic corrections as well as using the appropriated electron momentum distributions obtained from the calculations. It is worth noting that in the energy region $50 \text{ keV} < E_\gamma < 250 \text{ keV}$ (apart from the lowest energy and at the backward angle), it shows almost linear behavior for a given outgoing photon angle. Figure 6 shows our simulated Compton profile compared to the MCNP

simulation as well as the measured profile for the 88-keV monoenergetic gamma-ray. The sharp Compton edge from the MCNP simulation (due to two-body kinematics with electron at rest) smoothen and the entire profile is in better agreement with the measured profile.

Summary

We have used the theoretical calculated electron momentum distributions in Ge along with applying relativistic kinematics corrections in the simulation of the Compton profile. The results are in better agreement with the measurement compared to the results from the standard MCNP calculations.

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Figure Captions

Figure 1. A 88-keV monoenergetic gamma-ray energy spectrum of ^{109}Gd obtained from a high-purity germanium detector. The photo peak E_γ , Compton edge E_c , Compton profile, and multiple Compton scattering are labeled.

Figure 2. General interaction picture for photon-electron scattering

Figure 3. Relativistic kinematics (in polar plot) of photon scattering: 1) Head on with incoming K-shell electrons in Ge moving towards photons, 2) with electrons at rest, and 3) same as (1) with incoming electrons moving away from photons.

Figure 4. Unpolarized differential cross sections (in polar plot) for the cases (1), (2), (3) described in Figure 2.

Figure 5. The correction factor $S(E_\gamma, \theta)$ at the high statistics limit when the Ge crystal orientation is irreverent.

Figure 6. The Compton profile of 88-keV ^{109}Cd gamma-rays in a HPGe detector. (a) measured, (b) MCNP simulation, (c) MCNP simulation with our corrections.

Fig 1

Fig. 3

Fig. 4

Fig 5

Fig. 6