Benchmark of GEANT4 Treatment of Electron Backscattering from a Thin Film

Jianglai Liu, Brad Filippone, Caltech

September 13, 2007

Abstract

In this note, we summarize a benchmark study of the GEANT4 treatment of the e^- backscattering from a thin film in the energy range of the electrons from the neutron β decay.

1 Introduction

As discussed in [1], electron backscattering in the UCNA spectrometer can be categorized into four different types. They are illustrated in Fig. 1. Types I, II, and III can be distinguished using the

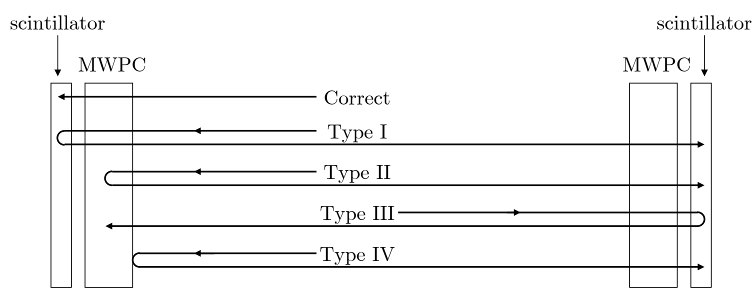


Figure 1: *Classification of backscattering events from Ref. [1].*

TDC timing and the MWPC information. Type IV, the electron backscattering from the front window (or dead layer) of the MWPC, is the only type that can not be measured experimentally. One therefore has to rely on a well-calibrated simulation to evaluate and correct for its effect. This motivates us to benchmark the GEANT4 treatment of such type of electron backscattering process in the neutron beta energy range. In Sec. 2, we present a simple calculation which gives the order magnitude of the effect that one might expect. In Sec. 3, some simulations with very simple geometry (and magnetic field) will be made and compared with theoretical calculation.

2 Theoretical Calculation

Electrons undergo multiple elastic scattering with the atomic electrons when they traverse the material. Backscattering, in effect, is a single or multiple scattering processes that makes the electron "turn around" and emit back from the incident surface of the material. To set the scale, for material such as carbon and an electron energy of 100 keV, the total elastic scattering cross section is about 5×10^{-19} cm^2 (see, e.g., Ref. [2]). The mean free path for such electrons in carbon is about 0.2 μm. So unless the thickness of the material is less than 0.2 μm, it seems that the single scattering approximation is not valid. On the other hand, if we are only interested in the backscattering, then large angle scattering is much more effective to turn the electron around. Therefore one expects that the 0.2 μm limit can be relaxed to some larger thickness. We shall present, hereafter, a calculation of the backscattering on a thin film *based on the single elastic scattering*, which should serve as a lower limit of the backscattering fraction, and provide some guidance to the energy and angle dependence of the backscattering fraction.

The differential cross section for electron elastically scattering with atomic electrons is given by the Mott formula:

$$\frac{d\sigma_{Mott}}{d\Omega} = \frac{Z^2\alpha^2}{4|\vec{p}|^2\beta^2\sin^4(\frac{\theta}{2})}(1-\beta^2\sin^2(\frac{\theta}{2}))\,. \tag{1}$$

In this equation, Z is the charge number of the target atom, α is the fine structure constant, θ is the scattering angle, and β and $\vec{p}$ are the (dimensionless) velocity and three-momentum of the electron. Strictly speaking, this formula is in the center of mass (CM) frame of the electron-atom system. For energy regime of the neutron beta decay, CM is practically the same as in the lab frame. The backscattering fraction (or probability) is an integral of this cross section over all scattering angles **that makes the electrons "turn-around"**.

2.1 Calculation of Normal Incidence Backscattering Fraction (NIBF)

As a starter, let us consider the normal incidence electrons: incoming electron perpendicular to the material surface (Fig. 2). Let us further assume that the detector acceptance covers the entire back angle, i.e. all electrons with scattering angle θ is $> \frac{\pi}{2}$ will be detected by the detector on the other side. Then NIBF can be calculated by integrating Eqn. 1 over the scattering angle from $\frac{\pi}{2}$ to π.

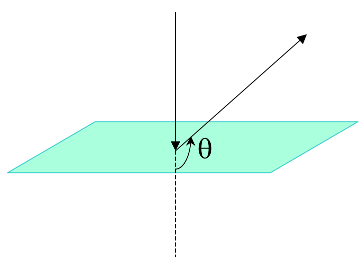


Figure 2: *Backscattering for electron normal incidence.*

Define $\sigma_{\theta_0} \equiv \int_{\theta_0}^{\pi} \frac{d\sigma_{Mott}}{d\Omega} d\Omega$. With Eqn. 1, we have

$$\sigma_{\theta_0} = \frac{2\pi Z^2\alpha^2}{4|\vec{p}|^2\beta^2}(2\frac{1+\cos\theta_0}{1-\cos\theta_0} + 4\beta^2\ln(\sin\frac{\theta_0}{2})) \tag{2}$$

Note that the 2π on the r.h.s. of the above expression is due to the integration over azimuthally symmetric ϕ dependence. The total normal incidence backscattering cross section can then be written by replacing θ_0 by $\pi/2$ in Eqn. 2:

$$\sigma_{nib} = \sigma_{\pi/2} = \frac{2\pi Z^2\alpha^2}{4|\vec{p}|^2\beta^2}(2-1.39\beta^2)\,. \tag{3}$$

The backscattering fraction for a single-element material is then simply

$$\eta_{nib} = \sigma_{\pi/2} \times t \times n_{tgt}\,, \tag{4}$$

where t is the target thickness and n_{tgt} is the target atom number density. For NIBF from a composite $E_1x_1E_2x_2\ldots$ (e.g. mylar = $C_6H_4O_2$) with the atomic and charge number A_i and Z_i for each element, the backscattering fraction η_{nib} is

$$\eta_{nib} = \sum_i x_i \sigma^i_{\pi/2} \times t_{tgt} \times \frac{\rho}{\sum_k x_k A_k} \mathcal{N}_A \,. \tag{5}$$

In this expression, ρ and $\mathcal{N}_A$ are the material density and the Avogadro's number, respectively, and $\sigma^i_{\pi/2}$ is obtained by replacing Z by Z_i in Eqn. 3.

2.2 NIBF with Magnetic Field Mirroring

To simulate the realistic detector acceptance, let us now consider the effect of the magnetic field. As shown in Fig. 3, electrons initially start off along z and the magnetic field there is 1 Tesla (also along z). The field adiabatically reduces into 0.6 Tesla, where the thin film is located. Electron

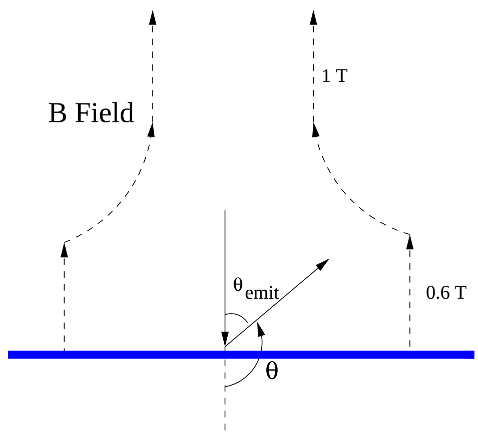


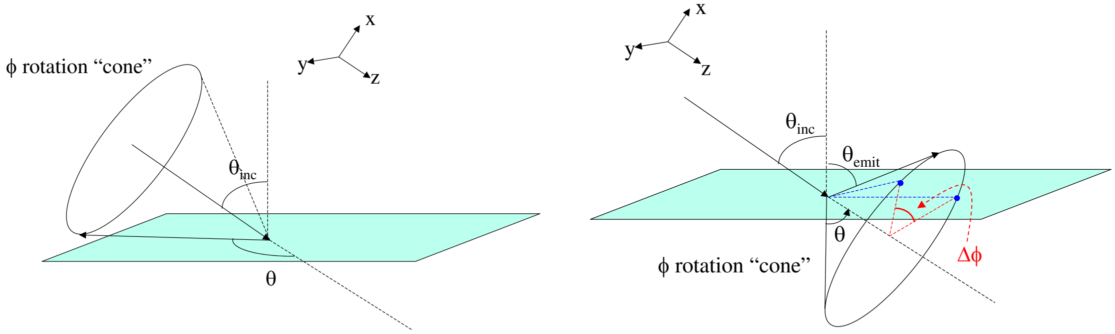
Figure 3: *Magnetic field configuration for mirroring of backscattered electrons.*

emitted from the surface with $\theta_{emit} > \sin^{-1}\sqrt{\frac{0.6}{1.0}} = 51^\circ$ will be "mirrored" back. So they will not be detected (misidentified) by the detector on the other side. In this case, to calculate the fraction of electrons backscattered into the other side of the detector, we simply replace θ_0, the lower limit of the integral over θ in Eqn. 2, by $180^\circ - 51^\circ = 129^\circ$.

2.3 Calculation of Oblique Incidence Backscattering Fraction (OIBF)

The calculation of NIBF above is greatly simplified due to the azimuthal symmetry (π integral can be simply pulled out). Now let us consider that the electron strikes the surface with θ_{inc} to the normal (=oblique incidence). A schematic view is shown in Fig. 4. All scattered trajectories for a given scattering angle θ are represented in the figure by a cone. Let us again assume that the detector acceptance covers the entire back angle, like in the case Sec. 2.1. The subtlety is that the range of the ϕ angle for backscattering depends on the scattering angle θ as follows. A) When $\theta < \pi/2 - \theta_{inc}$, the entire cone will be below the material surface. There is no backscattering by definition. B) When $\pi - \theta < \pi/2 - \theta_{inc}$, i.e. $\theta > \pi/2 + \theta_{inc}$, the entire cone will be above the surface (see Fig. 4(a)). Therefore any ϕ within 0 and 2π will correspond to backscattering, just like the situation in Sec. 2.1. C) When $\pi/2 - \theta_{inc} < \theta < \pi/2 + \theta_{inc}$, only part of cone is above the surface, as shown in Fig. 4(b). Therefore the integral over ϕ is less than 2π.

To calculate the range of ϕ for a given scattering angle θ (case C), let us consider the critical ϕ value when the emitting electron is in plane with the material surface. In this case, $\cos\theta_{emit} \equiv \hat{n} \cdot \hat{p} = 0$, where $\hat{p}$ is the final electron momentum direction and $\hat{n}$ is the normal of the surface



(a) $\Delta\phi = 2\pi$ (b) $\Delta\phi < 2\pi$

Figure 4: *Illustration of backscattering for oblique incident electrons with a full (a) and partial (b) range of ϕ angle.*

(pointing down). Let us now work in the "natural coordinate" of the incident electron (incident momentum along $\hat{z}$), as shown in Fig. 4(b). Then

$$\hat{n} = -\sin\theta_{inc}\hat{x} + \cos\theta_{inc}\hat{z}, \hat{p} = \sin\theta\cos\phi\hat{x} + \sin\theta\sin\phi\hat{y} + \cos\theta\hat{z}\,. \tag{6}$$

So

$$\hat{n}\cdot\hat{p} = -\sin\theta_{inc} sin\theta\cos\phi\ + cos\theta_{inc}\cos\theta = 0\,. \tag{7}$$

Therefore,

$$\phi_{crit} = \cos^{-1}\left[\frac{\cos\theta_{inc}\cos\theta}{\sin\theta_{inc}\sin\theta}\right]\,, \text{or} \int d\phi = 2\times\cos^{-1}\left[\frac{\cos\theta_{inc}\cos\theta}{\sin\theta_{inc}\sin\theta}\right]\,. \tag{8}$$

Based on the discussions above, the total oblique backscattering cross section for an incident angle θ_{inc} can now be calculated as

$$\sigma_{oib}(\theta_{inc}) = \int_{\frac{\pi}{2}-\theta_{inc}}^{\frac{\pi}{2}+\theta_{inc}} \frac{\sigma_{Mott}}{d\Omega}\times 2\cos^{-1}\left[\frac{\cos\theta_{inc}\cos\theta}{\sin\theta_{inc}\sin\theta}\right]\sin\theta d\theta + \int_{\frac{\pi}{2}+\theta_{inc}}^{\pi}\frac{\sigma_{Mott}}{d\Omega}\sin\theta d\theta\times 2\pi\,. \tag{9}$$

The 2nd term on the r.h.s. is just $\sigma_{\frac{\pi}{2}+\theta_{inc}}$ (Eqn. 2). The first term can be calculated by numerical integration.

Similar to Eqn. 5, the total fraction for oblique backscattering for a given incident angle θ_{inc} is now

$$\eta_{oib}(\theta_{inc}) = \sum_i x_i\sigma^i_{oib}\times\frac{t_{tgt}}{\cos(\theta_{inc})}\times\frac{\rho}{\sum_k x_k A_k}\mathcal{N}_A\,. \tag{10}$$

Note that the effective thickness of the film has been corrected by a factor of $1/\theta_{inc}$.

2.4 OIBF with Magnetic Field Mirroring

As discussed in Sec. 2.2, for a magnetic field configuration in Fig. 3, to backscatter into the detector on the other side, the emitting angle has to be less than 51°. In another word, the outgoing electron momentum has to be within a 51° cone around the surface normal. In this case, very similar to

Fig. 4, the range of ϕ angle for backscattering depends on the scattering angle θ as follows:

$$\begin{aligned}
&\pi - \theta < 51^\circ - \theta_{inc} \Rightarrow \theta \in (129^\circ + \theta_{inc}, \pi) \Rightarrow \int d\phi = 2\pi \\
&51^\circ - \theta_{inc} < \pi - \theta < 51^\circ + \theta_{inc} \Rightarrow \theta \in (129^\circ - \theta_{inc}, 129^\circ + \theta_{inc}) \Rightarrow \int d\phi < 2\pi \\
&\pi - \theta > 51^\circ + \theta_{inc} \Rightarrow \theta \in (0, 129^\circ - \theta_{inc}) \Rightarrow \int d\phi = 0\,.
\end{aligned} \tag{11}$$

It is important to note that due to the magnetic field, the range of the incident electron angle θ_{inc} (in the 0.6 T region) is from 0 to 51°. Therefore, the relations above is valid for all possible θ_{inc}.

For $\theta \in (129^\circ - \theta_{inc}, 129^\circ + \theta_{inc})$, the ϕ angle range can be calculated using Eqn. 7 with the modification that

$$\hat{n} \cdot \hat{p} = -\sin\theta_{inc} sin\theta \cos\phi \ + cos\theta_{inc} \cos\theta = -\cos 51^\circ\,. \tag{12}$$

The reason for $-\cos 51^\circ$ on the r.h.s. is that $\hat{n}$ is defined as the surface normal *pointing downward*. Therefore,

$$\phi_{crit} = \cos^{-1}\left[\frac{\cos\theta_{inc}\cos\theta + \cos 51^\circ}{\sin\theta_{inc}\sin\theta}\right], \text{or} \int d\phi = 2 \times \cos^{-1}\left[\frac{\cos\theta_{inc}\cos\theta + \cos 51^\circ}{\sin\theta_{inc}\sin\theta}\right]. \tag{13}$$

The total OIB cross section for a given θ_{inc} is now

$$\begin{aligned}
\sigma_{oib}(\theta_{inc}) = &\int_{129^\circ - \theta_{inc}}^{129^\circ + \theta_{inc}} \frac{\sigma_{Mott}}{d\Omega} \times 2\cos^{-1}\left[\frac{\cos\theta_{inc}\cos\theta + \cos 51^\circ}{\sin\theta_{inc}\sin\theta}\right]\sin\theta d\theta \\
&+ \int_{129^\circ + \theta_{inc}}^{\pi} \frac{\sigma_{Mott}}{d\Omega}\sin\theta d\theta \times 2\pi\,.
\end{aligned} \tag{14}$$

The total OIBF for this θ_{inc} can then be calculated using Eqn. 10.

Lastly, let us consider a realistic case where the initial electron momentum is isotropic in the 1 T region. The electrons, when hitting the film, has an incidence angle range from 0 to 51°. The total backscattering fraction is an average of $\eta_{oib}(\theta_{inc})$ (Eqn. 10) over the entire distribution of θ_{inc}:

$$\langle\eta_{oib}\rangle = \frac{\displaystyle\int_0^{51^\circ} \eta_{oib}(\theta_{inc})\frac{dN}{d\cos(\theta_{inc})}d(\cos\theta_{inc})}{\displaystyle\int_0^{51^\circ} \frac{dN}{d\cos(\theta_{inc})}d(\cos\theta_{inc})}\,. \tag{15}$$

Since the electron angular distribution is isotropic in the decay region (1 T), so

$$\frac{dN}{d\cos\theta_D} = \text{const}\,, \tag{16}$$

where $\theta_D \in [0, \pi/2]$ is the electron polar angle in the decay region. As discussed in Sec. 2.2, θ_D and θ_{inc} are related by

$$\frac{\sin(\theta_{inc})}{\sin\theta_D} = \sqrt{\frac{0.6}{1}} = 0.78\,. \tag{17}$$

It is then easy to show that

$$\frac{dN}{d\cos(\theta_{inc})} = \text{const} \times \frac{1}{0.78}\frac{\tan\theta_D}{\tan\theta_{inc}}\,. \tag{18}$$

Therefore, we have

$$\langle\eta_{oib}\rangle = \int_0^{51^\circ} \eta_{oib}(\theta_{inc})\frac{1}{0.78}\frac{\tan\theta_D}{\tan\theta_{inc}}d(\cos\theta_{inc})\,, \tag{19}$$

where $\eta_{oib}(\theta_{inc})$ is given by Eqn. 14. This can be evaluated, once again, via numerical integration.

3 GEANT4 Simulations and the Comparison with the Single-scattering Calculation

A simple GEANT4 (version 4.8.3) simulation program was developed to study the backscattering from a thin film. The geometry of the set up is shown in Fig. 5. A 3 meter long decay tube (yellow) is located in the 1 T region, where the initial electrons were generated. The detector packages (on both sides of the decay tube) were modeled by a window (green) backed by a detector disk (red) made out of vacuum (so no backscattering can occur on the detector itself).

Figure 5: *GEANT4*

The standard GEANT4 electromagnetic package was chosen in this simulation *without tuning*. The thickness of the film was chosen to be 25 μm in the simulation. This is simply based on statistical consideration. We chose the material of the film to be either mylar or Be since they are used as window materials in UCNA. Electrons are thrown towards a given side of the detector initially, and the backscattered fraction from the film can be calculated from the number of electrons detected by the detector on the other side [1]. The magnetic field can be switched between a 1 T uniform field, or a 1 T$\longrightarrow$ 0.6 T configuration like that in UCNA. To simulate NIB with full back angle acceptance (Sec. 2.1), the electrons were thrown out along the decay tube perpendicular to the window, with a uniform 1 T magnetic field in the entire volume. For NIB (OIB) with magnetic field mirroring, the field profile in Fig. 3 was used, and electrons were thrown perpendicular (or isotropically) toward the window.

The results of this simulation are summarized in Table 1. In this table, the electron backscattering fractions at various energies from 25 μm of mylar and Be films are listed for a) normal incidence with complete back angle acceptance ($=\eta_{nib}^{90^\circ}$), b) normal incidence with partial back angle acceptance corresponding to the field configuration in Fig. 3 ($=\eta_{nib}^{129^\circ}$), and c) oblique incidence with isotropically initial momentum and the field configuration in Fig. 3 ($=\eta_{oib}$). For brevity the statistical uncertainties are omitted in the table, but they are better than 15% even for the smallest backscattering fraction. For comparison, the calculated backscattering fraction based on the formalism in Sec. 2 are also listed in the table.

Material	thickness (μm)	E_e (keV)	$\eta_{nib}^{90^\circ}(\%)$ GEANT4	Calc	$\eta_{nib}^{129^\circ}(\%)$ GEANT4	Calc	$\eta_{oib}(\%)$ GEANT	Calc
mylar	25	100	0.99	1.06	0.71	0.22	1.70	0.43
mylar	25	200	0.38	0.25	0.21	0.048	0.59	0.10
mylar	25	300	0.23	0.11	0.11	0.019	0.19	0.043
mylar	25	400	0.16	0.06	0.07	0.010	0.10	0.024
Be	25	100	0.37	0.76	0.27	0.16	0.69	0.31
Be	25	200	0.20	0.18	0.09	0.035	0.32	0.073
Be	25	300	0.14	0.079	0.05	0.014	0.08	0.031
Be	25	400	0.07	0.044	0.03	0.007	0.04	0.017

Table 1: *Simulated (GEANT4) and calculated ("Calc") backscattering fractions from 25 μm mylar and Be films with various incident electron energy. See text for details.*

Several quick observations can be made from the table. First, in general GEANT4 gives larger

[1] No backscattering from the detector is possible since it is made out of vacuum.

backscattering fraction than the simple calculation. This indicates that the effect of the multiple scattering is not negligible. Second, the agreement between GEANT4 and the simple calculation is the best for $\eta_{nib}^{90^\circ}$, very roughly GEANT4 $\sim 2\times$ simple calculation. For $\eta_{nib}^{129^\circ}$ and η_{oib}, the difference is larger, ranging from a factor of 2 up to 7. This, once again, indicate that multiple scattering plays a rather important role for a 25 μm window. This is expected from the order of magnitude estimate given at the beginning of Sec. 2. Third, the energy dependence of the backscattering fraction from the simple calculation is very close to a $1/E^2$ (see Eqn. 1). GEANT4 predicts a slightly gentler dependence, e.g. from 100 to 200 keV, GEANT4 gives a factor of 2 to 3 reduction in the backscattering fraction instead of a factor of 4. This is a bit puzzling: multiple scattering and the energy loss in the window should bring a sharper dependence to the backscattering fraction.

In any case, the simple calculation should only serve as a lower bound of the backscattering fraction from the thin film due to its simplifying assumptions of the scattering process. In this regard, the GEANT4 prediction appears to be reasonable at the very least. Based on GEANT4, the backscattering fraction from the 25 μm windows of the MWPC should be small (about 0.2%), since the beta energy from neutron decay peaks around 300 keV.

References

[1] B. Plaster, et al., *Calibration of the electron spectrometer for a precision measurement of the neutron β-asymmetry*, UCNA internal report, Oct. 24, 2006.

[2] R. Browning, et al., J. Vac. Sci. Technol. B 9(6), Nov/Dec (1991).