THE HYBRID MODEL FOR SAMPLING MULTIPLE ELASTIC SCATTERING ANGULAR DEFLECTIONS BASED ON GOUDSMIT-SAUNDERSON THEORY

by

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An algorithm for the Monte Carlo simulation of electron multiple elastic scattering based on the framework of SuperMC (Super Monte Carlo simulation program for nuclear and radiation process) is presented. This paper describes efficient and accurate methods by which the multiple scattering angular deflections are sampled. The Goudsmit-Saunderson theory of multiple scattering has been used for sampling angular deflections. Differential cross-sections of electrons and positrons by neutral atoms have been calculated by using Dirac partial wave program ELSEPA. The Legendre coefficients are accurately computed by using the Gauss-Legendre integration method. Finally, a novel hybrid method for sampling angular distribution has been developed. The model uses efficient rejection sampling method for low energy electrons (<500 keV) and larger path lengths (>500 mean free paths). For small path lengths, a simple, efficient and accurate analytical distribution function has been proposed. The later uses adjustable parameters determined from the fitting of Goudsmith-Saunderson angular distribution. A discussion of the sampling efficiency and accuracy of this newly developed algorithm is given. The efficiency of rejection sampling algorithm is at least 50 % for electron kinetic energies less than 500 keV and longer path lengths (>500 mean free paths). Monte Carlo Simulation results are then compared with measured angular distributions of Ross *et al*. The comparison shows that our results are in good agreement with experimental measurements.

Key words: Monte Carlo, multiple scattering, Goudsmit-Saunderson, SuperMC, differential cross-section, angular distribution, ELSEPA

INTRODUCTION

During the passage of electron through the matter, it experiences a large number of elastic collisions with the atomic nuclei. This changes the electron's direction, but does not significantly change its energy. The number of such collisions is so large that a detailed Monte Carlo simulation of individual scattering events is almost impractical. The solution for incapacitating this difficulty is provided by the Condensed-history technique [1], in which the electron is followed in a series of steps, and a multiple scattering theory is used to group individual elastic scattering events. An accurate and efficient treatment of multiple scattering angular distributions is thus required in a general purpose Monte Carlo code such as SuperMC [2].

SuperMC is a general purpose, easy-to-use Monte Carlo simulation program, developed by FDS Team [2-5], for modeling and simulation of nuclear facilities. The released version of SuperMC can perform simulations for neutrons, photons and coupled neutron and photon transport, while Monte Carlo simulation of electron transport has been under development and will be released soon. This research work is the part of the development of electron transport. SuperMC has been applied to fusion reactor FDS I [6], FDS II [7], FDS III [8], ITER [9, 10] and other reactor studies [11, 12] and is also designed for the Monte Carlo based dose calculation engine of KylinRay (Accurate Radiotherapy System) [13].

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The multiple scattering probability distribution can be calculated through one of the multiple scattering theories of Goudsmit-Saunderson [14], Moliere [15] or Lewis [16]. Moliere's theory uses scaled angular variable to describe the distribution function which makes it fairly easy to sample angular deflections but the accuracy is limited because it is based on small angle approximation and also do not account the spin and relativistic effects. It is used in GEANT3 [17] and EGS4 [18]. The theory of Goudsmit-Saunderson (GS) [14] describes the "exact" multiple scattering distributions for an arbitrary differential cross-section and the distribution function can be applied for much smaller path lengths. It accounts the spin and relativistic effects and also differentiates between the scattering of electrons and positrons. Most of the Monte Carlo electron-photon transport codes such as ETRAN [19], EGS5 [20], PENELOPE [21], GEANT4 [22] uses Goudsmit-Saunderson theory or Lewis theory of Multiple scattering. EGSnrc [23] use a modified form of the Goudsmit-Saunderson theory that is based on the work of Kawrakow [24].

However, the random sampling from Goudsmit-Saunderson distribution function is complicated because it is based on the Legendre expansion of single scattering law. Therefore, previously, a huge database of pre-computed angular distributions for a set of pre-selected path lengths has been used for random sampling in many Monte Carlo codes, such as ETRAN [19], GEANT4 [22], and PENELOPE [21]. EGS5 [20] uses a Wentzel shape analytical function with adjustable parameters determined from the fitting of the GS distribution function, but the method is still computational extensive as it requires the calculation of GS distribution function at many angle points (~287 points).

In this paper, an efficient and accurate hybrid method for sampling angular distribution has been presented and it is based on Goudsmit-Saunderson theory of multiple scattering. Differential cross-sections (DCS) for electron and positron with kinetic energy range 1eV to 100 MeV and for Z = 1-95 have been calculated using Dirac partial wave program ELSEPA [25]. The Legendre coefficients in the single scattering distribution are accurately computed by using Gauss-Legendre integration method.

ELECTRON MULTIPLE ELASTIC SCATTERING

A brief review of Goudsmit-Saunderson theory of multiple elastic scattering [14] is presented in this section. We consider the multiple elastic scattering of electrons and positrons moving in an infinite homogeneous medium with kinetic energy E with N scattering centers per unit volume. The differential cross-section is assumed to be symmetric about the incident electron direction (*i. e.* depends on polar angle θ).

Angular distribution

The Goudsmit-Saunderson distribution of multiple scattering for arbitrarily large angles has the form

$$F_{\mathrm{GS}}(s,\theta) \quad \sum_{l\ 0}^{\infty} \frac{2l\ \ 1}{4\pi}\ \mathrm{e}^{\ -sG_l} P_l(\cos\theta) \qquad (1)$$

where θ is the angle between the initial and the final direction. The P_l's are Legendre polynomials, s is the path length (in gcm^{-2}). G_l's are Legendre coefficients, also called transport coefficients and can be calculated as

$$G_l \quad \frac{2\pi}{\lambda}\int_{1}^{1}[1 \quad P_l(\cos\theta)]\frac{1}{\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}d(\cos\theta) \qquad (2)$$

where $\mathrm{d}\sigma\ \mathrm{d}\Omega$ is the elastic differential cross-section as a function of polar angle for given E and Z. λ is the mean free path (mfp) and given as

$$\lambda^{\ 1} \quad N\sigma \quad \frac{N_{\mathrm{A}}\rho}{A_{\mathrm{w}}}\sigma \qquad (3)$$

where σ is the total elastic cross-section for given Z and E. N_{A} is the Avogadro's number, ρ – the mass density, and A_{W} – the atomic weight of the material.

The number of terms needed to make the Goudsmit-Saunderson series converge in eq. (1) increases as the path length decreases. However, the convergence of the series can be improved for smaller path lengths by separating the contribution from electrons that have experienced no collision [26]

$$\begin{aligned} F_{\mathrm{GS}}(s,\theta) \quad & \frac{\delta(\cos\theta\ \ 1)}{\pi}\mathrm{e}^{\ s/\lambda} \\ + & \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}[\mathrm{e}^{\ sG_l} \quad \mathrm{e}^{\ s/\lambda}]P_l(\cos\theta) \end{aligned} \qquad (4)$$

The first term of eq. (4) represents unscattered electrons.

Differential cross-sections database

Differential cross sections (DCS) for electron and positron with kinetic energy range 100 eV to 100 MeV and for Z = 1-95 have been calculated using Dirac partial wave program ELSEPA [25]. These differential cross sections account for screening, finite nuclear size, spin and relativistic effects. For given Z, electron and positron elastic DCS data is presented in tabulated form using a logarithmic grid of 91 kinetic energies E_{i}. For each energy in the grid, DCS is tabulated for 606 scattering angle points with a nearly logarithmic spacing near θ = 0 which allows cubic spline interpolation of $\ln(\mathrm{d}\sigma/\mathrm{d}\Omega$ in $\ln E$ and θ. Figure 1 shows the DCS for elastic scattering of electrons incident on lead and aluminum with various kinetic energies calculated by using ELSEPA [25].

MONTE CARLO SIMULATION

In this section, the Monte Carlo simulation of multiple elastic scattering is presented. In order to

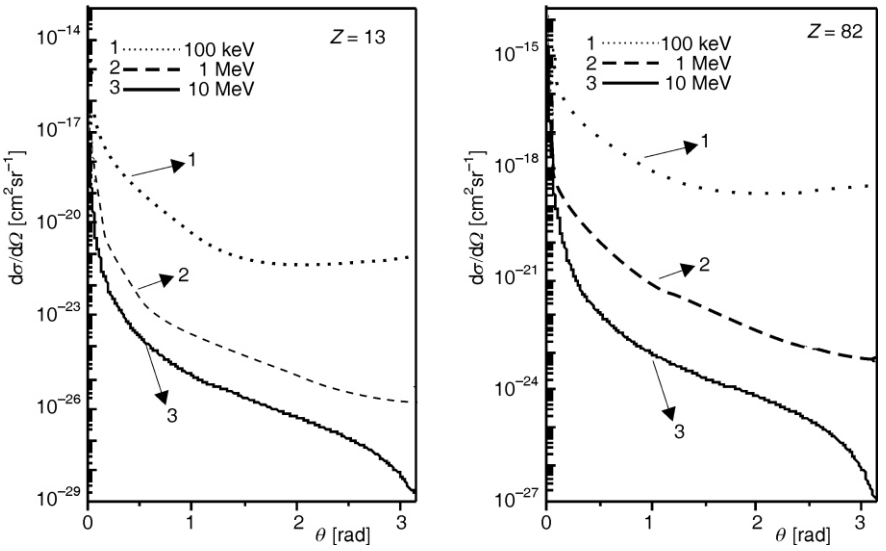

Figure 1. Differential cross section for elastic scattering of electrons incident on lead and aluminum with various kinetic energies calculated by using Dirac partial wave program ELSEPA [25]

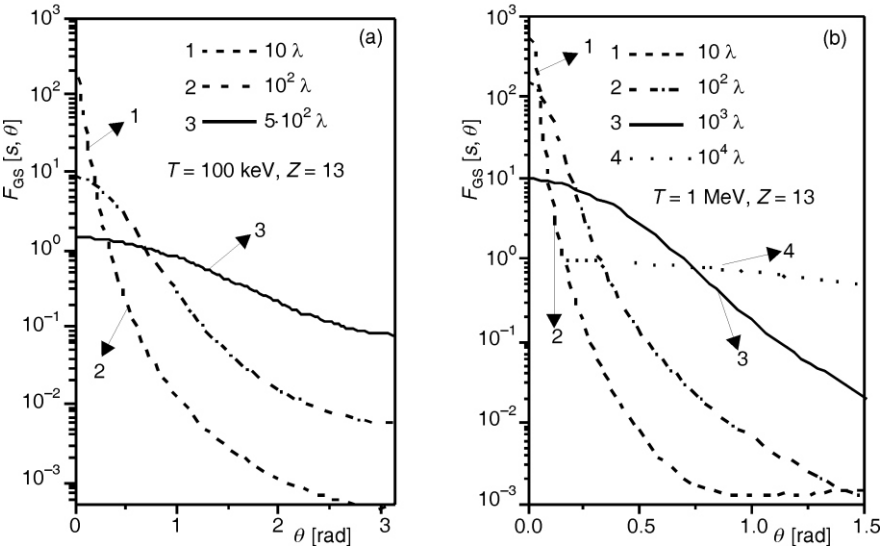

Figure 2. Goudsmit-Saunderson distribution (eq. 1) of (a) 100 keV and (b) 1 MeV electrons incident on aluminum

sample the angular deflections, one needs to accurately calculate the Goudsmit-Saunderson distribution function for given material (Z), electron kinetic energy (E) and path length (s).

Numerical calculation of GS distribution function

For the calculation of GS distribution function we started from the calculation of Legendre coefficients as described in eq. (2) for a given material (Z) and electron kinetic energy (E). Let μ $\cos\theta$ eq. (2) becomes

$$G_l \quad \frac{2\pi}{\lambda} \int_{1}^{1} [1 \quad P_l(\mu)] \frac{1}{\sigma} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \mathrm{d}\mu \tag{5}$$

Integrals in eq. (5) can be evaluated to very high accuracy with Gauss-Legendre quadrature formula. The n point Gauss-Legendre quadrature has the form

$$\int_a^b f(x)\mathrm{d}x \quad \frac{b \quad a}{2} \sum_{i \ 1}^{n} w_i f \quad \frac{b \quad a}{2} \xi_i \quad \frac{b \quad a}{2} \ w_i \quad \frac{2}{(1 \quad \xi_i^2 [P_{\mathrm{N}}(\xi_i)]^2} \tag{6}$$

where ξ_i are the n-zeros of the n^{th} order Legendre polynomial. We have used two points Gauss-Legendre quadrature to evaluate the integral in eq. (5) with ξ = = and $w_1 = w_2 = 1$. The maximum number of coefficients that can be obtained from our code are 20,000.

After the calculation of Legendre coefficients, the GS distribution of multiple scattering has been evaluated according to the eq. (1). We have used up to 1000 terms of the Goudsmit-Saunderson series and found that, for lead and aluminum, the convergence of the series can be achieved for pathlengths as low as 10 mfp at 1 MeV and for pathlengths as low as 5 mfp at 100 keV. Figure 2 shows the calculated multiple scattering angular distribution for 100 keV and 1 MeV electrons with various pathlengths incident on aluminum.

Hybrid sampling method

Unfortunately, sampling directly from GS distribution of multiple scattering is computationally extensive and previously very large pre-computed data tables have been used [19, 21, 22] with a limited accuracy due to the numerical integration and interpolation being used for sampling angular distributions. EGS5 [20] uses a Wentzel shape analytical function with adjustable parameters determined from the fitting of the GS distribution function, but this method is, however, still computationally extensive as it requires the calculation of GS distribution function at 287 angle points [20].

In this study, an efficient and accurate hybrid sampling method has been developed which uses efficient rejection sampling method for larger path lengths (~500 mfp and above) and for low electron energies (<500 keV) while for small path lengths, a simple, efficient and accurate analytical distribution function has been proposed. The later uses adjustable parameters determined from the fitting of Goudsmit-Saunderson angular distribution and requires less number of terms (~100 terms) for fitting as compared to EGS5 [20].

Rejection sampling, for low energy and longer path lengths

For low energy and longer path lengths (s mfp and $E < 500$ keV), a composite approach for direct and rejection sampling has been used. The multiple scattering angular distribution function $F(s\ \theta$ for a given E and Z is

$$F(s,\theta) \quad \sin\theta F_{GS}(s,\theta) \tag{7}$$

As can be seen from fig. 2, $F_{GS}(s,\theta)$ is relatively flat over the interval [0,] for longer path lengths and low electron kinetic energy and, therefore, can be used for rejection sampling while direct sampling (inverse-transform) method has been used to sample θ from the distribution $\sin\theta$ in the interval [0,].

Analytical function

Except for s 500 mfp and $E < 500$ keV, the angular distribution is sampled from a fairly simple and accurate analytical function with adjustable parameters determined from the fitting of GS distribution. For given s, E, and Z, the analytical function $G(\theta)$ has the form

$$G(\theta) \quad \begin{cases} \alpha\theta e^{\ \beta\theta}, & s \quad 100\,\text{mfp} \\ \alpha e^{1\ q\ e^{q}}, \quad q \quad \dfrac{\beta\ \theta}{\eta}, & s \quad 100\,\text{mfp} \end{cases} \tag{8}$$

where θ is the polar angle and can take values from 0 to . $\alpha, \beta,$ and η are adjustable parameters determined by fitting to the GS distribution function for given E, Z, and s. To achieve good accuracy we divided the polar angle range into 100 steps between 0 and with a higher density near 0 because the distribution is heavily forward peaked. The fits are accurate enough for sampling angular distribution of multiple scattering. Comparisons between the analytical function determined by eq. (8) and the original GS distribution function are plotted in fig. 3.

The uniqueness of the proposed analytical form is that $G(\theta)$ has analytical integral and the corresponding cumulative probability distribution function has analytical inverse for both cases, and therefore direct sampling procedure (inverse transform method) was applied to sample θ.

The polar angle is then sampled as

$$\theta \quad \begin{cases} \theta = -\dfrac{\ln(r_1 r_2)}{\beta}, \text{if } \theta \quad \pi, & s \quad 100\,\text{mfp} \\ \beta \quad \eta \ln 1 \quad \ln\dfrac{r_1}{C\alpha\eta} \quad e^{1\ e^{\frac{\beta}{\eta}}}, & s \quad 100\,\text{mfp} \end{cases} \tag{9}$$

where r_1 and r_2 are random numbers uniformly distributed over [0, 1]. C is normalization constant and can be calculated analytically. This algorithm requires either one log or one Log-Log and two exponential calculations in eq. (9). Besides this, the algorithm is efficient because the direct sampling method is used.

Sampling algorithm

Assembling all the sampling procedures, the algorithm for sampling angular deflections from GS distribution of multiple scattering for given E, Z, and s has the following compact form.

(1) Input: Electron energy (E), Material (Z), Path lengths (s).
(2) Output: Polar angle θ.

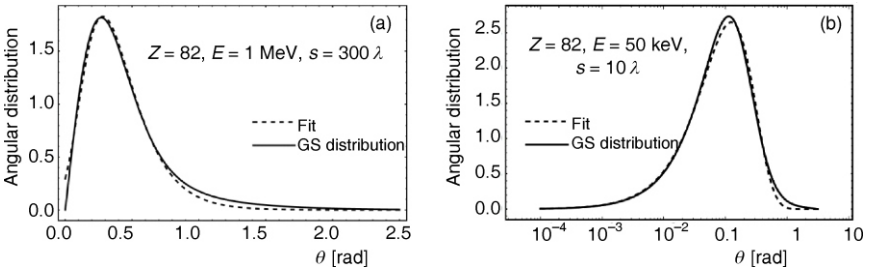

Figure 3. Comparisons of multiple scattering angular distribution of (a) 1 MeV and (b) 50 keV electrons incident on lead, obtained with GS distribution and analytical function (eq. 8). All plots are normalized to unity

(3) If E 500 keV and $s > 500$ mfp, use rejection sampling method as below.
(a) Calculate $F_{GS(max)} = F(0, s)$.
(b) Generate two random numbers r_1 and r_2 over the interval [0, 1].
(c) Sample θ from the distribution $\sin\theta$ as $\theta = \cos^{-1}(1 - 2r_1)$
(d) If r_2 $F_{GS}(\theta, s)/F_{GS(max)}$ accept θ, else, go to step ii.
Else: Sample θ from eq. (9)

Efficiency and accuracy of this sampling algorithm is discussed in the following section.

RESULTS AND DISCUSSION

Sampling accuracy

This section concerns the verification that the angular sampling algorithms work as expected. The verification is performed by comparing the Monte Carlo sampled angular distribution with the theoretical expressions. In fig. 4, the sampled angular distributions from rejection sampling are plotted with the theoretical expression given in eq. (7). The accuracy of angular sampling using analytical function, eq. (8), which is determined by fitting GS distribution has also been checked and the comparison is plotted in fig. 5. The smooth curves in figs. 4-5 are from theoretical expressions and histograms present sampled angular distribution from Monte Carlo simulation. All plots are normalized.

Sampling efficiency

The sampling efficiency of the angular sampling, based on the rejection sampling algorithm is plotted in fig. 6. The sampling efficiency is defined as the ratio of the accepted sampled values to the total number of trials. We have calculated the efficiency in terms of pathlengths (s) for 100 keV, 300 keV, and 500 keV electrons incident on aluminum and lead.

One can realize that the sampling efficiency based on rejection sampling method is generally very good for low energy electrons with longer pathlengths (>500 mfp) incident on lead. The sampling efficiency for aluminum decreases, at most, to 8 % at 500 keV electrons, when s = 500 mfp and then increases 35 % up to 3000 mfp. For 100 keV electrons incident on aluminum the sampling efficiency is at least 50 % for s 500 mfp. It can be seen from fig. 6 that the rejection sampling technique employed here is very efficient for electron kinetic energies less than 500 keV and pathlengths greater than 500 mfp.

Experimental verification

The multiple scattering angular distributions of 20 MeV electrons incident on aluminum have been compared with the measurements of Ross *et al*. [27]. The 1/e widths of the distributions ($\theta_{1/e}$) obtained with 20 MeV electrons incidents on Al foils of thickness 70.1 mgcm^{-2}, 140 mgcm^{-2}, 274 mgcm^{-2}, and 414 mgcm^{-2} are given in tab. 1. In general, the calculated distributions are narrower than the measured distributions. The maximum difference between the calculated and the measured distribution is 3.9 % .

The difference was calculated as the ratio of the difference between the calculated and measured values and the measured values. The difference shows that our calculated GS distribution is very much com-

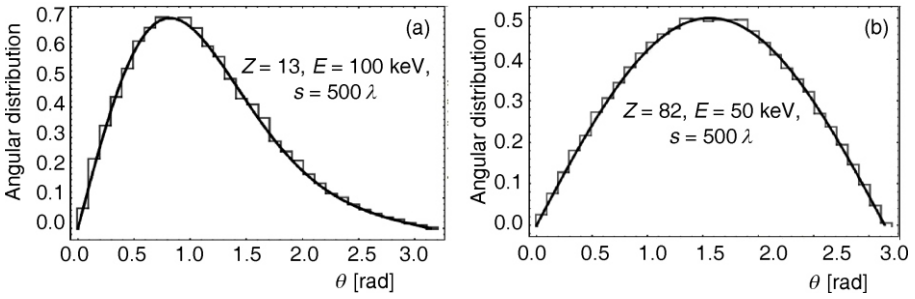

Figure 4. Multiple scattering angular distributions, for (a) 100 keV electrons incident on aluminum and (b) 50 keV electrons incident on lead

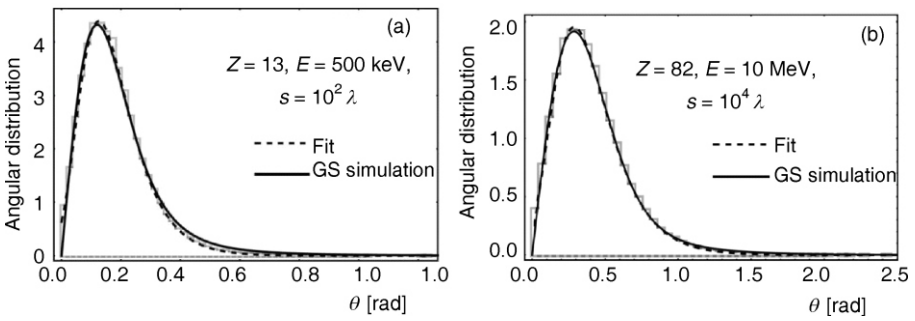

Figure 5. Multiple scattering angular distributions, for (a) 500 keV electrons incident on aluminum and (b) 10 MeV electrons incident on lead

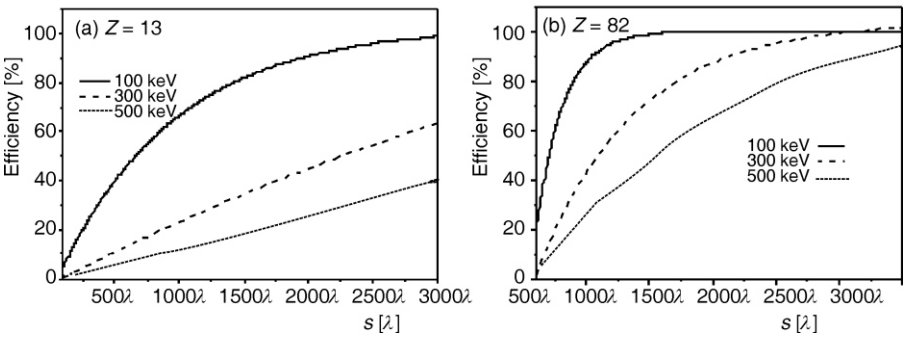

Figure 6. Sampling efficiency of eq. (7) for 100 keV, 300 keV, and 500 keV electrons incident on (a) aluminum and (b) lead and for pathlengths (500 λ -3000 λ)

Table 1. Comparison of the characteristic angle measured by Ross *et al*. [27] with the values calculated in this study

Thickness [mgcm^{-2}]	Calculated [degrees]	Measured [degrees]	Difference [%]
70.1	2.551	2.653	–3.8
140	3.345	3.484	–3.9
274	4.668	4.777	–2.3
414	5.703	5.865	–2.7

parable with the measured distributions of Ross *et al*. [27]. Hence, the Sampling of angular distributions is fully consistent with the experimental measurements.

CONCLUSIONS

It can be concluded that the proposed algorithm provides accurate and efficient methods for sampling multiple scattering angular deflections based on GS distribution function. The hybrid method provides very accurate treatment of photon angular distribution by low as well as high energy incident electrons. Figure 6 shows that the rejection sampling is very efficient for low electron kinetic energies (<500 keV and pathlengths longer than 500 mfp). The parameterization of the GS distribution function given by eq. (8) provides a very accurate fit as shown in fig. 3. Therefore, the simulated angular distribution is fully consistent with the most accurate and reliable theory at present. The sampling algorithm based on this method is relatively faster than previously developed approaches [20]. The experimental verification of our calculated GS distribution is very much comparable with the measured distributions of Ross *et al*. [27] and hence the Sampling of angular distributions based on this model is very accurate.

It is worth mentioning that the proposed algorithm for sampling multiple scattering angular distributions can be used for a wide range of incident electron energies and materials and hence suitable for general purpose Monte Carlo simulations.

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AUTHORS' CONTRIBUTIONS

M. A. Wasaye and H. Wang contributed equally to this work under the supervision of P. Long and H. Zheng. H. Naeem has carried out the experimental verification.

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ХИБРИДНИ МОДЕЛ ЗА УЗОРКОВАЊЕ УГАОНОГ СКРЕТАЊА ВИШЕСТРУКОГ ЕЛАСТИЧНОГ РАСЕЈАЊА ЗАСНОВАН НА ГАУДСМИТ-САУНДЕРСОНОВОЈ ТЕОРИЈИ

Приказан је алгоритам за Монте Карло симулацију електронског вишеструког еластичног расејања заснованог у оквиру SuperMC програма (Супер Монте Карло симулациони програм за нуклеарни и радијациони процес). Овај рад описује ефикасне и тачне методе помоћу којих се узоркује угаоно скретање при вишеструком расејању при чему се користи Гоудсмит-Саундерсонова теорија вишеструког расејања. Диференцијални пресек електрона и позитрона на неутралним атомима израчунат је помоћу програма ELSEPA који је заснован на Дираковом парцијалном таласу, а Лежандрови коефицијенти прецизно су израчунати помоћу методе Гаус-Леажандрове интеграције. На крају, развијена је нова хибридна метода за узорковање угаоне расподеле. Модел користи ефикасну методу одбацивања узорака за ниске енергије електрона (<500 keV) и веће дужине путева (>500 средњих слободних дужина). За мале дужине, предложена је једноставна, ефикасна и тачна, аналитичка функција расподеле која користи параметре подешавања одређене фитовањем Гаудсмит-Саундерсонове угаоне расподеле и приказана је дискусија о ефикасности узорковања и тачности ново развијеног алгоритма. Ефикасност алгоритма одбацивања узорака износи најмање 50 % за електроне са кинетичким енергијама мањим од 500 keV и већим дужинама путева (>500 средњих слободних дужина). Резултати Монте Карло симулације упоређени су са мереним угаоним расподелама Роса и сарадника (2008) и показана је добра сагласност.

Кључне речи: Монте Карло, вишеструко расејање, Гаудсмит-Саундерсон, SupieMC, диференцијални пресек за судар, угаона расподела, ELSEPA