Monte Carlo Calculations of Transmission of Electrons through Thin Foils

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A Monte Carlo method to calculate transmission of electrons through thin foils is described. Angular deflection due to multiple scattering, energy loss by ionization, and fluctuation in energy loss are taken into account. The calculations have been made for electrons normally incident on thin aluminum foils of various thicknesses. The results obtained are in fairly good agreement with other calculation and with the experimental results.

I. INTRODUCTION

The penetration of the fast electrons through the matter is the important subject of the theoretical and experimental investigations. It is characterized by multiple Coulomb scattering and statistical fluctuation in ionization energy loss. The transport properties of electrons are also of interest in connection with numerious experimental applications. When the absorber materials are thin enough compared to the range of incident electrons, the problems can be treated analytically and the satisfactory agreement between theory and experiment has been reported.[1]

The situation becomes more complicated when the absorber thickness increases. For this case, the energy loss and angular deflection can not be treated separately and theoretical treatment of the problem is very difficult. There are two techniques to study electron transport in the thick materials; the moments method and the Monte Carlo method. The moments method developed by Spencer[2] has been used to calculate the depth distribution of energy deposition in the materials. However, its application is limited only to media that are unbounded and homogeneous, and foil-transmission problems can not be treated by this method.

On the other hand, the Monte Carlo method can, in principle, offer the most accurate solutions for the electron transport problems in bounded media. This method is applicable to any energy range of electrons and to any geometry. The calculation is based on the simulation of the electron tracks by random sampling techniques. The number of Coulomb collisions undergone by a fast electron during the slowing-down process is quite large, so that the simulation of the individual collision is not feasible. Instead, the electron trajectory is divided into a number of short segments, such that the number of collisions along each segment is large, but the average angular deflection due to multiple scattering and the average energy loss by ionization per segment are small. This means that the results of analytical treatments of angular deflections and energy losses can give satisfactory approxi-

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mations to the net probability distributions in each segment. The angular deflections and energy losses sampled in each segment are then combined to construct a complete electron trajectory in the foil. By the use of such a procedure, the thick-foil transmission problem can be treated as a sequence of thin-foil ones, in which the electron behavior can be adequately represented by analytical forms.

The Monte Carlo method based on this approach has been outlined by Berger,[3] and the earlier references are cited therein. Recently, Sugiyama[4] performed Monte Carlo calculations for transport of fast electrons with energy higher than a few MeV and obtained the results in considerably good agreement with experimental data. Berger and Seltzer developed a computer code called ETRAN,[5] which is the most accurate and the most frequently used program at present. By the use of this code they calculated various quantities for electron transmission[6] and for production of bremsstrahlung radiation.[7] Using the same logic as those employed in the ETRAN code, several codes have been developed to permit the routine studying of the electron transport problems for one-dimensional multilayer targets,[8] cylindrical-geometry multimaterials,[9] and complex systems.[10]

Although the ETRAN code is accurate, takes into account many interactions between electron and atom, and has the flexibility of being able to calculate various quantities, it requires a large-memory and high-speed computer. In the case of radioactive sources, most electrons emitted from the source have the energy less than 2 MeV. It is worth while to develop a simple Monte Carlo code which can be used in this energy region.

In this paper is presented a brief description of a Monte Carlo program to study transmission of electrons through thin foils. This program includes electron multiple scattering and the effect of energy-loss straggling. The advantage is its simplicity and high speed. The present code does not require large-memory computer and is reasonably accurate. Calculations have been carried out with this code for monoenergetic electrons incident perpendicularly on the thin targets of various thicknesses. The results presented here include the transmission coefficient and the energy spectrum of transmitted electrons. Comparison is made with the experimental results and also with the calculated result from the ETRAN code of Berger and Seltzer.

All the the calculations in the present work have been performed on the FACOM 230–75 computer of the Data Processing Center of Kyoto University.

II. METHOD OF CALCULATION

The computer program has been written under the following assumptions:
1) An electron beam is incident normally on a foil.
2) The lateral extension of the foil is large enough compared to the electron range.
3) The electrons never return to the foil once they have left it.
4) The production of knock-on electrons by the inelastic Coulomb collisions is ignored.
5) The energy loss by radiation is neglected.
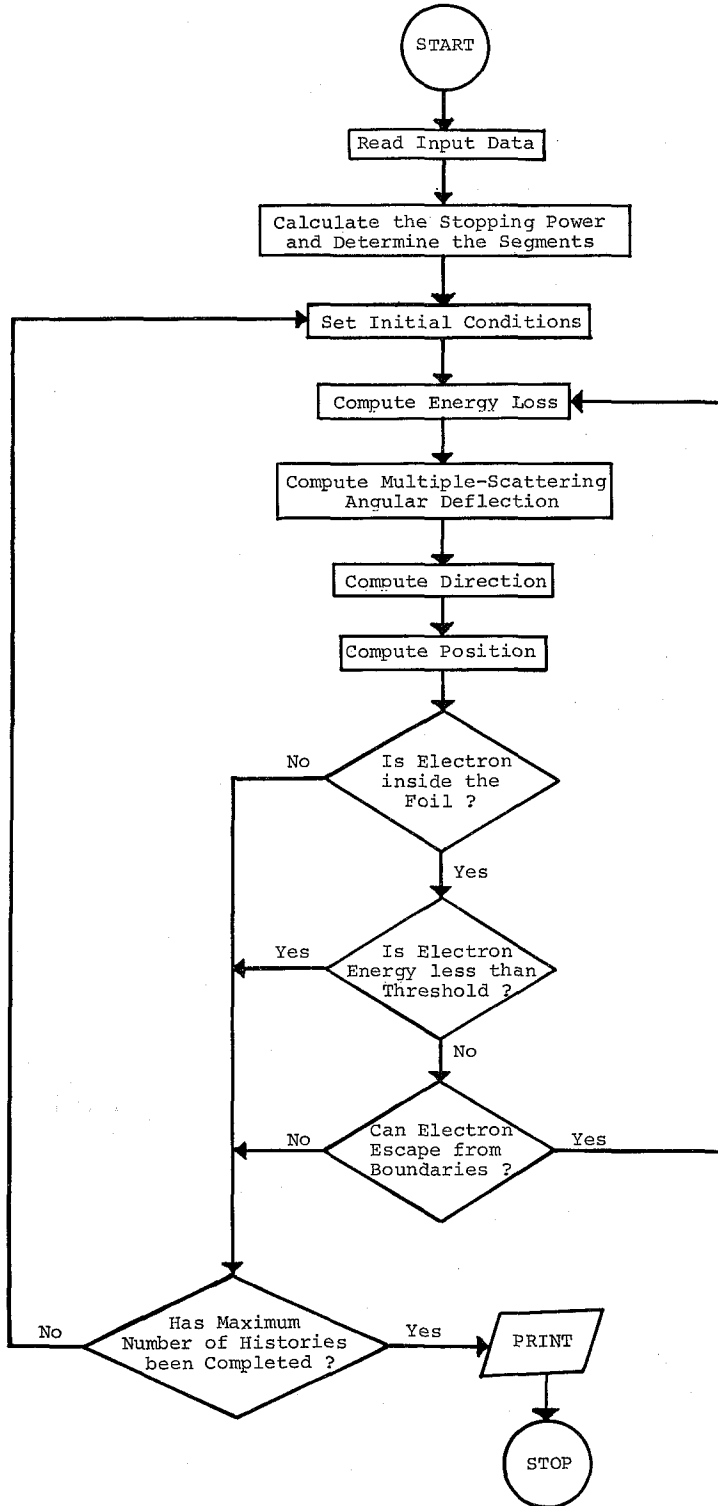
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Fig. 1. Schematic flow diagram of the program.

The flow diagram in Fig. 1 shows how each electron history is followed until the electron is absorbed in the foil or escapes from it. In the present code, the segment size is chosen by the logarithmic-spacing law and stopping power is determined from the continuous-slowing-down approximation. The energy-loss distribution in each segment is sampled from the Blunck-Leisegang formula and the multiple-scattering angular deflection is obtained from the Molière theory.

1. Division of Electron Track into Segments

The segment size is chosen so that the kinetic energy of the electron is, on the average, reduced by a constant factor $2^{-1/m}$ per segment. When the energy of the electron in the k-th segment is E_k, the size of the k-th segment is given by

$$t_k = \int_{E_{k-1}}^{E_k} \left| \frac{dE}{dx} \right|^{-1} dE , \qquad (1)$$

where $|dE/dx|$ is the mean energy loss per unit pathlength and

$$E_k = 2^{-1/m} E_{k-1} . \qquad (2)$$

This logarithmic spacing was chosen for the reason that the distribution of multiple-scattering angular deflections changes little from segment to segment. In the present work, we chose $m=16$. This means that the reduction of the energy in each segment is 0.9576.

2. Stopping Power and Mean Energy Loss

The mean energy loss per unit pathlength by collision is calculated in the continuous-slowing-down approximation. The resulting formula is[11]

$$\frac{dE}{dx} = 2C \, mc^2/\beta^2 \{B_0 - 2(\ln Z + \ln(I/(10Z)))\} , \qquad (3)$$

where

$$C = 0.1503 \, Z/A ,$$
$$B_0 = 21.683 + \ln T^2(T+2) - [1 + (2T+1)/(T+1)^2] \cdot \ln 2$$
$$+ 1/(T+1)^2 + \frac{1}{8}[T/(T+1)]^2 ,$$

and T is the initial kinetic energy of the electron in units of mc^2.

The mean excitation energy I is chosen from the empirical relation between I and Z as[12]

$$I/Z = 9.76 + 58.8 Z^{-1.19} \, \text{eV} . \qquad (4)$$

If the size of the segment is small, the energy loss in the segment can be assumed to be small compared to the energy of the electron. In this case, the mean energy loss in the segment is determined from

$$\overline{\Delta E} = \left| \frac{dE}{dx} \right| \cdot t , \qquad (5)$$

where t is the segment size.

3. Fluctuation in Energy Loss

When an electron with energy E_0 travels a distance t, it will suffer an energy loss ΔE by ionization. For the case that $\Delta E \ll E_0$, Landau[13] developed multiple scattering theory which gives the distribution of the energy losses. In his theory this distribution can be expressed in terms of a dimensionless parameter λ as

$$f(\Delta E, t)\mathrm{d}(\Delta E) = \phi(\lambda)\mathrm{d}\lambda , \tag{6}$$

where

$$\lambda = \frac{\Delta E - \overline{\Delta E}}{a \cdot t} + \ln[E_0/(a \cdot t)] - 1.116 , \tag{7}$$

$\overline{\Delta E}$ is the mean energy loss and

$$a = 0.154 \frac{Z}{A} \frac{\rho}{\beta^2} \quad \text{(MeV/cm)} .$$

The universal function $\phi(\lambda)$ has been evaluated by Landau and tabulated by Börsch-Supan.[14]

Blunck and Leisegang[15] have extended Landau theory by taking into account the binding effect of the atomic electrons to which the electron transfers its energy. According to their result, the distribution is given by

$$f(\lambda)\mathrm{d}\lambda = \sum_{\nu=1}^{4} \frac{c_\nu r_\nu}{(r_\nu^2 + b^2)^{1/2}} \exp\left\{-\frac{(\lambda - \lambda_\nu)^2}{r_\nu^2 + b^2}\right\}\mathrm{d}\lambda . \tag{8}$$

The parameters c_ν, λ_ν, and r_ν are determined from the least-squares fitting of the Landau function $\phi(\lambda)$ and have been listed by Blunck and Leisegang. The broadening parameter b in Eq. (8) has been estimated by Blunck and Westphal,[16] based on a Thomas-Fermi model of the atom and can be expressed as

$$b^2 = \frac{q \cdot \overline{\Delta E} \cdot Z^{4/3}}{(a \cdot t)^2} , \tag{9}$$

with $q \sim 20$ eV.

In the present work, the energy loss of the electron in each segment was sampled from the distribution derived by Blunck and Leisegang. The composition method to generate the random numbers according to Eq. (8) has been proposed by Sugiyama.[4] The frequency function of the distribution can be written as

$$f(\lambda) = \sum_{\nu=1}^{4} \alpha_\nu f_\nu(\lambda) , \tag{10}$$

where

$$\alpha_\nu = c_\nu r_\nu ,$$

$$f_\nu(\lambda) = \frac{1}{\sqrt{2\pi}\,\sigma_\nu} \exp\left\{-\frac{(\lambda - \lambda_\nu)^2}{2\sigma_\nu^2}\right\} ,$$

$$\sigma_\nu^2 = (\gamma_\nu^2 + b^2)/2 .$$

By using a uniform random number, an integer ν is chosen with the probability proportional to α_ν of being ν. Having selected the value of ν, a sample is drawn from the distribution with the frequency function $f_\nu(\lambda)$. Since $f_\nu(\lambda)$ is the normal distribution, the sample is obtained from
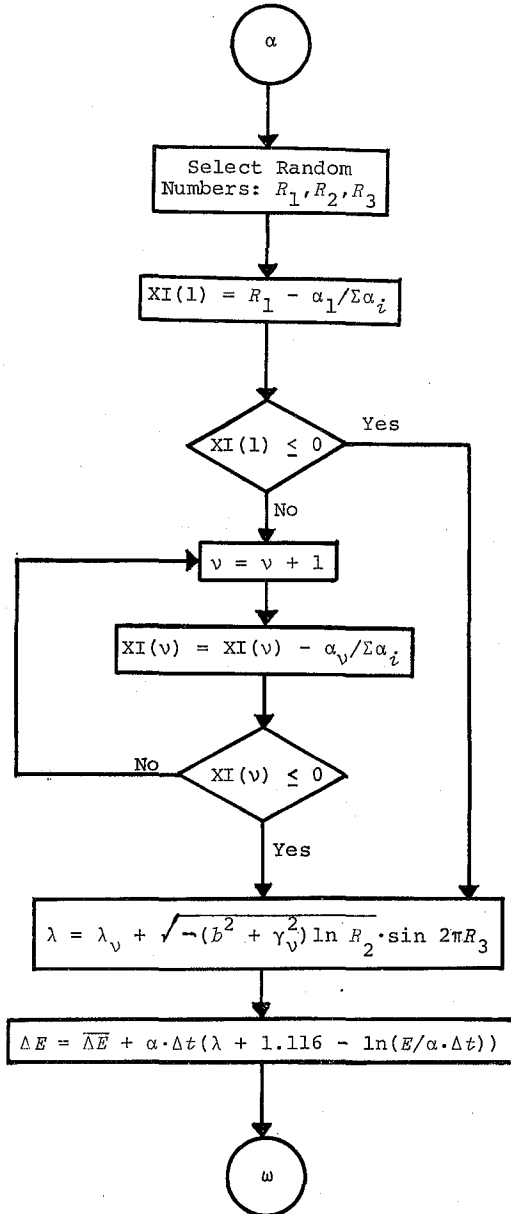

Fig. 2. Method of randomly selecting the energy-loss fluctuation from the Blunck-Leisegang theory.

$$\lambda = \lambda_\nu + \sigma_\nu \cdot \sqrt{-2 \ln R_1} \cdot \sin 2\pi R_2 , \tag{11}$$

where R_1 and R_2 are uniform random numbers in the interval $[0, 1]$. Then the value of ΔE is determined by using λ and t. The flow diagram of this procedure is shown in Fig. 2.

In order to test the validity of the present sampling method, the distribution of λ calculated from random sampling is compared with the $f(\lambda)$ function calculated analytically by the Blunck-Leisegang theory. The result is shown in Fig. 3.
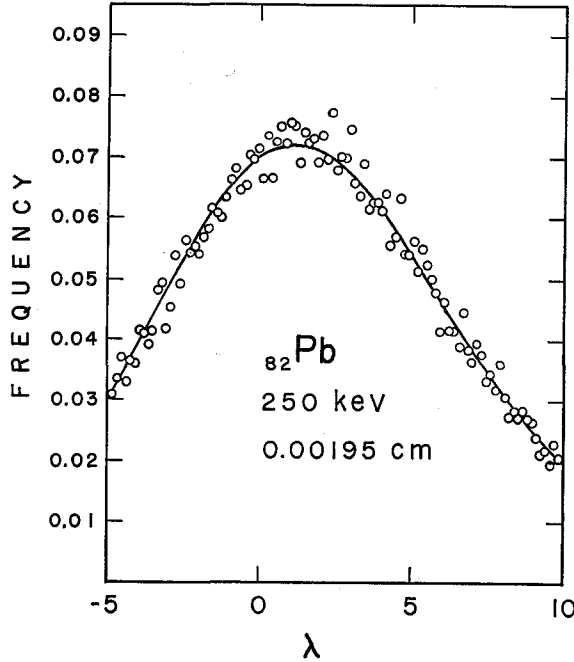

Fig. 3. Comparison of the distribution of random variates with the Blunck-Leisegang theory.

4. Angular Deflection by Multiple Scattering

When electrons traverse each segment of the material, they not only lose their energy, but they are also deflected laterally from their original paths. In the small–angle approximation, Molière[17] developed a theory which gives the angular distribution of multiple-scattering deflections. The applicability of this theory has been extended by Bethe[18] to large angles.

In the corrected Molière theory, the probability that an electron will have an angle between Θ and $\Theta+d\Theta$ after traversing a distance t can be written by

$$f(\Theta)\mathrm{d}\Theta = K \left(\frac{\sin \Theta}{\Theta}\right)^{1/2} \theta[f^{(0)}(\theta) + f^{(1)}(\theta)/B + \cdots]\mathrm{d}\theta , \tag{12}$$

where the reduced angle θ is

$$\theta = \frac{\Theta}{\chi_c \cdot \sqrt{B}} , \tag{13}$$

K is the normalization constant for the frequency function, and $f^{(0)}(\theta)$ and $f^{(1)}(\theta)$ are purely numerical functions tabulated by Molière and Bethe. The parameter χ_c is defined as

$$\chi_c^2 = 4\pi N t e^4 Z(Z+1)/(pv)^2 ,$$

where N is the number of atoms per cm^3, and p is the momentum and v the velocity of the electron, respectively.

The parameter B depends on the distance t and is obtained by solving the transcendental equation. This parameter can be expressed as a function of the number of collisions, n, during the traverse of the distance t and the relation between B and $\log_{10} n$ is tabulated by Molière. Instead of solving the transcendental equation, we expanded B is powers of $\log_{10} n$ and kept the first four terms. The coefficients of the third-order polynomial were determined by the least-squares method.

In order to sample the angular deflection from Eq. (12), the combination of the composition and the rejection methods was used. Following Messel et al.[19] and Sugiyama,[4] the expression (12) can be rewritten as

$$f(\Theta) = G(\Theta)\left[\alpha_1 f_1(\theta)g_1(\theta) + \alpha_m\left\{\frac{\alpha_2}{\alpha_m}f_2(\theta)g_2(\theta) + \frac{\alpha_3}{\alpha_m}f_3(\theta)g_3(\theta)\right\}\right], \tag{14}$$

where

$$G(\Theta) = (\sin\Theta/\Theta)^{1/2}, \quad \alpha_1 = 1-5/B, \quad f_1(\theta) = \theta f^{(0)}(\theta),$$

$$g_1(\theta) = 1, \quad f_2(\theta) = 1 \quad \text{if } \theta < 1,$$

$$\alpha_2 = [\theta\{5f^{(0)}(\theta) + f^{(1)}(\theta)\}/B]_{\max} = 4.1818/B,$$

$$f_3(\theta) = 2/\theta^3 \quad \text{if } \theta > 1,$$

$$\alpha_3 = [\theta^4\{5f^{(0)}(\theta) + f^{(1)}(\theta)\}/(2B)]_{\max} = 2.1947/B,$$

$$\alpha_m = \int_0^\infty \theta[5f^{(0)}(\theta) + f^{(1)}(\theta)]/B\,d\theta = 4.98/B.$$

The functions $g_2(\theta)$ and $g_3(\theta)$ are calculated from the table of Bethe and are given in the Tables I and II of Messel et al.[19] For $\theta < 4$, $g_3(\theta)$ is given to the constant value of 0.64 and the intermediate values of these functions are determined by interpolation from the tabulated values.

First, we choose an integer from 1 to 3 with probability proportional to α_i of being i. This is done by using the uniform random number distributed in $[0, 1]$. Then a sample is drawn from the distribution with frequency function $f_i(\theta)$, and the value is accepted or rejected by computing the value of $g_i(\theta)$ and comparing with a random variate. In the case of rejection, the process is repeated again and again until a value is finally accepted. The value of Θ is obtained by applying to transformation from the value of θ.

The value of Θ thus obtained is tested by using a uniform random number R_5 and only the values which fulfill the condition

$$\left(\frac{\sin \Theta}{\Theta}\right)^{1/2} > R_5, \qquad (15)$$

are accepted.

In Fig. 4, the flow diagram of this method is shown. The comparison of the random variates sampled from Eq. (14) with the frequency function is made in Fig. 5.
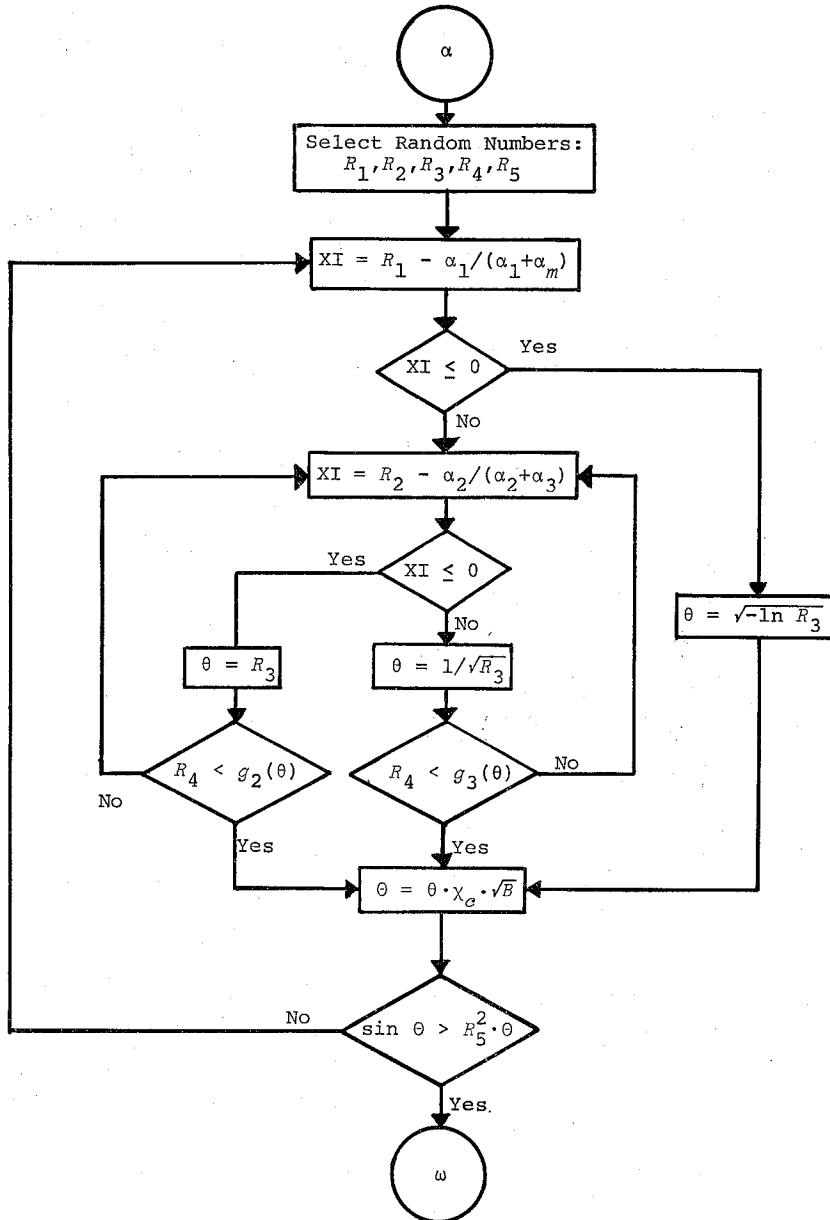

Fig. 4.　Method of randomly selecting the multiple-scattering angular deflection from the Molière theory.
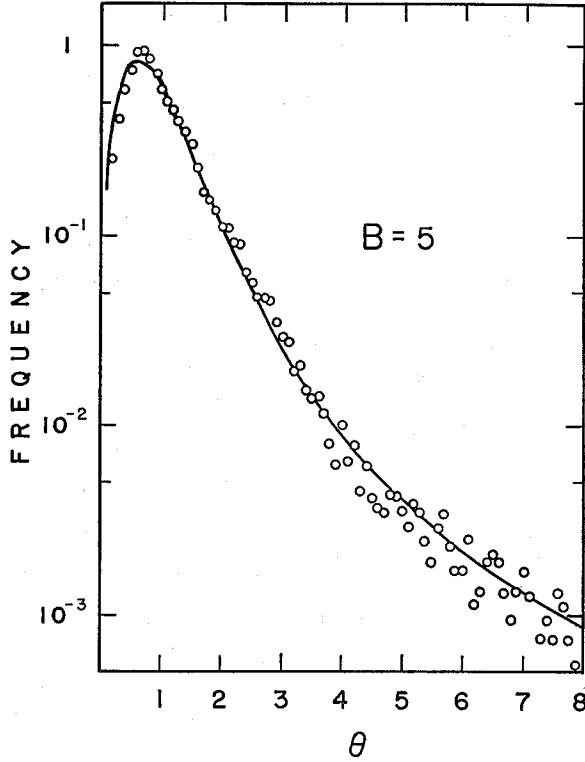
Fig. 5. Comparison of the distribution of random variates
with the Molière theory.

Sugimaya[4] proposed a method to correlate the energy-loss distribution which neglects the angular deflection and the angular deflection distribution which is derived from the continuous-slowing-down approximation. If Θ_m is the angular deflection estimated above, the angle can be corrected for the energy-loss fluctuation by the following relation:

$$\Theta = \Theta_m \frac{\Delta E}{\overline{\Delta E}} . \tag{16}$$

5. Changes in Direction and Position

We choose the z axis as polar axis and θ and ϕ are spherical coordinates in this system. Let (θ_n, ϕ_n) and $(\theta_{n+1}, \phi_{n+1})$ denote the directions of the electron at the beginning and at the end of a segment, and Θ and Ψ the polar and azimuthal multiple-scattering deflections in that segment. The values of θ_{n+1} and ϕ_{n+1} are determined from the well-known kinematic relations between change of direction and multiple-scattering deflection:

$$\cos \theta_{n+1} = \cos \theta_n \cos \Theta + \sin \theta_n \sin \Theta \cos \Psi , \tag{17}$$

$$\sin (\phi_{n+1} - \phi_n) = \frac{\sin \Theta \sin \Psi}{\sin \theta_{n+1}} , \tag{18}$$

(55)

$$\cos(\phi_{n+1}-\phi_n) = \frac{\cos\Theta - \cos\theta_n \cos\theta_{n+1}}{\sin\theta_n \sin\theta_{n+1}} .\tag{19}$$

The azimuthal deflection Ψ is distributed uniformly between 0 and 2π. The selection of Ψ is replaced by the selection of sine and cosine of the azimuthal angle and this selection is made by the rejection method of von Neumann.[20] The deflection angle Θ is selected by the technique described in the preceding section.

The position at the end of the segment (x', y', z') is determined from the position at the beginning of the segment (x, y, z) and the spherical coordinates (Θ, Ψ):

$$\left.\begin{aligned} x' &= x+t\cdot\sin\Theta\cdot\cos\Psi , \\ y' &= y+t\cdot\sin\Theta\cdot\sin\Psi , \\ z' &= z+t\cdot\cos\Theta , \end{aligned}\right\}\tag{20}$$

where t is the distance travelled by the electron in that segment.

6. Termination of History

According to the flow diagram shown in Fig. 1, an electron history is traced until the electron leaves the foil or is absorbed in it. The energy loss is estimated, angular deflection is calculated, and the position is determined. If the electron is inside the foil and has energy sufficient to escape from it, these procedures are repeated.

A history is terminated in the following cases:
1) The electron leaves the foil.
2) The electron energy falls below a certain cut-off energy.
3) The residual mean range is smaller than the distance to any boundaries of interest.

The last condition is estimated as follows; if the position of the electron is z and the coordinate of the boundary is z_B, the energy necessary to escape from the boundary is given by

$$E_B = \left|\frac{\mathrm{d}E}{\mathrm{d}x}\right|\cdot |z-z_B| .\tag{21}$$

When the electron energy is less than this value, the history is no longer followed.

III. SAMPLE CALCULATIONS AND COMPARISON WITH EXPERIMENTS

Various calculations of transmission electrons with the computer code based on the method described above have been made in order to compare with experimental data. The results of typical runs are presented.

The number transmission coefficients for aluminum foils are given in Fig. 6. The number transmission coefficient is defined as the ratio of the number of electrons emerging from the foil to the number of electrons impinging on the foil. Calculations were made for 250-keV electron beam perpendicularly incident on the foils. The results are based on a sample of 10,000 Monte Carlo histories. The transmission coefficient is presented as a function of the fractional true range z/r_0, where z is the
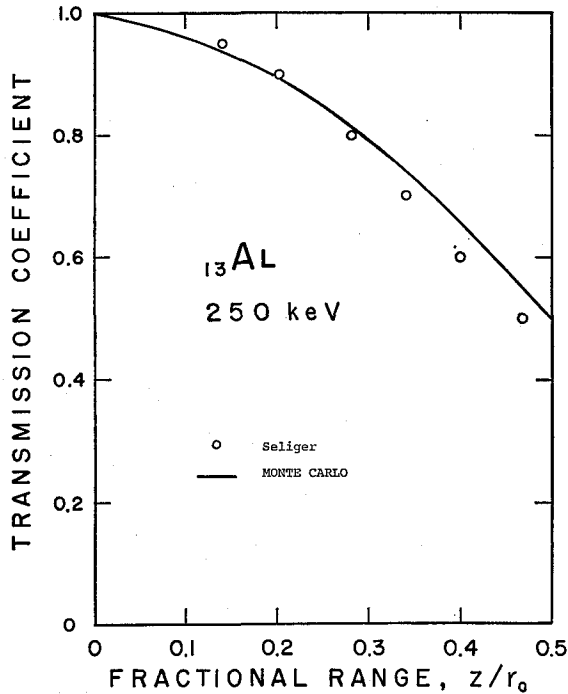
Fig. 6. Comparison of calculated number transmission coefficientes for aluminum foils with measured values of Seliger.

actual thickness and r_0 the mean range of the incident electrons.

The experimental values shown in the figure were obtained by Seliger.[21] He measured the transmissions of monoenergetic beams of electrons by the use of a 90-degree magnetic analyzer and a 2π GM counter, of which window is formed with the absorber material.

It can be seen from the figure that for small foil thickness there is good agreement. For larger thicknesses, the experimental points lie somewhat below the Monte Carlo results. This can be ascribed to the smallness of the number of segments. In the ETRAN code, each segment is divided into n equal sub-segments. Seltzer and Berger[6] tested the effect of varying n on the number transmission coefficients and showed that the transmission coefficient decreases with increasing n. They used $n=4$ for aluminum. However, the computer time needed for the calculations increases roughly in proportion to n.

In Fig. 7 is shown the energy spectrum of the transmitted electrons for an incident energy of 1 MeV and an aluminum target. The target thickness of 0.110 g/cm² corresponds to 0.2 of the electron range in aluminum at 1 MeV. The spectrum calculated by the Monte Carlo method is shown in histogram form. The result was obtained with a sample of 50,000 histories.

The transmitted energy spectrum for 1-MeV electrons incident perpendicularly on the aluminum foil has been measured by Rester and Derrickson.[22] A beam of
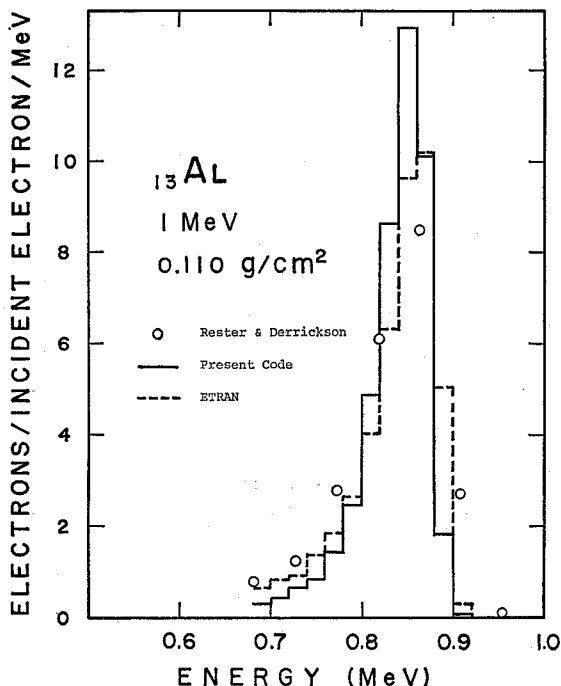
Fig. 7. Comparison of experimental and calculated energy
spectra of transmitted electrons. The incident
energy is 1 MeV and the foil thickness corresponds
to 0.2 of the range in aluminum at 1 MeV.

monoenergetic electrons was obtained from the 3-MeV Van de Graaff accelerator
and focused on the target foil by the use of an electrostatic quadrupole lens. The
energy spectra of the transmitted electrons were measured with a Si(Li) detector.
The results are plotted in the figure by open circles.

For comparison, the energy spectrum of transmitted electrons calculated by the
ETRAN code is also shown in the figure. The calculation was made by Rester and
Derrickson[22] in order to compare with their experimental result. This spectrum is
based on a sample of 15,000 Monte Carlo histories. It should be noted that this
calculation was made for slightly thinner foil (0.10 g/cm²).

It can be seen from the figure that the spectrum calculated with the present code
is fairly good agreement with the experimental data and also with the calculated
result of the ETRAN code.

ACKNOWLEDGMENT

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