Monte Carlo calculations for the design of Mott scattering spin polarimeters

S. Qiao[a] and A. Kakizaki
Synchrotron Radiation Laboratory, Institute for Solid State Physics, University of Tokyo, Tokyo 106, Japan

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Using the Monte Carlo method, we have calculated, for 50 keV electrons incident on a gold target, the dependence of the effective Sherman asymmetry function and scattered intensity on the target thickness and inelastic energy loss window for scattering angles from 90° to 180°. Our results show that, when the gold target is thicker than 700 Å or the inelastic energy loss window is larger than 1200 eV, the scattered intensity is maximum at a scattering angle of about 120°, and the effective Sherman function is almost constant over a wide range of scattering angles. Thus, for Mott scattering spin polarimeters, the electron detectors should be positioned at ±120°, and the larger the collection angle for scattered electrons, the higher the efficiency of the Mott polarimeter. © *1997 American Institute of Physics.* [S0034-6748(97)02911-0]

I. INTRODUCTION

Mott scattering is the most widely used experimental method to measure the electron spin polarization because of its high efficiency and excellent stability.[1,2] In this method, transversely polarized high energy electrons are scattered by a target of high atomic number, which results in a left–right asymmetry in the scattered intensities due to the spin-orbit interaction. If the Sherman asymmetry function, S, of the target is known, the transverse polarization component, P_t, of the incident electrons can be determined by the relation

$$P_t = A/S,$$

where the left–right scattering asymmetry

$$A = (N_L - N_R)/(N_L + N_R)$$

is related to the number of electrons scattered to the left, N_L, and right, N_R, respectively. The inverse square of the statistical error of the polarization measurement is proportional to

$$\epsilon = (I/I_0)S^2,$$

where I_0 is the number of electrons entering the polarimeter, and I is the total number of scattered electrons measured by the left and right detectors. ϵ is termed the figure of merit, or efficiency of the Mott polarimeter.[3]

The Sherman asymmetry function of some atoms are now well understood after extensive theoretical work initiated by Mott[4–8] more than 60 years ago. The error in calculating the Sherman function of the gold atom for 120 keV electrons and a 120° scattering angle is believed to be less than 2%. Figure 1 shows Lin's calculation of the Sherman function for 120 keV electrons incident on gold atoms.[7] The Sherman function has a peak at a scattering angle of 120°. So far, the electron detectors of a Mott polarimeter have usually been placed at a 120° scattering angle, and the reason for this is claimed to be that the Sherman function is at a maximum for a 120° scattering.[1] For the Sherman function of gold atoms, this is true. However, in constructing a Mott polarimeter, only a solid state target can be used and we have to replace the atomic Sherman function with the effective Sherman function, S_{eff}, in which the multiple and plural scattering are considered.

In practice, the effective Sherman function depends significantly on the energy of the incident electron and on the target thickness, e.g., in Fig. 1, the experimental results of Gellrich and Kessler[9] show that for 50 keV electrons scattered by a solid gold target, the maximum of the effective Sherman function is not at 120° and its absolute value is smaller than that calculated for an atomic target. On the other hand, the electron detectors of the spin polarimeter have a large collection angle to obtain a high efficiency, since the efficiency depends not only on the Sherman function but also on the scattering intensity, I/I_0. Because the scattered intensity is higher for a larger collection angle and the averaged Sherman function for a larger collection angle is smaller than its largest value, we have to balance the collection angle and the Sherman function. To estimate the optimum collection angle for the highest efficiency, we must know the effective Sherman function and scattered intensity of the target for different scattering angles. Therefore, when we design a Mott polarimeter to achieve a high efficiency, we should have a clear understanding about the spin-dependent scattering of electrons in a solid target.

There have been attempts to calculate the dependence of the effective Sherman function on the target thickness.[10,11] Wegener[10] considered two processes in his calculation; large-angle single scattering accompanied with small-angle multiple scattering and a process consisting of two large-angle single scattering events without small-angle multiple scattering. Braicovich and Michelis[11] added two other processes to be considered, namely the process consisting of two large-angle single scattering events accompanied by small-angle multiple scattering and the process of a succession of small-angle scattering events which allow the electrons to reach a large deflection angle. However, their results provided only qualitative understanding, because they did not consider every scattering process and had to make many approximations in their calculations. In contrast, the Monte Carlo method takes into account all possible processes and is much better suited to handling multiple scattering problems. Hnizdo[12] calculated the relation between the effective Sherman function and the target thickness using the Monte Carlo

[a]Present address: Surface and Interface Engineering Laboratory, The Institute of Physical and Chemical Research, 2-1 Hirosawa, Wako, Saitama 351-01, Japan.

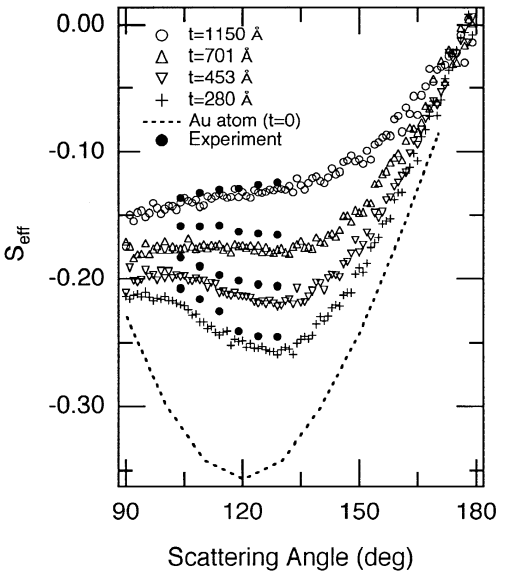

FIG. 1. The calculated effective Sherman functions for different scattering angles for 280, 453, 701, and 1150 Å gold targets. The experimental results (Ref. 9) and the theoretical Sherman function for gold atoms (Ref. 7) are also shown.

method and obtained good agreement with experiments. However, he restricted his calculation only to the case of 120° scattering and made some approximations for the calculation of successive small-angle scatterings.

Recently, retarding-potential Mott polarimeters[1] have become one of the most widely used spin polarimeters due to their small size, relatively low operating voltage, etc. For this kind of polarimeter, the relation of the effective Sherman function to the target thickness is not important and only the relation to the energy loss window is applicable. Unfortunately, relating the effective Sherman function to the energy loss window, neither calculation nor accurate experimental results have been reported so far. In this work, we have calculated, for 50 keV electrons incident on a gold target, the dependence of the effective Sherman function and the scattered intensity on the target thickness and inelastic energy loss windows for scattering angles from 90° to 180°.

II. THE MONTE CARLO CALCULATION

For a polarized electron beam, the scattering cross section can be calculated from the Dirac equation, a relativistic generalization of the Schrödinger equation. The solution of the electron scattering problem is given by two scattering amplitudes, f and g, where f is the amplitude of the scattering wave with spin direction unchanged and g is the amplitude of the spin-flip scattering wave as a result of the spin-orbit coupling. The spin-dependent scattering of electrons can be completely described by the four functions, I, S, T, and U, which are

$$I=|f|^2+|g|^2,$$

$$S=i(fg^*-f^*g)/(|f|^2+|g|^2),$$

$$T=(|f|^2-|g|^2)/(|f|^2+|g|^2),$$

$$U=(fg^*+f^*g)/(|f|^2+|g|^2),$$

and their physical meanings are as follows. I is the differential cross section for an unpolarized beam. S is the asymmetry or Sherman function which gives the transverse polarization of the scattered electrons for an unpolarized incident beam or the left–right scattering asymmetry for a completely transversely polarized incident beam. T and U describe the rotation of the polarization vector $\mathbf{P}$ during the scattering process. The spin-dependent differential scattering cross section $d\sigma/d\Omega$ can be written as

$$d\sigma(\theta,\varphi)/d\Omega=I(\theta)(1+S\mathbf{P}\cdot\mathbf{n}),$$

where $\mathbf{n}=\mathbf{n}_1\times\mathbf{n}_2/\sin\theta$ is the unit vector normal to the scattering plane, and $\mathbf{n}_1$ and $\mathbf{n}_2$ are unit vectors in the direction of the electron motion before and after the scattering, respectively. If we introduce

$$L=U\sin\theta+T\cos\theta,$$

$$R=U\cos\theta-T\sin\theta,$$

the rotation of $\mathbf{P}$ can then be written as[12]

$$\begin{aligned} P'_x&=(LP_x-RP_y)/(1+SP_z),\\ P'_y&=(LP_y+RP_x)/(1+SP_z),\\ P'_z&=(S+P_z)/(1+SP_z), \end{aligned} \tag{1}$$

where the incident polarization vector (P_x,P_y,P_z) is given in the coordinate system spanned by the unit vectors $\mathbf{n}_1$, $\mathbf{n}\times\mathbf{n}_1$, and $\mathbf{n}$, and the final polarization (P'_x,P'_y,P'_z) in the coordinate system spanned by $\mathbf{n}_2$, $\mathbf{n}\times\mathbf{n}_2$, and $\mathbf{n}$.

When the scattering angle is small enough, the scattering asymmetry is negligible and the impact parameter is large. In this case, the scattering of electrons can be approximated to the process that the electrons are deflected by a macroscopic transverse electric field. Then the above functions of the polarization rotation can be approximated as

$$\begin{aligned} P'_x&=P_x\cos\alpha+P_y\sin\alpha,\\ P'_y&=-P_x\sin\alpha+P_y\cos\alpha,\\ P'_z&=P_z, \end{aligned} \tag{2}$$

where $\alpha=(1-\beta^2)^{1/2}\theta$ and β is the ratio of velocity of the electrons to that of light.[12] Therefore, if we know the functions of I, S, L, and R, we can trace the position, direction of motion, and polarization of electrons through successive scattering events by the Monte Carlo method.

Equation (2) is in fact a linear translation of the polarization, so the total rotation of the polarization after j successive small-angle scatterings can be given as a translation:

$$\begin{aligned} \mathbf{P}'&=A\mathbf{P},\\ A&=A(\theta_j)\ldots A(\theta_2)A(\theta_1), \end{aligned} \tag{3}$$

where $A(\theta_i)$ is the translation matrix of the scattering i. In Hnizdo's calculations,[12] he supposed that the small-angle multiple scatterings could be approximated to a single scattering event with a scattering angle satisfying a certain distribution and the rotation of the polarization could be calculated by Eq. (2) using the scattering angle of that single scattering event. But it can be proved, when considering the problem in three-dimensional space, that if the total scattering angle of two successive scatterings θ_1, θ_2 is θ, $A(\theta)$ is

in general not equal to $A(\theta_2)A(\theta_1)$, where all the translation matrices, $A(\theta)$, $A(\theta_1)$, and $A(\theta_2)$ are calculated using Eq. (2). In our calculation, every small-angle scattering event is sampled from $I(\theta)$ directly and the rotation of the polarization during every small-angle scattering event is calculated by Eq. (3).

At first, we consider a transversely polarized electron beam of a certain energy being incident normally on a target film of a given thickness. The distance d traveled by the electron between two successive collisions is sampled from the distribution

$$f(d)=\Sigma\ \exp(-\Sigma d),$$

where Σ is the total scattering cross section per unit volume of the target. The scattering angle, θ, is sampled from the differential cross section, $I(\theta)$, and the azimuthal angle of every scattering event is sampled from a uniform distribution between 0 and 2π. The inelastic energy loss is taken into account by restricting the total distance $D_{\max}$ which the electrons can travel using the relation

$$D_{\max}=\Delta E/(dE/dS),$$

where dE/dS is the rate of inelastic electron energy loss with distance and ΔE is the inelastic energy loss window determined by the energy discrimination level in the scattered electron measurements. When the total distance that the electron has traveled is larger than $D_{\max}$, it can no longer be detected and a new incident electron is considered.

Since we are interested in backscattering where the polarization of the incident electron is perpendicular to the scattering plane, the following calculation procedure is used to save the computing time. In this procedure, we trace the electron motion and calculate the polarization translation matrix A using Eq. (3) for successive small-angle scattering events untie a large angle scattering event occurs and then the total scattering polar angle $\Delta\theta$ and azimuthal angle $\Delta\varphi$ are calculated. $\Delta\theta$, $\Delta\varphi$, and A of every multiple small-angle scattering sequence and $\Delta\theta$ and $\Delta\varphi$ of every large-angle scattering event are recorded until the electron has traveled a distance greater than $D_{\max}$ in the target or leaves the target. If the electron is backscattered, i.e., exits from the incident surface, the polarization of the incident electron is set perpendicular to the scattering plane defined by the incident and outgoing direction of the electron with respect to the target. The rotation of the polarization of the electrons in the large- and small-angle multiple scattering events are calculated by Eqs. (1) and (3), respectively.

The spin dependence of the scattering intensity is included by multiplying the statistical weight of the electron by a factor of $(1+SP_n)$ in every large-angle scattering event. Then the effective Sherman function is calculated using

$$S_{\text{eff}}=1-N_{\text{sta}}(\theta)/N(\theta),$$

where $N(\theta)$ is the number of electrons whose total scattering angle is θ, and $N_{\text{sta}}(\theta)$ is the sum of the statistical weights of these electrons. The scattered intensity for a certain scattering angle θ can be calculated by

$$I(\theta)/I_0=N(\theta)/N_{\text{total}},$$

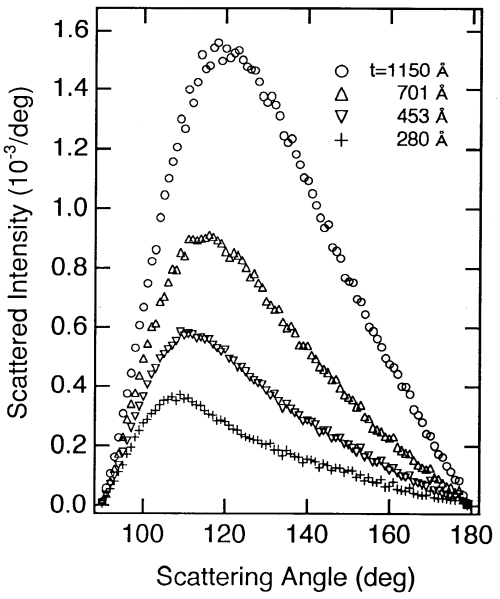

FIG. 2. The calculated scattered intensities for different scattering angles for 280, 453, 701, and 1150 Å gold targets.

where N_{total} is the total number of incident electron considered.

The dependence of the effective Sherman function and the scattered intensity on the energy loss windows can be obtained by setting the target thickness to be infinite and changing $D_{\max}$.

III. RESULTS AND DISCUSSION

We have carried out Monte-Carlo calculations for 50 keV electrons scattered by a gold target. $I(\theta)$ was taken from the literature[13] by interpolation. The Sherman function, $S(\theta)$, for gold atoms is taken from Lin's result,[7] and $R(\theta)$ and $L(\theta)$ from Ref. 14. The energy loss rate for 50 keV electron in gold is about 3 MeV cm^2/g.[15] In Gellrich and Kessler's measurement, the discrimination level was set to be 12.5% lower than the energy of the incident electrons. In order to compare with their experimental results, we use the same discrimination level, i.e., the inelastic energy loss window is taken to be about 6 keV and the maximum travel distance $D_{\max}$ to be 1.0×10^{-4} cm in the calculations for different target thicknesses. The results of calculations for different target thicknesses show that in changing $D_{\max}$ from 1×10^{-5} to 5×10^{-5} cm, the effective Sherman function decreases by 25%, and in changing $D_{\max}$ from 1×10^{-4} to 5×10^{-4} cm, it only decreases by less than 2%. This implies that the results are not sensitive to the choice of $D_{\max}$ provided larger than 1.0×10^{-4} cm. The critical scattering angle, which separates large-angle scattering processes from small-angle ones, was chosen to be 0.1 rad. The value of 0.1 rad is a tradeoff between accuracy and the computing time. In fact, tests revealed that, when this value changes from 0.5 to 0.05 rad, the effective Sherman function only decreases by 0.7%.

Figure 1 shows the calculated effective Sherman function at different scattering angles for 280, 453, 701, and 1150 Å thick gold targets. In this figure we also show the experimental results[9] and the Sherman function for gold atoms.[7]

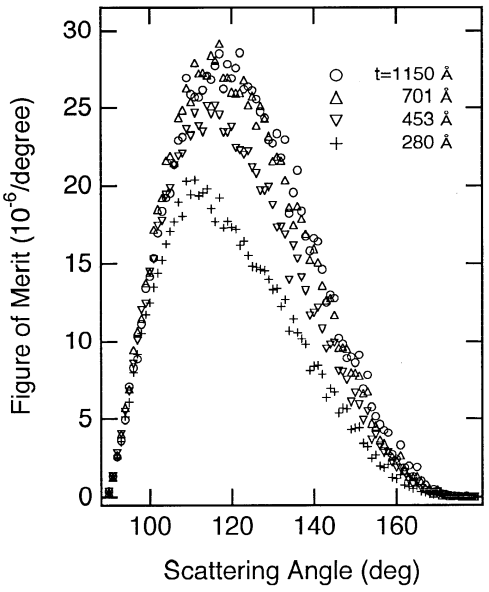

FIG. 3. The calculated figure of merit for different scattering angles for 280, 453, 701, and 1150 Å gold targets.

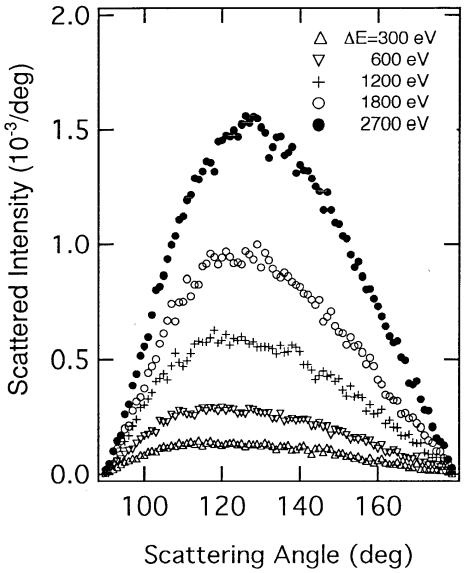

FIG. 5. The calculated scattered intensities for different scattering angles for 300, 600, 1200, 1800, and 2700 eV inelastic energy loss windows.

The results of this work agree quite well with the experimental values, which indicates that the Monte-Carlo method is reliable for our problem. A slightly higher effective Sherman functions predicted by our calculations compared with the experimental data can be attributed to inelastic effects. Values for $I(\theta)$ and $S(\theta)$ for 50 keV electrons were used in our calculation routine, but in fact, after being scattered in the target, the electrons will lose energy and $I(\theta)$ on the small scattering angle side will increase and $S(\theta)$ will decrease. Either of these two factors will result in a larger effective Sherman function in our calculations.

The results of the scattered intensity I/I_0 for these target thicknesses are shown in Fig. 2 and the results of the figureof merit, $(I/I_0)S_{\text{eff}}^2$ are shown in Fig. 3. When the target gold film is thicker than 700 Å, which is the thickness usually used in conventional Mott polarimeters, the effective Sherman functions are almost constant for a very wide scattering angle range around 120°. On the contrary, the scattered intensities change sharply with the scattering angle and the peak shifts from 108° to 120° when the thickness of the target changes from 280 to 1150 Å. The peak of the scattered intensity near 120°, instead of that of the Sherman function, is a primary reason why we can get high efficiencies by putting the detectors at a 120° scattering angle. From Fig. 3, we can see that the maximum of the figure of merit shifts from 110° to 117° when the sample thickness varies from 280 to 1150

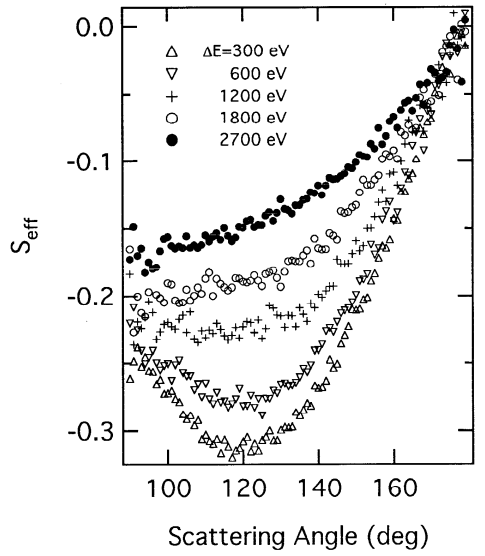

FIG. 4. The calculated effective Sherman functions for different scattering angles for 300, 600, 1200, 1800, and 2700 eV inelastic energy loss windows.

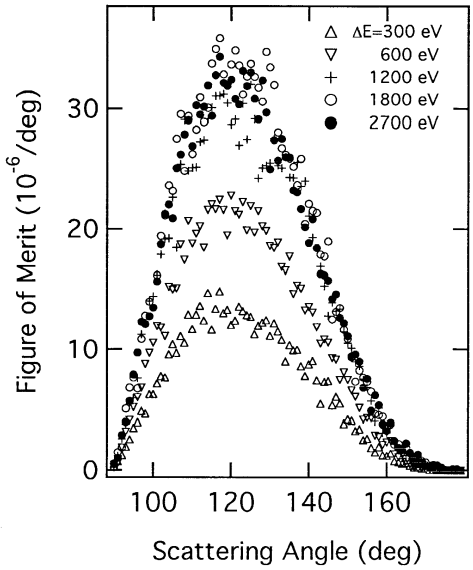

FIG. 6. The calculated figure of merit for different scattering angles for 300, 600, 1200, 1800, and 2700 eV inelastic energy loss windows.

Å. Therefore, in a strict sense, the detectors should be placed at different positions for different thicknesses of the target.

Our results for the above three functions for 300, 600, 1200, 1800, and 2700 eV inelastic loss windows are shown in Figs. 4, 5, and 6, respectively. When the energy loss window is larger than 1200 eV which is usually used in a retarding-type Mott polarimeter, the effective Sherman functions are also almost constant in a wide scattering angle range. The scattering intensity peak shifts from 120° to about 128° when the energy loss window changes from 300 to 2700 eV. The peak position of the figure of merit is almost independent of the variation of the energy loss window and is about 120°.

In conclusion, we have carried out a Monte Carlo calculation to obtain scattered intensity and effective Sherman functions for 50 keV electrons for various scattering angles. Since the effective Sherman function is practically almost constant over a wide range of scattering angles, for both conventional and retarding-type Mott polarimeters, a larger collection angle for the scattered electrons results in a higher efficiency.

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