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Multiple Scattering in Solids based on Statistical Model

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Angular distribution caused by multiple scattering in the small-angle approximation has been calculated, according to the theory derived by Sigmund and Winterbon. In this formula for the angular distribution, single-scattering cross section of elastic collision based on classical mechanics introduced by Lindhard et al. is used and we employed Thomas-Fermi-Moliere potential in the cross section. Multiple scattering distributions have been calculated for various combinations of projectiles and targets and compared with several experimental results.

Keywords: multiple scattering; statistical model; Thomas-Fermi-Moliere potential; elastic collision

1. Introduction

The angular broadening of the beam takes place after a well-collimated ion beam passes thorough a foil. Significant deflections of trajectory of each incident particle result mainly from multiple nuclear collisions because electronic scattering generally does not cause deflections. The information of multiple scattering is one of main issues in atomic and nuclear physics. For example, in the region of beam foil spectroscopy, multiple scattering is often an undesirable phenomenon. The angular divergence and lateral spread of beam in a target foil have to be considered in the construction of an apparatus because of diminishing the resolution of the experiment. From a theoretical point of view, the screened ion-atom potential is estimated by multiple scattering approach.

So far multiple scattering has been investigated experimentally and theoretically. For many combinations of projectiles and targets, experimental multiple scattering data have been obtained [1–3, 5] in the incident energy ranges from 14keV to 7.2MeV and for the combinations of incident ions with atomic number Z_1 for $1 \le Z_1 \le 18$ and target atoms with atomic number Z_2 for $6 \le Z_2 \le 28$. Some experiments [1–3] showed good agreement with theory; however deviations were obtained for the other experiments [5]. The information on the above literature was introduced by H. H. Andersen et al. [6]. Many authors have presented multiple scattering theories [7–9, 12, 13] and review articles have been given by Scott [10] in 1963 and Sigmund [11] in 2004. Using small angle approximation, Moliere [7], Meyer [8] and Sigmund and Winterbon (SW) [9] developed well known analytical formulae. Meyer and SW made use of the differential scattering cross section based on Thomas-Fermi (T-F) model which was developed by Lindhard et al. [14]. On the other hand, Goudsmit and Saunderson [12] and Lewis [13] treated theories without small angle approximation.

The present paper reports on theoretical studies of multiple scattering based on SW [9]. In section 2, an elastic scattering cross section and a multiple scattering formula are described on the basis of Lindhard et al. and SW, respectively. The theoretical results of present approach are compared with several experimental results in Sec. 3.

2. Theory

2.1 Differential elastic scattering cross section

In this section, we introduce a scattering cross section of binary collision to calculate the angular distribution of multiple scattering. The differential cross section of elastic collision $d\sigma$ based on the method derived by Lindhard et al. [14] is used in this paper. Lindhard et al. obtained $d\sigma$ by classical mechanics and their calculation was based on the interatomic potential of Thomas-Fermi model

$$V(r)=\frac{Z_1Z_2e^2}{r}u\left(\frac{r}{a}\right), \tag{1}$$

where e is the elementary charge, r is the distance between nuclei, a is a screening length and $u(r/a)$ is the screening function. By considering the relationship between small scattering angle θ and the impact parameter p by means of impulse approximation, in the center of mass system (C.M.S.), they showed the formula,

$$\theta=\frac{b}{p}g\left(\frac{p}{a}\right), \tag{2}$$

where

$$g\left(\frac{p}{a}\right)=\int_0^{\pi/2}d\varphi\cos(\varphi)\left\{u\left(\frac{p}{a\cos(\varphi)}\right)-\frac{p}{a\cos(\varphi)}u'\left(\frac{p}{a\cos(\varphi)}\right)\right\}, \tag{3}$$

$$b=\frac{Z_1Z_2e^2}{E}\ .$$

Here b is the collision diameter in Rutherford scattering and E is the kinetic energy of a particle with the reduced mass. They, then, replaced in eq. (2) θ with $2\sin\left(\theta/2\right)$. The expansion was performed on the grounds that the case of using power law potential provided the correspondence between analytical formulae of small angle and wide angle. The cross section is finally written as follows,

$$d\sigma=\pi a^2\frac{f\left(t^{1/2}\right)}{2t^{3/2}}\ , \tag{4}$$

where $t^{1/2}=\varepsilon\, sin\left(\theta/2\right)$ and $\varepsilon=a/b$ are the non-dimensional variables. The function $f(t^{1/2})$ is

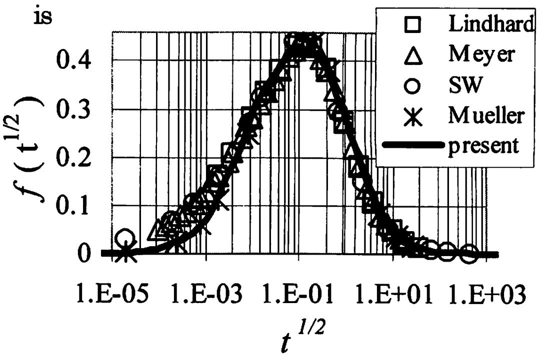

Fig.1. The comparison of scattering functions calculated by Lindhard et al. [13] (open squares), Meyer [8] (open triangles), SW [9] (open circles), Mueller [14] (asterisks) with the present result (solid line).

estimated numerically by using a Thomas-Fermi (T-F) potential.

The function, $f(t^{1/2})$, is dependent upon interaction potential. Meyer[8], SW[9], and Mueller[15] also evaluated $f(t^{1/2})$. Meyer made use of a T-F potential and SW used a three-parameter form, which represents various interatomic potentials. Mueller derived a fitting form, which describes T-F-Moliere potential. In the present treatment, T-F-Moliere potential is employed. The comparison with them is shown in Fig. 1. The function $f(t^{1/2})$ in our case is expressed as

$$f\left(t^{1/2}\right)=X\left(\frac{g^2(X)}{g(X)-X\dfrac{dg}{dX}}\right)\ , \tag{5}$$

where

$$t^{1/2}=\frac{g(X)}{2X}\ , \tag{6}$$

$$g(X)=\int_0^{\pi/2}d\varphi\cos(\varphi)\left\{\sum_{i=1}^{3}\alpha_i\exp[-\beta_iX/\cos(\varphi)]+\sum_{i=1}^{3}\frac{\alpha_i\beta_iX}{\cos(\varphi)}\exp[-\beta_iX/\cos(\varphi)]\right\},$$

(7)

$$X = p/a. \tag{8}$$

In eq. (7), the values of parameters are $\alpha_1 = 0.10$, $\alpha_2 = 0.55$, $\alpha_3 = 6.0$, $\beta_1 = 6.0$, $\beta_2 = 1.20$, $\beta_3 = 0.30$.

2.2 Multiple scattering

We consider the angular distribution of ions penetrating a foil of thickness x. The formula of multiple scattering is based on the theory of SW [9]. The angular distribution at $x+\delta x$ changes from the distribution at x after the particles traveled δx in the matter. There are two phenomena that some particles change its directions due to nuclear collisions and the others without nuclear collision. The distribution at $x+\delta x$, therefore, is the following expression

$$\begin{aligned} f(x+\delta x,\vec{\alpha}) &= n\delta x \int d\sigma(\vec{\alpha}'\to\vec{\alpha}) f(x,\vec{\alpha}') \\ &+ \left[1-n\delta x \int d\sigma(\vec{\alpha}\to\vec{\alpha}')\right] f(x,\vec{\alpha}), \end{aligned} \tag{9}$$

where $\vec{\alpha}$ and $\vec{\alpha}'$ are the two dimensional angles and n is the number of atoms per unit volume. Four assumptions are used here. (I) neglect of energy loss, (II) binary collision with azimuthally symmetrical scattering, (III) small scattering angle in each event of collision and (IV) random homogeneous distribution of scattering centers in space. The differential scattering cross section, therefore, is considered as a function of the relative deflection $|\vec{\phi}| = |\vec{\alpha}-\vec{\alpha}'|$ because of azimuthal symmetry. Considering the limit, $\delta x \to 0$, we get

$$-\frac{\partial f(x,\vec{\alpha})}{\partial x} = n \int d\sigma(\phi)\left[f(x,\vec{\alpha}) - f(x,\vec{\alpha}+\vec{\phi})\right]. \tag{10}$$

Here we define the two-dimensional Fourier transformation as follows

$$\begin{aligned} f(x,\vec{\alpha}) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\vec{k}\, \tilde{f}(x,\vec{k}) e^{i\vec{k}\cdot\vec{\alpha}}, \\ \tilde{f}(x,\vec{k}) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\vec{\alpha}\, f(x,\vec{\alpha}) e^{-i\vec{k}\cdot\vec{\alpha}}, \end{aligned} \tag{11}$$

and then eq. (10) becomes the differential equation

$$\frac{\partial \tilde{f}(x,\vec{k})}{\partial x} = -n\tilde{f}(x,\vec{k}) \int d\sigma(\phi)\left[1-e^{i\vec{k}\cdot\vec{\phi}}\right]. \tag{12}$$

The solution of the above equation is

$$\tilde{f}(x,\vec{k}) = C e^{-nA(k)x}, \tag{13}$$

$$A(\vec{k}) = \int d\sigma(\phi)\left[1-e^{i\vec{k}\cdot\vec{\phi}}\right], \tag{14}$$

and using the initial condition, $f(0,\alpha) = \delta(\alpha)$, we obtain

$$\begin{aligned} C &= \tilde{f}(0,\vec{k}), \\ &= \frac{1}{2\pi}. \end{aligned} \tag{15}$$

In eq. (11), integrating azimuthal angle and using $d\sigma(\phi) = \Theta(\phi) d\Omega = \Theta(\phi)\phi\, d\phi\, d\chi$, we find

$$\begin{aligned} A(k) &= \int_0^{\infty} \Theta(\phi)\phi d\phi 2\pi\left[1-\frac{1}{2\pi}\int_0^{2\pi} d\chi e^{ik\phi\cos(\phi)}\right], \\ &= \int_0^{\infty} d\sigma(\phi)\left[1-J_0(k\phi)\right], \end{aligned} \tag{16}$$

where J_0 is the zero-order Bessel function of the first kind. Inserting eq. (13) in eq. (11), we get by the same manner as $A(k)$ is treated

$$f(x,\vec{\alpha}) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} d\vec{k}\, e^{-nA(k)x} e^{i\vec{k}\cdot\vec{\alpha}},$$

$$= \frac{1}{(2\pi)^2} \int_0^\infty dk k \int_0^{2\pi} d\psi e^{-nA(k)x} e^{ik\alpha\cos(\psi)},$$
$$= \frac{1}{2\pi} \int_0^\infty dk k e^{-nA(k)x} J_0(k\alpha) \,. \tag{17}$$

Using the differential scattering cross section showed by Lindhard et al. and the small angle approximation, we can rewrite eq. (17) as follows

$$f_1(\tau,\tilde{\alpha}) = \int_0^\infty dz z e^{-\tau\Delta(z)} J_0(z\tilde{\alpha}), \tag{18}$$

where

$$\Delta(z) = \int_0^\infty d\tilde{\phi} \frac{f(\tilde{\phi})}{\tilde{\phi}^2} \left[1 - J_0(z\tilde{\phi})\right] \,,$$
$$\tilde{\phi} = t^{1/2} = \frac{E_1 a}{2 Z_1 Z_2 e^2} \phi \,,$$
$$\tau = \pi a^2 N x \,,$$
$$\tilde{\alpha} = \frac{E_1 a}{2 Z_1 Z_2 e^2} \alpha \,,$$
$$z = k \frac{2 Z_1 Z_2 e^2}{E_1 a} \,.$$

Here, E_I is the energy of incident particle, τ is the reduced thickness, α is the total scattering angle, $\tilde{\alpha}$ is the reduced scattering angle and z is the non–dimensional variable. We note that the formula of the scattering distribution in reduced scattering angle is independent of the energy of projectiles.

There are various screening lengths, a_B, a_F, a_L and a_{ZBL}, proposed by Bohr [16], Firsov [17], Lindhard et al. [14] and Ziegler et al. [18], respectively, of the following forms:

$$a_B = \frac{a_0}{\left(Z_1^{2/3} + Z_2^{2/3}\right)^{1/2}} \,, \tag{19}$$

$$a_F = \frac{0.8853\, a_0}{\left(Z_1^{1/2} + Z_2^{1/2}\right)^{2/3}} \,, \tag{20}$$

$$a_L = \frac{0.8853\, a_0}{\left(Z_1^{2/3} + Z_2^{2/3}\right)^{1/2}} \,, \tag{21}$$

$$a_{ZBL} = \frac{0.8853\, a_0}{\left(Z_1^{0.23} + Z_2^{0.23}\right)} \,. \tag{22}$$

We adopt a_L in the present study.

3. Results and Discussions

In this section, the results of eq. (18) are compared with several experimental results. All the measured and theoretical distributions are normalized to the maximum value. The scattering distribution is obtained as a function of the reduced thickness and reduced angle. The reduced thickness includes the screening length a, which has been calculated according to Lindhard et al. [14]. In the reduced units, the results of calculations are independent of the incident energy of particles, but depend upon the reduced thickness. Hence, for different combinations of Z_1, Z_2, and incident energy E_1, the same angular distributions are obtained in case of the same reduced thickness.

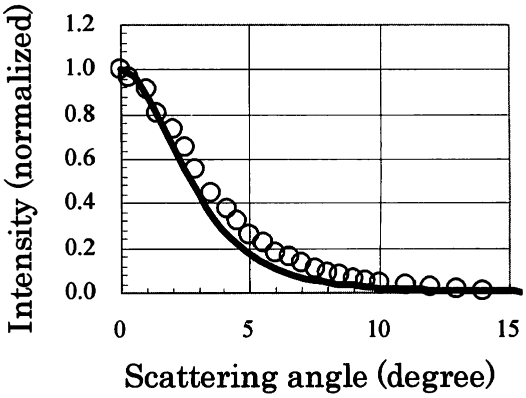

Fig. 2. Scattering distribution of 50keV proton transmitted through a 20μg/cm² nickel foil. The open circles and solid line refer to the experimental results obtained by Schaffler [1, 4] and the present result, respectively. The vertical and the horizontal axes are the normalized intensity and the scattering angle in degree, respectively.

In Fig.2, 3 and 4, the measured scattering distributions of 50keV proton[1], 54keV argon[2] and 7.2MeV neon[3] passing through nickel, aluminum and carbon foils with the thickness 20μg/cm^2, 2.5μg/cm^2 and 12μg/cm^2, respectively, are shown by open circles. Also the corresponding theoretical results are shown by solid lines. We have taken out measured values for the above three experiments from the literature written by Moller et al. [4]. The reader, therefore, is recommended to see the original reports [1–3]. In the above three

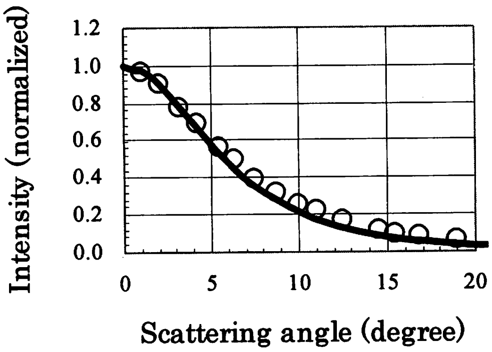

Fig. 3. Scattering distribution of 54keV argon transmitted through a 2.5μg/cm^2 carbon foil. Open circles and solid line refer to the experimental results obtained by Hogberg [2, 4] and the present result, respectively. The vertical and the horizontal axes are the normalized intensity and the scattering angle in degree, respectively.

experiments, we can say that the theoretical curves explain very well the trend of the experimental data. In Fig.2, we have not employed the screening length a of two atoms but single atom, because proton has no bound electron. Namely, for the combination of proton and nickel, the screening length a has been calculated in the condition that Z_1 is zero.

For Li incidence on Al, Co and Si targets [5], is found disagreement, while for the combination of Li and C, the experimental and theoretical results are in agreement as shown in Fig. 5 and 6. As pointed out in the previous section, in reduced scattering angle, the angular distribution is independent of the energy of the incident particles but dependent upon

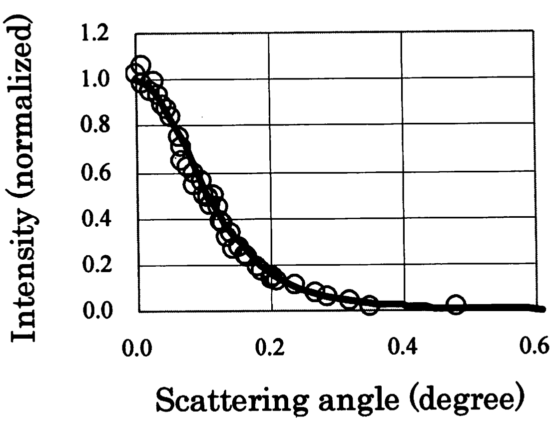

Fig. 4. Scattering distribution of 7.2MeV neon transmitted through a 12μg/cm^2 aluminum foil. Open circles and solid line refer to the experimental results obtained by Spahn [3, 4] and the present result, respectively. The vertical and the horizontal axes are the normalized intensity and the scattering angle in degree, respectively.

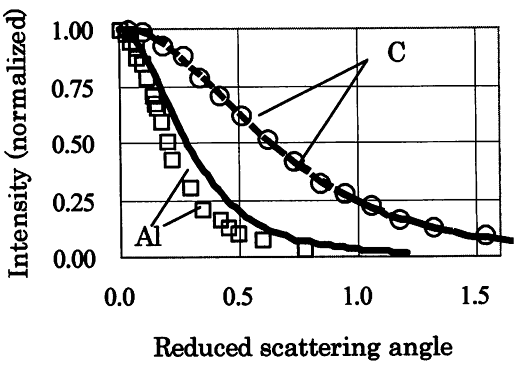

Fig. 5. Scattering distribution of lithium transmitted through a 170 Å aluminum foil and 155 Å carbon foil. Open circles and open squares refer to the experimental results on Al and C, respectively, obtained by Schwabe et al. [5]. The solid line and dashed line denote the present results for Al and C, respectively. The vertical and the horizontal axes are the normalized intensity and the reduced scattering angle, respectively. The incident energies are 14, 20, 28, 35, 43 and 50keV.

the reduced thickness. The results measured at different energies in Fig. 5 and 6 lay on the unique curves, respectively. The foil thicknesses of Al, C, Co and Si are 170, 155, 210 and 700[Å], respectively. In Fig.5 and 6, the measured data for different energies are intermingled, and therefore we recommend the reader to refer to the original papers [5] for detailed experimental results.

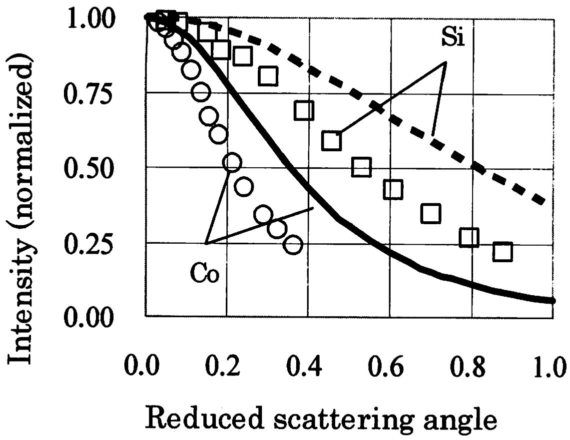

Fig. 6. Scattering distribution of lithium transmitted through a 210 Å cobalt foil and 700 Å silicon foil. Open circles and open squares correspond to the experimental results on Co and Si, respectively, obtained by Schwabe et al. [5]. The solid line and dashed line denote the present results for Co and Si, respectively. The vertical and the horizontal axes are the normalized intensity and the reduced scattering angle, respectively. The incident energies are 28, 35, 43 and 50keV.

Schwave et al. [5] fitted the theoretical distributions of Meyer's theory to the experimental ones by changing screening length a for combinations of Z_1 and Z_2. From the above comparisons and the suggestion of Schwabe et al. [5], it is inferred that more realistic inter-atomic potential could provide a better correspondence between theory and experiment. Finally we add a few comments that SW's treatment dropped off the function $f_2(\tau, \tilde{\alpha})$ appeared in Meyer's [8]. This is valid, judging from the normalization of the distribution function. H. H. Andersen et al. [6] suggested that the experimental results showed narrower distributions than theoretical ones in case of the target film including grains huger than or approximately equal to 100[Å].

4. Conclusion

The theoretical results in this paper are agreement with the published experimental data when the following combinations of projectiles and targets are used: p–Ni, Ne–Al, Ar–C and Li–C. On the other hand, there are discrepancies between the calculated data and experimental ones for combination of Li–Al, Li–Co and Li–Si.

We can say that it is useful to apply T-F-Moliere potential to the multiple scattering theory of SW and agreement between experimental and theoretical results is obtained while for some combinations of Z_1 and Z_2 the differences between them are shown.

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