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ENHANCED ION BACKSCATTERING NEAR 180° SCATTERING ANGLES

IN THE TWO-ATOM SCATTERING MODEL

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IN THE TWO-ATOM SCATTERING MODEL*

Ordean S. Den

ABSTRACT

An analytical two-atom scattering model has been developed to treat the recent discovery of the enhancement near 180° of Rutherford backscattering yields from disordered solids. In contrast to conventional calculations of Rutherford backscattering that treat scattering from a single atom only (the backscattering atom), the present model includes the interaction of a second atom lying between the target surface and the backscattering atom. The projectile ion makes a glancing collision with this second atom both before and after it is backscattered. A weighted average is made over all possible positions of this second atom. The model predicts an enhancement effect whose physical origin arises from the tolerance of path for those ions whose ingoing and outgoing trajectories lie in the vicinity of the critical impact parameter. Results using Molière scattering show how the yield enhancement depends on ion energy, backscattering depth, exit angle, scattering potential, atomic numbers of the projectile and target, and target density. In the model the critical impact parameter and critical angle play important roles. It is shown that these quantities depend on a single dimensionless parameter and formulas accurate to better than 1% are given for them.

INTRODUCTION

An unusual enhancement of the yield of low MeV ions backscattered from the near-surface regions of solids for scattering angles very near 180° was discovered recently at Oak Ridge National Laboratory by Pronko, Appleton, Holland and Wilson.^{1,2} The enhancement over that expected for Rutherford scattering occurs at angles a few tenths of a degree from 180° backscattering and increases rapidly as the beam axis

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is approached. Typically, the enhancement, which may be a factor of two or larger, is a maximum when the ions are backscattered from depths of about 5 to 10 nm. The effect has been observed¹⁻⁷ for a wide variety of amorphous and polycrystalline solids using H^+ and He^+ beams of energies from 0.2 to 2.5 MeV.

Barrett⁸ suggested that this enhancement effect is a consequence of a correlation between the ingoing and outgoing paths of the backscattered ion, and computer simulation results by Crawford,⁹ by Jakas and Baragiola¹⁰ and by Barrett et al.¹¹ have confirmed this suggestion. The computer simulations of Barrett et al.¹¹ are in excellent agreement with the experimental data. Barrett¹¹ also suggested that the two-atom scattering (blocking) model¹² might give some insight into this phenomenon.

The present report develops a two-atom scattering model¹² in detail to treat the enhancement of ion backscattering yields from amorphous solids. An abbreviated account of this work was reported recently;¹³ however, page limitations of the conference proceedings precluded publishing many of the important mathematical details and results. Therefore, it was felt desirable to write an expanded report which included all of the relevant details. It is found that the model gives a simple physical picture for the origin of the enhancement effect and reproduces its typical features.

BASIC FORMULATION

In conventional Rutherford backscattering calculations¹⁴ applicable to the near surface region of amorphous solids, an ion interacts with a single atom, the backscattering atom. In the present

two-atom model an ion interacts with two atoms: one atom produces the Rutherford backscattering and another closer to the surface scatters the ion through a small angle both before and after the backscattering event. Although there may be additional collisions in an actual solid, the present development treats only the most important ones. The structureless target consists of randomly located atoms and the analysis is based on classical scattering theory.

Let a uniform ion beam of intensity I_0 be normally incident upon the target and consider that the backscattering occurs at depth D from an atom at some fixed point B (see Fig. 1). Locate an atom A at some arbitrary position in a plane at distance l above the backscattering plane. (Later, an integration is performed over all possible atom A sites lying between the point B and the target surface.) The perturbation of the particle flux due to the scattering by atom A causes a redistribution of the flux particles hitting the backscattering atom B . For instance, an incident ion with an impact parameter s is scattered thru a small angle η and arrives at point B when the projected distance $l\theta$ between A and B satisfies the equation

$$l\theta = s + l\eta, \quad (1)$$

where the small angle approximation is used. Since the scattering angle η , for repulsive potentials, increases with decreasing s , Eq. (1) predicts a minimum or critical angle $\theta = \theta_c$ when $s = s_c$ as shown in the top of Fig. 2. (Because of this extremum, backscattered ions whose ingoing and outgoing trajectories pass within a broad neighborhood of the critical impact parameter s_c emerge at an angle close to the surface normal. In this model this tolerance of path is the

basic reason for the enhancement of the backscattering yield). The minimum value of θ produces a shadow or blocked region behind atom A where no particles can penetrate. Since the position of the backscattering atom B is taken as fixed, this means that it is impossible for an ion to reach point B if it is scattered from any A atom lying within a circular region of radius $\lambda\theta_c$. The center of this circle is the point at which a vertical projection of point B intersects the plane containing atom A. The flux density hitting the backscattering atom B is readily found from Eq. (1) to be

$$I_i(\theta) = \begin{cases} 0 & \theta < \theta_c \\ I_0 \frac{s}{\lambda^2 \theta} \left| \frac{ds}{d\theta} \right| & \theta > \theta_c \end{cases} \quad (2)$$

A general feature of $I_i(\theta)$ is that it is highly peaked near θ_c and approaches a constant I_0 for $\theta \gg \theta_c$ as illustrated in the bottom of Fig. 2. It is noted that for any given value of θ there are two values of the impact parameter s that contribute to the intensity. It may be helpful to think of atoms A and B as making up a dipole. Then the angle θ in Eq. (2) is the orientation of the dipole axis with respect to the incident beam direction.

Next, consider an isotropic angular distribution of particles starting back toward the surface from the backscattering atom B. These particles are scattered by atom A before they exit thru the surface (see Fig. 1). The number of particles scattered per unit solid angle at angle θ' (measured from the axis of the dipole BA) is proportional to

$$f(\theta') = \begin{cases} 0 & \theta' < \theta'_c \\ \frac{s'}{\lambda^2 \theta'} \left| \frac{ds'}{d\theta'} \right| & \theta' > \theta'_c \end{cases} \quad (2a)$$

Here the angle θ' is given by

$$\lambda \theta' = s' + \lambda \eta' \quad (1a)$$

where the ion scattering angle η' is a function of the impact parameter s' . Since the angles θ' and η' are small the distance between atoms A and B is λ . The critical angle θ'_c is found from the extremum of Eq. (1a), which results in a shadow region behind atom A (as viewed from atom B) exactly analogous to that discussed before.

It is noted that there is an exact similarity between Eqs. (1) and (1a) and between Eqs. (2) and (2a) although they have a different physical content. For instance, Eq. (2) gives the flux density hitting the backscattering atom when an initially uniform parallel beam of incident particles is scattered. On the other hand, Eq. (2a) gives the angular distribution of flux intensity resulting from the scattering of an initially isotropic angular distribution. The exact similarity between Eqs. (1) and (1a) is a consequence of the small angle approximation. It may be noted also that when the energy of the ingoing and outgoing ion is the same (no energy loss on backscattering) then the functional forms for the scattering angles η and η' in Eqs. (1) and (1a) respectively are identical.

Three more factors are important in developing an expression for the backscattered intensity. First, the connection between the

ingoing and outgoing flux is the Rutherford backscattering event. Since Rutherford scattering changes little over an angular range of a few degrees from 180° , one can simply use the total Rutherford backscattering cross section σ_R for that cone. Second, all possible positions of the perturbing atom A relative to the backscattering atom B need to be included. For a random solid the spatial distribution function for finding atom A in a small volume of thickness Δl is simply $N l^2 \theta \Delta l d\theta d\phi$, where N is the atomic density and ϕ is the azimuthal angle [see Eq. (5)]. Here cylindrical coordinates are used with atom B and the surface normal defining the cylindrical axis. Third, the two atom model assumes that there is only one significant scattering before the incident particle strikes the backscattering atom. The probability for a single scattering with an impact parameter s is assumed to be $\exp(-\pi s^2 ND)$. This exponential factor seems reasonable since it gives the probability that there is no atom within a cylindrical volume of radius s and height D .

Now combining the three factors above with Eqs. (1) and (2), the backscattering intensity per steradian, $I(\psi)$, at small exit angle ψ is

$$I(\psi) = I_0 \sigma_R \sum \Delta l \iint \frac{s}{l^2 \theta} \left| \frac{ds}{d\theta} \right| f(\theta') e^{-\pi s^2 ND} N l^2 \theta d\theta d\phi, \quad (3)$$

where the summation extends over all atomic layers between the backscattering plane and the surface of the target.

Since the angles θ' , θ and ψ are small their functional relationship can be obtained most easily by making use of the fact that small angles can be treated as vectors. If one assumes that atom A is stationary from the time the ion makes a glancing collision on its

inward trajectory until it makes a subsequent glancing collision on its outward trajectory, then from the kinematics the following vector equation results,

$$\vec{\theta}' = \vec{\psi} - \vec{\theta} \quad (4)$$

The equivalent scalar equation is

$$\theta'^2 = \psi^2 + \theta^2 - 2\psi\theta\cos\phi, \quad (5)$$

where ϕ is the azimuthal angle between the vectors $\vec{\psi}$ and $\vec{\theta}$.

By changing variables from θ to s Eq. (3) simplifies to

$$\chi(\psi) = \frac{I(\psi)}{I_0 \sigma_R} = \sum \frac{\Delta \ell}{D} \int_0^\infty \int_0^{2\pi} f(\theta') e^{-\pi s^2 ND} ND s d\phi ds, \quad (6)$$

where $\chi(\psi)$ is the normalized yield. In Eqs. (3) and (6) the angle ψ is written as a scalar because the yield is azimuthally symmetric about the target normal. Equation (6) is the central result of this paper and will be evaluated in the next section.

Before evaluating Eq. (6) it seems useful to discuss a related quantity which sheds some insight on the above development. This quantity is the total integrated flux that hits the backscattering atom B after deflection by some A atom. The expression for this quantity is

$$\begin{aligned} I_1 &= I_0 \sigma_R \sum \Delta \ell \iint \frac{s}{\ell^2 \theta} \left| \frac{ds}{d\theta} \right| e^{-\pi s^2 ND} N \ell^2 \theta d\theta d\phi \\ &= I_0 \sigma_R \sum \frac{\Delta \ell}{D} \int_0^\infty \int_0^{2\pi} e^{-\pi s^2 ND} ND s ds d\phi. \end{aligned} \quad (7)$$

It is seen that the only difference between Eq. (7) and Eq. (3) is the presence of the factor $f(\theta')$ in the latter. This is the factor, of course, that accounts for the deflection of the projectile by atom A on its outward trajectory as was discussed previously [Eq. (2a)].

Equation (7) can be integrated immediately and equals

$$I_i = I_o \sigma_R \int \frac{\Delta l}{D} \left\{ (1 - e^{-\pi s_c^2 ND}) + e^{-\pi s_c^2 ND} \right\} \\ = I_o \sigma_R \quad (8)$$

This result shows that the total flux $I_o \sigma_R$ hitting the backscattering atom B is independent of the deflection by atom A. It is seen, therefore, that no enhancement can occur unless the scattering of the projectile on its outgoing trajectory is included. By including $f(\theta')$ as in Eqs. (3) and (6) one allows for correlations between the incoming and outgoing trajectories which makes possible an enhancement in the backscattering yield.

The term in parentheses in Eq. (8) is the result of integrating Eq. (7) from $s = 0$ to $s = s_c$ and, therefore, is the fraction of flux having impact parameters less than the critical impact parameter s_c that is focussed from a given plane to atom B. The second term $\exp(-\pi s_c^2 ND)$ is the fraction that is focussed with impact parameters greater than s_c . The enhancement in the backscattering is expected to be greatest when these two factors are about equal, i.e. $\pi s_c^2 ND = 0.693$, since then the backscattered projectile will have the highest probability for both its ingoing and outgoing trajectory to be in the vicinity of s_c . This point will be treated further in the discussion.

CALCULATIONS

The scattering of the moving ion by the stationary target atom is described using the Molière approximation^{15,16} to the Thomas-Fermi potential. In the small angle impulse approximation¹⁷ the scattering angle is

$$\eta(x) = \frac{b}{a} \{0.6K_1(6x) + 0.66K_1(1.2x) + 0.105K_1(0.3x)\}, \quad (9)$$

where x is the ratio of the impact parameter s to the Thomas-Fermi screening distance, $a = 0.04683 Z_2^{-1/3}$ (nanometers). Here $b = Z_1 Z_2 e^2 / E$ where E is the kinetic energy of the ion and $Z_1 e$, $Z_2 e$ are the nuclear charges of the ion and target atom respectively. The quantity K_1 is a modified Bessel function of the third kind. Using Eq. (9) one can calculate directly the critical angles and scattering patterns given by Eqs. (1)-(2a), (a discussion of these quantities is given in Appendix A and B). For light ions hitting heavy targets it is quite accurate to assume that the ion loses no energy on backscattering, therefore, $\theta'_c = \theta_c$ since the equations giving η and η' in Eqs. (1) and (1a) respectively, are then identical. Numerical methods were used to evaluate Eq. (6) because of complexities in the function $f(\theta')$. (An approximate method to solve Eq. (6) is given in Appendix D.) For instance, it does not seem possible to get a closed analytical expression for $f(\theta')$ using a realistic screened Coulomb potential such as the Molière. A Taylor's expansion shows that the singularity in $f(\theta')$ is of the form $(\theta' - \theta_c)^{1/2}$ so Gauss-Mehler quadrature methods were used to evaluate the inner integral over ϕ . The integral over s

was done using a Simpson quadrature technique. The summation in Eq. (6) was typically done by subdividing the region between the surface and the Rutherford backscattering plane into 10 atomic layers.

The three upper graphs of Fig. 3 show results of evaluating the double integral of Eq. (6) (omitting the summation) for 1 MeV He ions backscattered from amorphous Pt at a depth of $D = 5 \text{ r.l.}$. Each of the three graphs shows three distinct regions: an enhancement of the yield at very small ψ , then a deficit region ($\chi < 1.0$), and finally a slight enhancement beginning at $\psi \approx 2\theta_c$. The enhancement at very small ψ is due to backscattered ions whose ingoing and outgoing trajectories both pass through the same neighborhood of the critical impact parameter s_c of the perturbing atom. For $\psi = 0$ it can be shown that the yield has a logarithmic singularity. The deficit region arises from the blocking or shadowing produced by the perturbing atom on the backscattered ions. The slight enhancement at $\psi > 2\theta_c$ occurs from ions whose inbound trajectories are near s_c and whose outbound trajectories are near the s_c located on the far side of the perturbing atom. Overall there is particle flux conservation, for instance, if the ordinate is multiplied by $\sin \psi$, it is found that the two enhancement regions are exactly compensated by the deficit region. (Compensation is discussed in Appendix C.) The bottom curve in Fig. 3 is the calculated backscattering yield found by summing over all focussing layers ($\Delta z = 0.1D$). It is seen that the enhancement at small ψ is still present, but now the enhancement at larger angles disappears because an enhancement in one layer is cancelled by deficits in other layers.

Equation (6) has been evaluated for several ion-target parameters and results are shown in Figs. 4-9. Figure 4 shows that the yield enhancement is greatest at some intermediate depth and that it is small at both shallow and relatively large depths. In Fig. 5 it is seen that the peak in the normalized yield increases and shifts toward greater depth for decreasing ψ . Figure 6 shows that the yield at $\psi = 0.1^\circ$ increases and peaks at shallower depths with decreasing ion energy. Figure 7 illustrates the yield dependence on the atomic density. Figure 8 shows the influence of the scattering potential on the yield when the screening distance is changed. Shown in Fig. 9 is the yield at $\psi = 0.1^\circ$ for four different target materials. For Al it is seen that the yield is less than unity for depths greater than about 10 nm. This simply means that at these relatively large depths the enhancement is occurring at angles of ψ smaller than 0.1° (this may be inferred from the trend in Fig. 4). Many of the above results may be scaled to other systems by noting that the atomic number and energy of the ion appear only in the combination $Z_1 Z_2 e^2 / E$. For instance, the same results are predicted for 0.5 MeV protons as for 1.0 MeV alpha particles.

Further insight into the results can be obtained by utilizing the results of Eq. (8). There it was pointed out that the enhancement is expected to be greatest when the flux arriving at the backscattering atom is split by the critical impact parameter into two equal fractions. For orientation purposes take as a zeroth approximation $s_c^2 = b_c^2 = Z_1 Z_2 e^2 / E$. (Coulomb scattering, see Appendix B for Molière scattering). The small enhancement at shallow and large depths shown in Fig. 4 is now explainable

as follows: For shallow depths (small D and λ) most of the ions arrive at the backscattering atom having had impact parameters with atom A that are greater than s_c . On the other hand, at large backscattering depths most of the ions have had impact parameters smaller than s_c .

From Eq. (8) the two fractions of flux from a given focussing plane are equal when $\pi N D s_c^2 = 0.693$. Using $s_c^2 = b\lambda$ and a focussing plane midway between the surface and the backscattering plane ($\lambda = D/2$), the above equality becomes $\pi N Z_1 Z_2 e^2 D^2 = 1.386 E$. For 1 MeV He ions backscattered from Pt this expression predicts the maximum in the enhancement to occur at a depth $D = 5.4$ nm which is in fair agreement with the result shown in Fig. 6. This expression enables one to predict also how the enhancement peak shifts in depth when E or N is varied. The predictions are in qualitative agreement with the results shown in Figs. 6 and 7. The shift of the enhancement peak to greater depths with decreasing ψ as seen in Fig. 5 can be qualitatively understood as follows: As noted in the top three graphs of Fig. 3 a focussing plane contributes to the enhancement for values of $\psi \gtrsim 0.4 \theta_c$ ($\theta_c = 2 \sqrt{b/\lambda}$, Coulomb scattering). This means that as ψ decreases, focussing planes with larger λ are able to contribute and the result is that the enhancement peak shifts to greater depth.

CONCLUSION

The overall features of the results of the two-atom model are confirmed by experiment. The main differences are that the model predicts smaller enhancements whose maxima occur at somewhat shallower depths. As an illustration, predictions of the two-atom model are

compared with computer simulation results of Barrett et al.¹¹ and with experimental measurements¹ in Fig. 10. In this example the model predicts yields that are too little especially at very small ψ . The most probable reason for this underprediction is that glancing collisions in addition to those included in the two-atom model are contributing to the enhancement effect. It should be mentioned that including the effects of nuclear recoil and depth resolution of the detector in the model would lead to poorer agreement.

It has been shown that the two-atom model gives a simple picture of ion path tolerance near the critical impact parameter as the physical origin of the enhancement in the backscattering yield. The model reproduces the typical features of the effect and its dependence on the various physical parameters. It is to date the only analytical model that gives quantitative predictions and an explanation in terms of basic mechanisms of the enhancement effect. The simplicity and rapidity with which one can do exploratory calculations makes it a complementary approach to the detailed computer simulation methods. The model may also serve as a building block upon which a more general model may be built.

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APPENDIX A: Function $f(\theta)$ of Eqs. (2) and (2a)

For Coulomb (Rutherford) scattering the function $f(\theta)$ in Eq. (2a) takes on a very simple form¹⁸

$$f(\theta) = \begin{cases} 0 & \theta < 2\sqrt{b/l} \\ \frac{1}{2} \left[\left(1 - \frac{4b}{l\theta^2}\right)^{1/2} + \left(1 - \frac{4b}{l\theta^2}\right)^{-1/2} \right] & \theta > 2\sqrt{b/l} \end{cases} \quad (\text{A-1})$$

where the Coulomb critical angle is $2\sqrt{b/l}$ ($b=Z_1Z_2e^2E^{-1}$). The critical impact parameter for Coulomb scattering is $\sqrt{bl}$. For Coulomb scattering the contribution to $f(\theta)$ from impact parameters greater than the critical impact parameter is $0.5(f(\theta)+1)$ and from those smaller than the critical impact parameter is $0.5(f(\theta)-1)$. For large θ the latter quantity goes asymptotically into the ordinary Rutherford scattering law (impulse approximation). Although these Coulomb expressions are sometimes used in making estimates when discussing blocking phenomena, they are frequently not very accurate. In general, one needs a more accurate interaction potential, such as the Molière, which includes the screening of the nuclear charges. Figure 11 shows a universal curve for the ratio of the Molière scattering angle to the Rutherford scattering angle b/s , both calculated using the impulse approximation.

For the Molière potential it does not seem possible to find a closed expression for $f(\theta)$ or even for the critical angle or critical impact parameter. However, in the vicinity of the critical angle θ_c a Taylor's expansion of θ as a function of $(s-s_c)$, where terms higher than the quadratic are dropped, yields

$$f(\theta) = \frac{\lambda s_c}{\lambda^2 \theta \sqrt{\theta - \theta_c}} \quad (\text{A-2})$$

where $2\lambda^{-2} = \frac{d^2 \eta}{ds_c^2}$ is the second derivative of the scattering angle (Eq. 9) with respect to the impact parameter evaluated at the critical impact parameter. Equation (A-2) shows the square root nature of the singularity at $\theta = \theta_c$. It should be stressed that Eq. (A-2) is only accurate for θ very close to θ_c and that it is necessary, in general, to evaluate $f(\theta)$ numerically.

APPENDIX B: Universal Expressions for Molière Critical Angle

It was pointed out previously¹⁹ that within the impulse approximation the ratio of the Molière critical angle θ_c to the Coulomb critical angle $2\sqrt{b/l}$ is a function of a single parameter $\alpha = \frac{bl}{a^2}$. A similar result obtains for the ratio of the Molière critical impact parameter s_c to the Coulomb critical impact parameter $\sqrt{bl}$. Figure 12 shows a universal graph of these ratios as a function of $2\sqrt{\alpha}$. It is seen that the Molière critical angle is always less than the Coulomb critical angle. The Molière critical impact parameter is usually smaller than the Coulomb critical impact parameter except for a region in which it can be about 1% larger.

The following empirical expressions are found to give these ratios to an accuracy of better than 1%.

$$\frac{\theta_c}{2\sqrt{b/l}} = \begin{cases} 1.0 - 0.24 \sqrt{\alpha} + 0.04 \alpha & 0 < \alpha < 5 \\ 0.799 - 0.091 \ln \alpha + 0.0016 \sqrt{\alpha} & 5 < \alpha < 2500 \end{cases} \quad (B-1)$$

$$\frac{s_c}{\sqrt{bl}} = \begin{cases} 1.0 & 0 < \alpha < 0.1 \\ 1.03 - 0.08 \sqrt{\alpha} + 9.6 \times 10^{-5} \alpha^2 & 0.1 < \alpha < 25 \\ 0.969 - 0.0892 \ln \alpha & 25 < \alpha < 2500 \end{cases} \quad (B-2)$$

where $\alpha = \frac{bl}{a^2}$, that is, the square of the ratio of the Coulomb critical impact parameter to the Thomas-Fermi screening distance. It should be mentioned that the above universal expressions and the results of Fig. 12 for the Molière critical angle and impact parameter

are also valid when the screening distance a is a function of both Z_1 and Z_2 as occurs in both the Firsov and Lindhard screening expressions.

The expressions given in Eqs. (B-1), (B-2) and Fig. 12 cover a very wide range of ion-target combinations and ion energies. The expressions, therefore, are expected to be useful to calculate two-atom critical angles and critical impact parameters which may be used in making estimates in a wide variety of blocking phenomena.¹⁹⁻²⁸

It can also be shown that the ratio $s_c/\lambda\eta_c$ is a function of α only. Here s_c and η_c are related to θ_c by $\lambda\theta_c = s_c + \lambda\eta_c$ (extremum of Eq. 1). It is seen that the radius of the shadow cone $\lambda\theta_c$ consists of two parts: s_c which may be termed the geometric part and $\lambda\eta_c$ the part due to the scattering. Figure 13 shows a universal plot for the ratio $s_c/\lambda\eta_c$ where it may be noted that the two parts become equal in the Coulomb limit ($\alpha \rightarrow 0$). For power law scattering $\eta \sim s^{-n}$ it has been shown by Mashkova and Molchanov^{23,29} that the ratio is simply n . Thus, the graph in Fig. 13 shows immediately what power potential approximates Molière scattering for a given value of $\frac{Z_1 Z_2 e^2 \lambda}{E a^2}$.

APPENDIX C: Compensation

A quantity of interest in blocking phenomena is compensation, that is, to what extent the missing particles from the region $\theta < \theta_c$ of the scattering pattern $f(\theta)$ [Eq. (2a) and Fig. 2] show up as excess particles in the region $\theta > \theta_c$. Here it will be shown that total compensation results for any screened Coulomb scattering whereas Rutherford scattering gives only one-half compensation. The total number of missing particles in the deficit is $\pi\theta_c^2$. The excess of particles between the angles θ_c and θ_m is given by

$$2\pi \int_{\theta_c}^{\theta_m} [f(\theta) - 1] \theta d\theta. \quad (C-1)$$

For any arbitrary screened Coulomb potential the above equation can be integrated and gives

$$\pi \left[\frac{s_u^2 - s_l^2}{\ell^2} - \theta_m + \theta_c^2 \right] = \pi \left[-\frac{s_l^2}{\ell^2} - \frac{2s_u n(s_u)}{\ell} - n^2(s_u) + \theta_c^2 \right] \quad (C-2)$$

where s_l and s_u are the lower and upper roots, respectively, of $\theta_m = s\ell^{-1} + n(s)$ [Eq. (1) in text]. For large θ_m the terms $s_l^2\ell^{-2}$ and $n^2(s_u)$ go to zero, therefore only the term $2s_u n(s_u)\ell^{-1}$ needs to be examined. For any screened Coulomb potential this term goes to zero for large s_u since n goes to zero faster than s^{-1} ; the result is total compensation. For Rutherford scattering, however, $n = b/s$ so that $2s_u n(s_u)\ell^{-1} = 2b\ell^{-1} = \frac{\theta_c^2}{2}$. Therefore, even in the limit of very large θ_m there is only one-half compensation.¹⁸ In contrast, for most cases of Molière scattering over 50% compensation is already achieved when $\theta_m \approx 1.2 \theta_c$. In Fig. 14 the fractional compensation, given by Eq. (C-2)

divided by $\pi\theta_c^2$, is plotted as a function of θ/θ_c for Molière and Rutherford scattering. Here θ_c is computed for each of the curves and, therefore, has a different value for each. The compensation curve for Rutherford scattering is universal. On the other hand, for Molière scattering the fractional compensation for a given θ/θ_c depends on b , a , and λ , although the dependence on these parameters is rather weak.

Although compensation seems difficult or perhaps impossible to demonstrate analytically for the backscattering yield $\chi(\psi)$ of Eq. (6), numerical calculations confirm that total compensation exists for Molière scattering.

APPENDIX D: Approximate Formula for Enhancement

An approximate method for solving Eq. (6) for the enhancement $\chi(\psi)$ will be discussed here. The function $f(\theta')$, which typically has a shape as shown in Fig. 2, is approximated as a Dirac delta-function plus a step function.

$$f(\theta') = \frac{\theta_c}{2} \delta(\theta' - \theta_c) + u(\theta' - \theta_c) \quad (D-1)$$

where

$$u(\theta' - \theta_c) = \begin{cases} 0 & \theta' < \theta_c \\ 1 & \theta' > \theta_c \end{cases}.$$

The magnitude of the coefficient preceding the delta function is chosen to account for all of the particles emitted between the angles 0 and θ_c , that is full compensation. When the above form of $f(\theta')$ is substituted into Eq. (6) the integration over variable ϕ can be performed analytically giving the result

$$1 + \left[\frac{\Delta \ell}{D} \left\{ \int_{s_L}^{s_U} g(s) ds \right\} \right] \quad \psi < 2\theta_c \quad (D-2)$$

$$\chi(\psi) = 1 + \left[\frac{\Delta \ell}{D} \left\{ \int_{s_L}^{s_m} g(s) ds + \int_{s_n}^{s_U} g(s) ds \right\} \right] \quad \psi > 2\theta_c \quad (D-3)$$

where

$$g(s) = 2NDse^{-\pi'0s^2} \left\{ \frac{\theta_c^2}{\sqrt{4\theta_c^2\psi^2 - (\theta_c^2 + \psi^2 - \theta_c^2)^2}} - \cos^{-1}\left(\frac{\theta_c^2 + \psi^2 - \theta_c^2}{2\theta\psi}\right) \right\}.$$

Here s_l and s_u are the smaller and larger roots, respectively, of $\psi + \theta_c = s/l + n(s)$ (Eq. 2) and s_m and s_n are the smaller and larger roots of $\psi - \theta_c = s/l + n(s)$. The scattering angle n is given by Eq. (7); however, a useful approximation is

$$n = be^{-0.6x}(x^{-1} + 0.08 + 0.02x + 0.004x^2 + 0.0009x^3), \quad (D-4)$$

which agrees with the results of Eq. (7) to within 1% in the important range $0.5 < x < 3.5$ and to within 2% for $0 < x < 10$.

In general it is necessary to evaluate the remaining integrals in Eqs. (D-2) and (D-3) numerically. This has been done for 1 MeV He ions backscattered from Pt and the results are displayed in Fig. 14 together with the more exact Molière results for comparison. It is seen that using a delta function plus a step function in evaluating Eq. (6) give enhancements some 50% higher. In fact it is found that results from Eqs. (D-2) and (D-3) are higher for all the cases shown in Figs. 3-10 found by solving Eq. (6) more exactly. Thus it might be expected that the results of this approximate method might agree more closely with experiment than solving the two-atom model exactly. It should be stated that the approximation introduced in Eq. (D-1) for $f(\theta')$ is for the backscattered beam only, since the incoming beam $I_i(\theta)$ (Eq. 2 in text) hitting the backscattered atom is treated correctly throughout.

Finally, an approximate solution to Eq. (D-2) for small ψ is

$$x(\psi) = 1 + \frac{C_1 D^{\frac{n+6}{2(n+1)}_b \frac{5}{2(n+1)}_a \frac{5(n-1)}{2(n+1)}}}{\sqrt{\psi}} \left(1 - C_3 D^{\frac{n}{n+1}_b - \frac{1}{n+1}_a - \frac{n-1}{n+1}_\psi} \right) x$$

$$\exp\left(-C_2 D^{\frac{n+3}{n+1}_b \frac{2}{n+1}_a \frac{2(n-1)}{n+1}}\right), \quad (D-5)$$

where power law scattering ($n \sim s^{-n}$) is assumed. For $n = 1$ (MeV energies)

$C_1 = \pi$, $C_2 = \pi/2$ and $C_3 = 1/2$. For $n = 3/2$ (lower energies) $C_1 = \pi$,

$C_2 = 4/5 \pi$ and $C_3 = 2/5$. The angle ψ is measured in radians.

Equation (D-5) is very approximate in several ways, for instance, the

square root of ψ singularity is a consequence of the delta-function

approximation introduced above. A more exact solution of Eq. (6)

shows that the singularity is logarithmic. Although Eq. (D-5) is not

quantitatively accurate, it does predict qualitatively the enhancement

dependence upon the various parameters.

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Fig. 1. Typical trajectory of an ion in the two-atom model. The ion makes glancing collisions with atom A before and after being backscattered by atom B. The ion exits the solid at an angle ψ which is measured with respect to the surface normal. The scattering angles are not drawn to scale, but are exaggerated for clarity.

Fig. 2. Top diagram: A plot of Eq. (1) for $\ell = 2\text{nm}$. Molière scattering, Eq. (9), is used and $Z_1 = 2$, $Z_2 = 78$, and $E = 1\text{ MeV}$. Lower diagram: two atom blocking pattern (Eq. 2 with $I_0=1$) for above case. Curve a corresponds to ions whose impact parameters are less than s_c and curve b to those greater. Curve c is the sum of a and b.

Fig. 3. Top three graphs: Calculated contributions of three selected atomic layers to the backscattering yield for 1 MeV He ions backscattered from amorphous Pt at depth $D = 5$ nm. It is noted that the point $\psi = 2\theta_c$ depends on ℓ (Eq. 1 and Appendix B).

Fig. 4. Calculated backscattering yield vs angle for 1 MeV He ions from different depths in amorphous Pt.

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Fig. 5. Calculated ion backscattering yield vs depth for different exit angles ψ for 1 MeV He ions from amorphous Pt.

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Fig. 6. Calculated He ion backscattering yield in amorphous Pt vs depth for different ion energies.

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Fig. 7. Calculated backscattering yield in Pt for 1 MeV He ions for different atomic densities (the normal density $N = 66.4$ atoms/nm³ curve is dashed for clarity).

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Fig. 8. Calculated backscattering yield in Pt for 1 MeV He ions for different atomic screening distances ($a = 0.011$ nm is normal).

Fig. 9. Calculated backscattering yield vs depth for 1 MeV He ions for different amorphous solids.

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Fig. 10. Comparison of the two-atom model results with experiment^{1,2} and computer simulations¹⁰ for 1 MeV He ions backscattered from amorphous Pt. The open circles include depth resolution appropriate to the detector used in the experiment.

Fig. 11. Universal curve for the ratio of the Molière scattering angle (Eq. 9) to the Rutherford scattering angle $Z_1 Z_2 e^2 E^{-1} s^{-1}$ as a function of reduced impact parameter s/a (a is the screening distance).

Fig. 12. (A) Universal curve for the ratio of the critical angle (Eq. 1) for Molière scattering to that of Rutherford scattering vs dimensionless parameter (l is the distance between the two atoms).

(B) Universal curve for the ratio of the critical impact parameter (Eq. 1) for Molière scattering to that of Rutherford scattering vs dimensionless parameter. See Appendix B for further discussion of curves A and B.

Fig. 13. Universal curve for the ratio of the Molière critical impact parameter to Molière critical scattering angle times atom separation distance l vs dimensionless parameter. See Appendix B for further discussion.

Fig. 14. Fractional compensation (Eq. C-2 divided by $\pi\theta_c^2$) for Molière scattering and Rutherford scattering as a function of θ/θ_c . See Appendix C for details.

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Fig. 15. A comparison of the calculated backscattering enhancement in the two-atom model for 1 MeV He ions in Pt using the delta function plus step function approximation (Eqs. D-2, D-3) and the more exact method (Molière scattering in Eq. 6).