large, which is to be expected from the essential similarity in the gross features of the spectra of these two modifications. Such a similarity was also noted between cubic and hexagonal modifications of SiC by Spitzer, Kleinman, and Walsh.[22]

[22] W. G. Spitzer, D. Kleinman, and D. Walsh, Phys. Rev. **113**, 127 (1959); W. G. Spitzer, D. A. Kleinman, and C. J. Frosch, *ibid.* **113**, 133 (1959).

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Theory of Electron Backscattering*

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An exact integral equation is derived for the backscattering coefficient as a function of energy and angle. The equation has an approximate symmetry which allows one to determine the conditions under which backscattering will be independent of the energy of the incident electrons. The validity of some approximations is discussed, and a possible method for obtaining numerical solutions is proposed. It is found that small and large-angle individual scatterings are of about equal importance. For those electrons that have lost very little energy, the equation can be solved exactly, and some interesting results are obtained.

1. INTRODUCTION

WHEN a beam of electrons is directed against a thick solid target, many of the electrons stop in the target but some are scattered back out. These are the backscattered electrons.[1] Over the past few years a considerable amount of experimental information has been collected [2–6] and from an empirical point of view there now exists a fairly complete picture of the phenomenon. On the other hand, attempts at a theoretical interpretation of the data[7–10] have been based on rather severe approximations and have met with only limited success. The purpose of this paper is to present a reformulation of the problem which circumvents many, but by no means all of the difficulties which one encounters in trying to treat backscattering through the usual methods of multiple-scattering theory.

Mathematically, the problem can be formulated as follows. Given a uniform, monoenergetic flux of electrons incident on a semi-infinite block of scattering material, what is the energy and angular distribution of electrons that are scattered back out? In order to solve this problem using standard multiple-scattering theory, one must find the distribution function for the electrons at each point within the block. A more economical method would be to obtain an equation for the distribution of backscattered electrons alone, thereby freeing ourselves from the unnecessary task of finding the distribution within the block. In the following section we will derive an integral equation for the backscattering coefficient as a function of energy and angle. An application of this equation to the energy dependence of the backscattering coefficient is given in Sec. 3. Section 4 contains a critical analysis of some

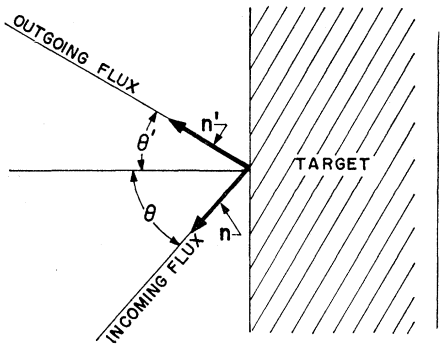

FIG. 1. Kinematics.

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[1] Secondary electrons are also emitted. Experimentally, it is usually assumed that an electron emerging from the target with an energy of more than 50 eV has been backscattered.
[2] E. Stenglass, Phys. Rev. **95**, 345 (1954).
[3] P. Palluel, Compt. Rend. **224**, 1492 (1947).
[4] H. Kanter, Ann. Physik **20**, 144 (1957).
[5] K. Wright and J. Trump, J. Appl. Phys. **33**, 687 (1962).
[6] H. Kulenkampff and K. Rüttiger, Z. Physik **137**, 426 (1954).
[7] H. Bethe, Ann. Physik **5**, 325 (1940).
[8] G. Archard, J. Appl. Phys. **32**, 1505 (1961).
[9] T. Everhart, J. Appl. Phys. **31**, 1483 (1960).
[10] W. Bothe, Z. Naturforsch. **4a**, 542 (1949).

approximate methods along with some interesting numerical results based on the assumption that small-angle scattering is unimportant. Finally, in Sec. 5 we discuss the possibility of more extensive calculations.

2. THE BASIC EQUATION

Given a uniform flux of electrons incident on a plane surface (Fig. 1), we define the backscattering coefficient R to be

$$R(\mathbf{n},E;\mathbf{n}',E')=\frac{\text{outgoing flux per unit solid angle per unit energy interval}}{\text{incident flux}}, \tag{1}$$

where E=incident energy, E'=outgoing energy, $\mathbf{n}$=unit vector *antiparallel* to the incoming direction, $\mathbf{n}'$=unit vector *parallel* to the outgoing direction. One will note that the quantity measured in the laboratory is not R, but $R(\mathbf{n},E,\mathbf{n}'E')\sec\theta\cos\theta'$, where θ is the angle between the $\mathbf{n}$ and the normal to the surface. This is due to the fact that we have assumed a uniform, infinitely broad, incoming beam whereas in the laboratory the incoming beam is confined to a thin pencil.

To derive an integral equation for R, we will follow a chain of thought that has proven to be very fruitful in similar contexts and generally goes under the title of "invariant imbedding." Our application of these ideas will be of the most rudimentary nature. For a thorough exposition of this manner of thinking and its many applications, the interested reader is referred to the review article of Bellman, Kalaba, and Wing.[11] The basic idea is very simple. Suppose we add a thin layer of the same material to the surface of our target thereby increasing its thickness by an amount Δt. Since we have assumed that our target was already infinitely thick, the backscattering coefficient must remain unchanged. If we take the new layer to be differentially thin, this simple device will lead to an integral equation for R.

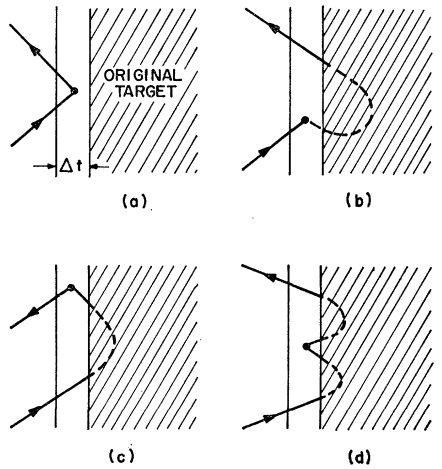

FIG. 2. New paths created by increasing the thickness of the target. The dots represent a single elastic or inelastic collision in the new layer, and the broken lines indicate backscattering in the original target.

[11] R. Bellman, R. Kalaba, and G. Wing, J. Math. Phys. **1**, 280 (1960).

As notational difficulties would tend to obscure the basic simplicity of the argument, we will not follow the derivation in mathematical detail. The reader, if so inclined, can easily fill in the gaps.

Apart from normalization factors, the backscattering coefficient $R(\mathbf{n},E;\mathbf{n}',E')$ is imply the probability that an electron will follow any path which can lead to backscattering from the state $(\mathbf{n},E)$ to the state $(\mathbf{n}',E')$. By adding a layer of scattering material we have created some new paths. These are the paths where the electron makes a collision, either elastic or inelastic, somewhere in the new layer. They are illustrated schematically in Fig. 2. Note that we need not consider paths where the electron makes two or more collisions in the added layer since the probability that an electron will follow one of these paths is of order $(\Delta t)^2$. To calculate the *increase* in R due to fact that we have added some extra paths, we must add up the probabilities that an electron will follow each of the new paths. Referring to Fig. 2 we see that the sum over paths of type (a) is simply a normalization factor times the atomic cross section. Again, apart from normalization factors, the paths of type (b) can be summed by multiplying the atomic cross section for scattering from the state $(E,\mathbf{n})$ to a state $(E'',\mathbf{n}'')$ times the "original" backscattering coefficient $R(\mathbf{n}'',E'';\mathbf{n}',E')$ and summing over all intermediate states $(\mathbf{n}'',E'')$. Paths of type (c) are treated similarly. The sum over paths of type (d) contains the atomic cross section times the square of the "original" backscattering coefficient and a double summation over intermediate states.

Since the total variation in R must be zero, the increase in probability of backscattering due to the increased number of available paths must be exactly cancelled by a decrease in the probability that an electron will follow one of the old paths; i.e., a path along which it makes no collisions in the added layer. It is immediately obvious that the net probability that an electron will follow one of the original paths is decreased since the probability that an electron will pass twice through the new layer without making a collision is less than one. More specifically, the *reduction* in the probability that an electron will follow one of the old paths is simply the "original" backscattering coefficient times the total probability that the electron will make a collision as it passes twice through the new layer.

At this point we make the usual assumption that inelastic collisions with the atomic electrons contribute only to energy loss and do not change the incident electrons' direction of motion. This simplification is not in principle necessary, but it is a very good approximation and has the pleasant feature that the cross sections for angular deflection and energy loss become independent. Combining this assumption with the analysis of the preceding paragraphs, one finds that R satisfies the integral equation

$$\begin{aligned}&[(\sigma_T(E)+\omega_T(E))\sec\theta+(\sigma_T(E')+\omega_T(E'))\sec\theta']\\&\qquad\times R(\mathbf{n},E;\mathbf{n}',E')\\&=\sigma(E,-\mathbf{n}\cdot\mathbf{n}')\sec\theta'\delta(E-E')\\&\quad+\int_{E'}^{E}[\omega(E,E'')\sec\theta R(\mathbf{n},E'';\mathbf{n}',E')\\&\quad+\omega(E'',E')\sec\theta' R(\mathbf{n},E;\mathbf{n}',E'')]dE''\\&\quad+\int[\sigma(E,\mathbf{n}\cdot\mathbf{n}'')\sec\theta'' R(\mathbf{n}'',E;\mathbf{n}',E')\\&\quad+\sigma(E',\mathbf{n}''\cdot\mathbf{n}')\sec\theta' R(\mathbf{n},E;\mathbf{n}'',E')]d\mathbf{n}''\\&\quad+\int_{E'}^{E}\int\int R(\mathbf{n},E;\mathbf{n}'',E'')\sigma(E'',-\mathbf{n}''\cdot\mathbf{n}''')\\&\qquad\times\sec\theta''' R(\mathbf{n}''',E'';\mathbf{n}',E')dE''d\mathbf{n}''d\mathbf{n}''',\end{aligned}\tag{2}$$

where $\sigma(E,\cos\Theta)$ is the atomic cross section for elastic scattering through an angle Θ, $\omega(E,E')$ is the atomic cross section for an inelastic collision leading to an energy loss $E-E'$, $\sigma_T(E)$ and $\omega_T(E)$ are the total elastic and inelastic cross sections, $\sec\theta$ is the secant of the angle between $\mathbf{n}$ and the normal, and the angular integrations run over the hemisphere of unit vectors pointing out of the target. The first term on the right of Eq. (2) is the probability that an electron will follow one of the new paths of type (a). In accord with our assumption that inelastic collisions do not cause angular deflection, we have included only the elastic cross section in this term. The two single integrals are the sum over paths of types (b) and (c) and the triple integral is the sum over paths of type (d). Finally, the left-hand side is the net reduction in the probability that an electron will follow one of the old paths. The geometrical factors $\sec\theta$ are the usual ones which arise because the effective volume of the layer available for scattering into a direction $\mathbf{n}$ is proportional to $\Delta t\sec\theta$. In writing down Eq. (2) we have omitted a factor $\Delta t\times$(number of atoms per unit volume) which multiplies each term as it is of no consequence. Physically, this means that backscattering is independent of the density of the scattering material.

For future purposes it is convenient to write Eq. (2) in the form

$$\begin{aligned}&\int_{E'}^{E}\int[\delta(E-E'')\omega_T(E)-\omega(E,E'')]\\&\qquad\times\sec\theta''\delta(\mathbf{n}-\mathbf{n}'')R(\mathbf{n}'',E'';\mathbf{n}',E')dE''d\mathbf{n}''\\&\quad+\int_{E'}^{E}\int R(\mathbf{n},E;\mathbf{n}'',E'')[\delta(E''-E')\omega_T(E')\\&\qquad-\omega(E'',E')]\sec\theta'\delta(\mathbf{n}'-\mathbf{n}'')dE''d\mathbf{n}''\\&=\sigma(E,-\mathbf{n}\cdot\mathbf{n}')\sec\theta'\delta(E-E')\\&\quad+\int_{E'}^{E}\int[[\sigma(E,\mathbf{n}\cdot\mathbf{n}'')-\delta(\mathbf{n}-\mathbf{n}')\sigma_T(E)]\\&\quad\times\sec\theta''\delta(E-E'')R(\mathbf{n}'',E'';\mathbf{n}',E')]dE''d\mathbf{n}''\\&\quad+\int_{E'}^{E}\int[R(\mathbf{n},E;\mathbf{n}'',E'')[\sigma(E'',\mathbf{n}'\cdot\mathbf{n}'')\\&\quad-\delta(\mathbf{n}'-\mathbf{n}'')\sigma_T(E'')]\sec\theta'\delta(E''-E')]dE''d\mathbf{n}''\\&\quad+\int_{E'}^{E}\int_{E'}^{E''}\int\int R(\mathbf{n},E;\mathbf{n}'',E'')\\&\quad\times\sigma(E'',-\mathbf{n}''\cdot\mathbf{n}''')\sec\theta'''\delta(E''-E''')\\&\qquad\times R(\mathbf{n}''',E''';\mathbf{n}',E')dE''dE'''d\mathbf{n}''d\mathbf{n}''',\end{aligned}\tag{3}$$

where $\delta(\mathbf{n}-\mathbf{n}')$ is the delta function on the unit sphere.

In the remaining sections of this paper we will restrict ourselves to electron energies that are nonrelativistic but large compared to the binding energy of the atomic electrons. This is a permissible limitation since from the form of Eq. (2) it is apparent that for a given maximum value of E and minimum value of E', R does not depend on reflection coefficients whose energy indices lie outside this range. Under these conditions the elastic cross section is simply the Rutherford cross section[12]

$$\sigma(E,\cos\Theta)=\frac{Z^2e^4}{4E^2}\frac{1}{(1-\cos\Theta+\gamma)^2},\tag{4}$$

where γ is the screening parameter. The inelastic cross section can be sufficiently well approximated by[13]

$$\omega(E,E')=\frac{\pi e^4Z}{E}\frac{1}{(E-E')^2},\quad \epsilon_{\max}>E-E'>\epsilon_{\min}\tag{5}$$

where $\epsilon_{\min}$ and $\epsilon_{\max}$ are the minimum and maximum energy losses.[13] For our purposes it is sufficient to know that $\epsilon_{\max}$ is proportional to E and that the usual range-

[12] N. Mott and H. Massey, *Theory of Atomic Collisions* (Oxford University Press, New York, 1949).
[13] M. Livingston and H. Bethe, Rev. Mod. Phys. **2**, 245 (1937).

energy relation is given by[12]

$$\int_0^E \omega(E,E')(E-E')dE' = -\frac{dE}{dx} = \frac{2\pi Ze^4}{E}\ln\left(\frac{2E}{I}\right), \quad (6)$$

where the unit of length has been chosen so that there is one atom per unit volume and I is a mean ionization potential.

In writing down Eq. (3) we have placed the factors in a particular order to bring out the fact that the integrations over energy and angle can be considered as matrix multiplications. This observation leads to a more economical notation and allows us to use the methods of matrix analysis to manipulate the equation. We consider $R(\mathbf{n},E;\mathbf{n}',E')$ as a matrix with two sets of indices, $\mathbf{n}$ and E, and define the following matrices

$$S_B = 4(e^4Z^2)^{-1}\sigma(E, -\mathbf{n}\cdot\mathbf{n}')\sec\theta'\delta(E-E'), \quad (7a)$$

$$S_F = 4(e^4Z^2)^{-1}[\sigma(E,\mathbf{n}\cdot\mathbf{n}')-\delta(\mathbf{n}-\mathbf{n}')\sigma_T(E)] \times\sec\theta'\delta(E-E'), \quad (7b)$$

$$W = (2\pi e^4Z)^{-1}[\delta(E-E')\omega_T(E)-\omega(E,E')] \times\sec\theta'\delta(\mathbf{n}-\mathbf{n}'). \quad (7c)$$

Equation (2) can now be written as

$$WR+RW = (Z/8\pi)(S_B+S_FR+RS_F+RS_BR). \quad (8)$$

Owing to the fact that none of the matrices S_B, S_F, and W commute, Eq. (8) cannot be solved explicitly. We can, however, put it in a more advantageous form. It is a standard theorem of matrix calculus[14] that a formal solution to (8) is given by

$$R = \frac{Z}{8\pi}\int_0^\infty \exp(-Wt)(S_B+S_FR+RS_F+RS_BR) \times\exp(-Wt)dt, \quad (9)$$

which holds provided that the integral converges. To see that the integral does converge one need only consider the physical meaning of the exponentials. Writing the matrix $\exp(-tW)$ in the form

$$\exp(-tW) = P(E,E';t\sec\theta)\delta(\mathbf{n}-\mathbf{n}'), \quad (10)$$

we find that P satisfies the differential equation and boundary condition

$$\frac{d}{d(t\sec\theta)}P(E,E';t\sec\theta) = (2\pi e^4Z)^{-1}\int_{E'}^{E}[\omega(E,E'')-\delta(E-E'')\omega_T(E)] \times P(E'',E',t\sec\theta)dE'', \quad (11)$$

$$P(E,E';0) = \delta(E-E'),$$

from which one easily sees that $P(E,E';t\sec\theta)$ is simply the probability that an electron will suffer an energy loss $E-E'$ while traversing a path of length $t\sec\theta$ where the unit of distance is chosen such that $2\pi e^4Z \times$(number of atoms per unit volume)$=1$. Now for fixed E and E', P tends rapidly to zero for large t and the integral converges. Landau[15] has given explicit expressions for the function P so we now have an equation that can, at least in principle, be solved by successive approximations.

Equations (8) and (9), being quadratic in R, most likely have more than one solution. Obviously the physically interesting solution has the property that, considered as a function of Z, it tends smoothly to zero for small Z. We will now give a heuristic proof that Eq. (9) has a unique solution with this property. Strictly speaking, the atomic screening radius γ and the minimum energy loss $\epsilon_{\min}$ are functions of Z. In the next section, however, we will see that the dependence of R on these quantities is rather unimportant and to a good approximation we can take the matrices S_F, S_B, and W to be independent of Z. With this assumption one can easily see that Eq. (9) has a unique formal solution as a power series in Z. To see that this series is, in fact, convergent we need only observe that an expansion of R in powers of Z corresponds exactly to an expansion in the number of times an individual electron is elastically scattered before leaving the target. Now a large number of scatterings requires a long time spent in the target, but for a given energy loss very long paths are highly improbable. Therefore, for fixed $E-E'$, the coefficient of Z^N must tend to zero for large N and the series converges. Since we have found that (8) has a unique solution which is analytic around $Z=0$, any extraneous solutions must have some singular behavior for small Z.

3. DEPENDENCE ON THE INCIDENT ENERGY

Perhaps the most striking experimental observation is that the number of backscattered electrons and their distribution in energy and angle are, over a broad range of energies, very nearly independent of the incident energy. The first application of our formalism will therefore be to investigate the energy dependence of R. Since the parameters γ and $\epsilon_{\min}$ appearing in (5) are rather poorly known functions of E and Z, our first task must be to see if R is sensitive to moderate variations of these parameters. For fast incident electrons both γ and $\epsilon_{\min}/E$ are very small numbers, generally being on the order of 10^{-3}. In the limit as γ and $\epsilon_{\min}$ tend to zero both the elastic and inelastic cross sections diverge, but one can easily verify that they have the symbolic expansions

$$\sigma(E,\mathbf{n}\cdot\mathbf{n}') = \sigma_T(E)\delta(\mathbf{n}-\mathbf{n}')-e^4Z^2(2E)^{-2} \times\ln(1/\gamma)\delta'(1-\mathbf{n}\cdot\mathbf{n}')+O(1), \quad (12)$$

$$\omega(E,E') = \omega_T(E)\delta(E-E')-2\pi Ze^4E^{-1} \times\ln(2E/I)\delta'(E-E')+O(1), \quad (13)$$

[14] R. Bellman, *Introduction to Matrix Analysis* (McGraw-Hill Book Company, Inc., New York, 1960).

[15] L. Landau, J. Phys. 8, 201 (1944).

where the symbol $O(1)$ has been used to denote finite terms independent of γ or $\epsilon_{\min}$ plus terms which vanish as γ or $\epsilon_{\min}$ tends to zero and we have used Eq. (6) to simplify (13). Referring to Eq. (3) we see that the terms proportional to σ_T and ω_T drop out so the dependence of R on $\epsilon_{\min}$ and γ is only logarithmic.

Upon inserting the cross sections (4) and (5) into Eq. (2), one can verify by a simple change of variables that if $R(\mathbf{n},E;\mathbf{n}',E')$ is a solution so is $\lambda R(\mathbf{n},\lambda E;\mathbf{n}',\lambda E')$ where λ is any positive number, *provided* that one neglects the energy dependence of the logarithms $\ln(1/\gamma)$ and $\ln(2E/I)$ appearing in (12) and (13). When the latter is a good approximation we can apply our uniqueness "theorem" which then yields

$$R(\mathbf{n},E;\mathbf{n}'E')\approx\lambda R(\mathbf{n},\lambda E;\mathbf{n}',\lambda E'). \tag{14}$$

Physically this means that increasing the incoming and outgoing energies in the same proportion will leave the whole backscattering process unchanged, except for a scaling factor which is precisely that needed to keep the integrated coefficient at a constant value.

While it is reassuring to derive this well verified symmetry from theory, it is perhaps more important to investigate the conditions under which it is valid. To begin with, Eq. (14) does not hold unless we can neglect the energy dependence of the logarithms in (12) and (13). Roughly speaking, this requires that the incident energy be greater than the K-shell binding energy of the scatterer. For carbon the K-shell energy is roughly 300 eV and one finds experimentally that the total backscattering coefficient is very nearly constant for $E\gtrsim 500$ eV.[2,3] On the other hand, the K-shell energy of silver is about 25 keV and one indeed finds that the number of backscattered electrons does not become constant until E is on the order of 15 keV.[2,3] A second breakdown of (14) occurs when the angle of incidence is near 90° (Fig. 1). In this case the incoming electrons can take full advantage of the forward peak in the Rutherford cross section which is extremely sensitive to γ. With an incident angle of 80°, Kanter[4] has found that the energy distribution of electrons backscattered from aluminum varies considerably for incident energies between 10 and 70 keV even though the K-shell energy of aluminum is on the order of 1.5 keV. Since backscattering is largest at grazing incidence, this breakdown of (14) for $\theta\approx 90°$ will have a disproportionate effect when the incident flux is isotropic. Formally, Eq. (14) breaks down near $\theta=90°$ because $\ln\gamma$ multiplies an angular derivative which becomes very large when the initial direction is parallel to the surface of the target. Finally, if the relativistic cross sections, rather than those given by (4) and (5) are used in Eq. (2), one finds that the resulting equation has a different dependence on the energy variables and (14) no longer holds. Experimentally[5] one finds that in the relativistic region the backscattering coefficient is not independent of the incident energy, but shows a marked decrease from the nearly constant nonrelativistic value.

4. APPROXIMATIONS

Most theories of electron transport are based on the assumption that electrons lose energy continuously according to the usual range-energy relationship. This is definitely an approximation since energy loss, like angular deflection, is a stochastic process. To determine the accuracy of this approximation when applied to backscattering, we must examine the integrals on the left-hand side of Eq. (3). For simplicity, we will consider only the first integral and assume that the integration over the angular delta function has already been carried out. The inelastic cross section $\omega(E,E'')$ is very strongly peaked near $E=E''$, which suggests that we change the lower limit of integration from E' to zero and, keeping E' fixed, expand $R(\mathbf{n},E'';\mathbf{n}',E')$ in a Taylor series around $E''=E$. The zeroth-order term in the expansion is exactly cancelled by the $\delta(E-E'')\omega_T(E)$ term and the first integral becomes

$$\sec\theta\left[\int_0^E \omega(E,E'')(E-E'')dE''\right]\frac{\partial}{\partial E}R(\mathbf{n},E;n',E')$$
$$-\tfrac{1}{2}\sec\theta\left[\int_0^E \omega(E,E'')(E-E'')^2dE''\right]\frac{\partial^2}{\partial^2 E}$$
$$\times R(\mathbf{n},E;\mathbf{n}',E')+\cdots. \tag{15}$$

According to (6) the first term in (15) can be written as

$$-\sec\theta\frac{dE}{dx}\frac{\partial}{\partial E}R(\mathbf{n},E;\mathbf{n}',E').$$

On the other hand, in the continuous approximation the probability of energy loss per unit path length $\omega(E;E')$ would be

$$(dx)^{-1}\delta[E-E'-(dE/dx)dx].$$

In this case ω_T is simply $(dx)^{-1}$, and upon inserting these expressions into the first term on the left-hand side of (3) and taking the limit $dx\to 0$, one finds that the continuous energy loss approximation is exactly equivalent to keeping only the first term in (15). Since $\omega(E,E'')$ is peaked near $E=E''$, the coefficient of the first term in (15) will be considerably larger than the coefficients of the higher order terms so that dropping these terms will be a good approximation unless R is so rapidly varying that the higher derivatives are large. To estimate these derivatives one must remember that we are considering R as a function of E for fixed E'. Experimentally one finds that for low-Z targets, R is a

slowly varying function and the approximation should be very good but for high-Z targets R changes by an order of magnitude between $E/E'=1$ and $E/E'=2$. A rough calculation indicates that for Z greater than about 40, the second term in (15) can be nearly as large as the first. One cannot, therefore, expect a theory based on a continuous energy loss to give detailed, quantitative results for high-Z materials. This conclusion is in agreement with Monte Carlo calculations carried out by MacCallum,[16] who found that calculations based on the usual range-energy relationship gave the details of the energy distribution of backscattered electrons correctly only for low-Z scatterers.

The easiest way to incorporate this approximation into the present formalism is through Eq. (9). If the energy loss is assumed to take place continuously, the function $P(E,E';t\sec\theta)$ defined in (10) is obviously just a delta function whose argument is determined by the range-energy relation which in terms of t is given by $dE/dt=-E^{-1}\ln(2E/I)$. If we want our solution to obey Eq. (14) we must neglect the energy variation of the logarithm in which case the range-energy relation can be integrated analytically and we find

$$P(E,E';t\sec\theta)=2E'\delta(E^2-E'^2-Ct\sec\theta), \quad (16)$$

where $C=2\ln(2E/I)$. There is, of course, some ambiguity in assigning a numerical value to the "constant" $\ln(2E/I)$. However, one will note that (16) is simply a restatement of the Thompson-Whiddington law[9] and Terrill[17] has found that this simplification of the range-energy relationship is fairly accurate provided that one takes $C\approx 10$. Since one might argue that this value of C is not the proper one to use in backscattering problems, it is interesting to observe that C can be determined directly by studying the behavior of R in the limit $E'\to E$. Clearly an electron which has lost very little energy cannot have spent enough time in the target to have been scattered more than once, which means that in the limit $E'\to E$ the first-order term in an expansion of R in powers of Z is exact. This term can be obtained simply by setting $R=0$ on the right hand side of Eq. (9).

At this point it is convenient to introduce some notation which will be used throughout the rest of this section. Since we will be interested only in solutions which satisfy Eq. (14), it is advantageous to work with the dimensionless function

$$r(\mathbf{n},\mathbf{n}';\xi)=E\cos\theta' R(\mathbf{n},E;\mathbf{n}',E'), \quad (17)$$

where $\xi=E'/E$ and the factor $\cos\theta'$ has been added to facilitate comparison with experimental data. That r is a function only of E'/E follows directly from (14).

Substituting (16) into Eq. (9) and integrating over the delta functions, one easily verifies that to order Z

$$r(\mathbf{n},\mathbf{n}';\xi)=\frac{Z}{4\pi C}\frac{\xi\cos\theta\cos\theta'}{\cos\theta+\xi^2\cos\theta'}\frac{1}{(1+\mathbf{n}\cdot\mathbf{n}'+\gamma)^2}. \quad (18)$$

Taking $C=10$, we find that for $\xi=1$ and $\theta=0$ (normal incidence) r should behave as shown in Fig. 3. The curves are in excellent agreement with the experimental points of Kulenkampff and Rüttiger.[6] One will note that in the limit $\xi\to 1$ it is not an approximation to neglect the energy dependence of the $\ln(2E/I)$ term in the range-energy relation which means that for $\xi=1$ Eq. (18) is, within the approximation of continuous energy loss, exact and C has the unambiguous value of $2\ln(2E/I)$ where E is the incident energy. Since the experimental points were taken at 30 keV, this would yield an ionization potential $I\approx 400$ eV independent of Z whereas one usually takes $I\approx(13.4\text{ eV})Z$. This is indeed a remarkable occurrence for which there appears to be no immediate explanation.

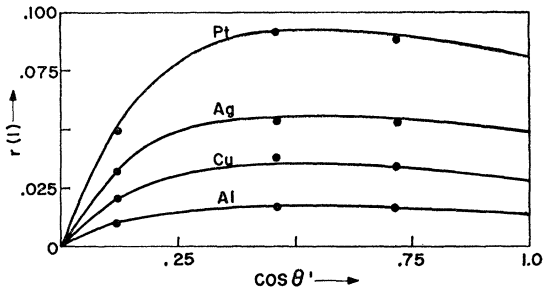

FIG. 3. Behavior of r for $\xi=1$ and normal incidence. The dots are the experimental points of Kulenkampff and Rüttiger (Ref. 6).

Recently there have been attempts to explain backscattering in terms of a single large-angle scattering.[9,10] Since a theory that includes only a single scattering necessarily corresponds to the first term in an expansion of R in powers of Z, it must be exact in the limit $Z\to 0$, and one might hope that it would be valid for low-Z materials of experimental interest. Further motivation for this approach can be found in the fact that for Z between 6 and 40 the total backscattering coefficient for normal incidence is about $0.013Z$ which is suggestive of a first-order term in Z. However, for $\theta=0$, Eq. (18) yields a total coefficient of $[8C]^{-1}[1-\ln 2]Z+0(Z^2)$ which for $C=10$ is about $0.004Z$. Everhart[9] has suggested treating C as a phenomenological parameter which should be adjusted to give the observed backscattering. In view of the accuracy with which Terrill's value reproduces the experimental points at $\xi=1$ this is hardly a permissible procedure. Moreover, the energy distribution of backscattered electrons predicted by (17) is in violent disagreement with experiment so we are forced to the conclusion that a single-scattering theory is not valid for realistic values of Z. Apparently the linear behavior of the total coefficient for low-Z materials is accidental.

[16] C. MacCallum, Bull. Am. Phys. Soc. **5**, 379 (1960).
[17] H. Terrill, Phys. Rev. **22**, 101 (1923).

Having found that a theory based on a single large-angle scattering is not realistic, one might be tempted to go to the opposite extreme and use a small-angle approximation in which one keeps only the forward peak of the cross section. The possibility of constricting a quantative theory of this sort is imbedded in what is perhaps the most interesting question in backscattering theory: Which is the more important, small- or large-angle scattering? One way to answer this question is simply to chop off the small-angle part of the Rutherford cross section, calculate the resulting backscattering coefficient, and compare the results with experiment. We have made a number of such calculations by iterating Eq. (9) in the continuous energy-loss approximation (16). Other motivations for the calculations were the hope that we might obtain quantitative results for low-Z targets and to find out if matrix equations like (9) are suitable for machine calculations. More specifically, we replaced the Rutherford cross section $[1-\cos\Theta+\gamma]^{-2}$ with $[1-\cos\Theta]^{-2}\exp[-b^2/(1-\cos\Theta)^2]$ and iterated (9) starting with $R=0$. As long as Z was not large or b too small, the iterates converged satisfactorily becoming almost constant after about six iterations. However, for large Z or very small b satisfactory convergence could be obtained only for values of ξ close to one. This was due to the fact that the matrix S_F is the difference between two terms which partially cancel each other, and if either S_F or R becomes too large or rapidly varying, the equation becomes numerically unstable. For this reason, the method is not practical for applications of the theory and it would not be worth while to go into the details.

Some typical results obtained for $b=0.1$ are shown in Figs. 4 and 5. While the calculated curves lie considerably lower than the experimental ones, the results are remarkable considering that we have in effect said that if an electron is not scattered through an angle greater than about 25°, it is not scattered at all. Particularly surprising is the fact that the calculated curve for copper is about as close to the experimental one as it is for aluminum, even though the atomic number of copper is over twice that of aluminum. This appeared to be a general trend. Our results for carbon and silver were percentage wise, in about the same agreement as those for copper and aluminum. Apparently the physical reason for this is that the increased probability of small angle scattering in the higher Z materials is being compensated for by the shorter time which a typical backscattered electron spends in the target. One will also note that the relative discrepancy between the calculated and observed curves is larger for $\theta'=83°$ than for $\theta'=43°$. This is to be expected since the points at $\theta'=83°$ corresponds to deflection through a smaller angle, which is more likely to be effected by small-angle scattering. As the cutoff angle was decreased, the calculated points rose towards the experimental values. However, the difference between the curves computed with cutoffs of 25° and 12° was only about 15% which indicates that the bulk of the discrepancy is due to scattering at angles well inside the forward peak of the Rutherford cross section. The conclusion is that quite independently of Z, about half the backscattering arises from a relatively small number of large-angle scatterings, with the remainder being due to the diffusive effects of small-angle scattering. In retrospect, this is not a surprising result since the mean-square scattering angle is on the order of γ so one needs roughly γ small-angle scatterings to deflect an electron through 90°, but about one out of every γ collisions will give rise to a single scattering through an angle greater than 90°.

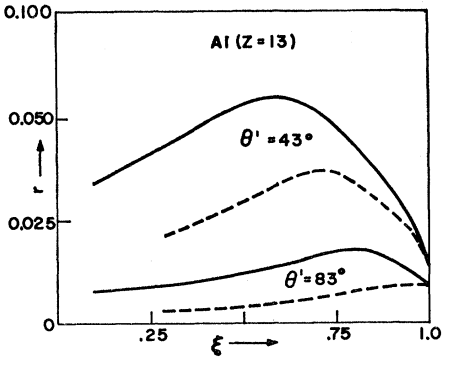

FIG. 4. Results of the cutoff calculations (dashed line) for normal incidence compared with the experimental data (Ref. 6) of Kulenkampff and Rüttiger (solid line).

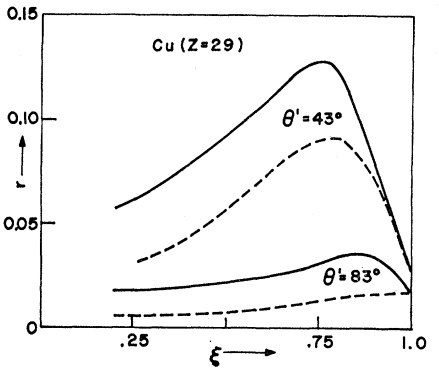

FIG. 5. Results of the cutoff calculations (dashed line) for normal incidence compared with the experimental data (Ref. 6) of Kulenkampff and Rüttiger (solid line).

5. A POSSIBLE METHOD FOR NUMERICAL SOLUTION

The main result of the previous section was that backscattering is a very complicated problem. For one thing, we found that both the forward peak of the scattering cross section and the details of its large-angle tail are important. Also, it appears that for high-Z materials one must include the stochastic nature of energy loss. For these reasons it seems very doubtful that a simplified treatment will ever lead to more than

a crude estimate of the total coefficient. Barring the appearance of an entirely new formalism, if one wishes to make quantitative calculations, he is faced with either resorting to the Monte Carlo method or attempting a numerical solution of one of the present equations. Leaving aside, for the moment, the difficulties arising from the peak in the Rutherford cross section, let us consider some pertinent properties of Eq. (2).

The factors $\sec\theta$ appearing in (2) blow up at $\theta=90°$. Since the laboratory coefficient $R\sec\theta\cos\theta'$ is well behaved at $\theta=90°$ the integrand remains finite. In carrying out our cutoff calculations we approximated the angular integrals with a Gaussian quadrature scheme which avoids the ambiguous points at $\theta=90°$ and found that these apparent divergences caused no difficulty.

Since the problem has rotational symmetry around an axis perpendicular to the target, $R(\mathbf{n},E;\mathbf{n}',E')$ has the property that its average over the azimuthal angle of either $\mathbf{n}$ or $\mathbf{n}'$ is equal to its average over the azimuthal angle of both $\mathbf{n}$ and $\mathbf{n}'$. Using this property, one readily verifies that averaging (2) over the azimuthal angles of $\mathbf{n}$ and $\mathbf{n}'$ yields an equation for the corresponding average of R. The resulting equation is still of the matrix form (8) and the same techniques can be applied to both the full and averaged equations. This procedure will greatly reduce the number of points needed to carry out the angular integrations.

Another simplification arises if the solution is required to satisfy (14). As one would expect, (2) then becomes an equation for the dimensionless function r defined in (17) and the number of energy variables is cut in half. We have pointed out that $R(\mathbf{n},E;\mathbf{n}',E')$ is independent of reflection coefficients whose energy indices are greater than E or less than E' which means that the integral equation for r is of the Volterra type as far as the ξ variable is concerned. One can therefore compute r out to some minimum value of ξ without having to find the function for smaller values of ξ. The validity of forcing R to satisfy (14) is, however, not *a priori* known.

The major stumbling block will, of course, be the strong forward peak in the Rutherford cross section. One will note, however, that the matrix W is also ill behaved, but when it was exponentiated to obtain Eq. (9) its singular behavior ceased to cause any difficulty. The latter equation can be obtained by multiplying (8) from both right and left by $\exp(-Wt)$, noticing that the left-hand side is a total derivative and integrating from zero to infinity. More generally, suppose we take any matrix function $A(t)$ which has the properties, $A(0)=I$ and $A(\infty)=0$, and carry out the same manipulations. One easily verifies that the analog of (9) is then

$$\begin{aligned}
R&=\frac{Z}{8\pi}\int_0^\infty A(t)[S_B+B_1(t)R+RB_2(t)\\
&\qquad\qquad +RS_BR]A(t)dt,\\
B_1(t)&=\frac{8\pi}{Z}\left[-A^{-1}(t)\frac{d}{dt}A(t)-W+\left(\frac{Z}{8\pi}\right)S_F\right],\\
B_2(t)&=\frac{8\pi}{Z}\left[-\left[\frac{d}{dt}A(t)\right]A^{-1}(t)-W+\left(\frac{Z}{8\pi}\right)S_F\right].
\end{aligned}\tag{19}$$

The game is now to choose A so that the matrices B_1 and B_2 are well behaved. The ideal choice would be $\exp[-(W-Z/8\pi S_F)t]$, but from the analog of Eq. (11) one finds that the $(\mathbf{n},E;\mathbf{n}',E')$th element of this matrix is the probability that an electron will be scattered from the state $(\mathbf{n},E)$ to the state (n',E') while passing through a slab of thickness t, provided that one only includes scatterings such that the electron is always traveling into the target. Evaluating this matrix would be as difficult a problem as solving the original equation. On the other hand, the theory of small-angle multiple scattering[18,19] has provided a number of approximate evaluations of this matrix. These approximations are only valid for small-angle deflections, but one will note that this is all that is needed to insure that B_1 and B_2 are well behaved. The scheme is, therefore, to calculate $\exp[-(W-Z/8\pi S_F)t]$ in some tractable small-angle approximation, use this matrix for $A(t)$ in (19), and solve the resulting equation by iteration starting with $R=0$. Any reasonable approximation for the above exponential should remove most of the small-angle scattering from B_1 and B_2, and the successive iterates should converge like an expansion in the number of large-angle scatterings. Our experience with the cutoff calculations described in the previous section indicate that such a series would converge rapidly after about five iterations. Furthermore, any iterative solution to (19) is clearly well behaved for small Z, so if the iterates converge they are guaranteed to yield the correct solution. The author has not investigated the above scheme in detail but preliminary investigations indicate that it may lead to a practical method for obtaining numerical results.

ACKNOWLEDGMENTS

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[18] W. Scott, Rev. Mod. Phys. **35**, 231 (1963).
[19] H. Bethe, M. Rose, and L. Smith, Proc. Am. Phil. Soc. **78**, 573 (1938).