# Explanation for the 180° Rutherford Backscattering Anomaly in Solids

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An explanation is given for the unusual enhancement in the Rutherford backscattering yield at 180° found by Pronko and co-workers. It involves a nonstochastic dependence between inward and outward trajectories of backscattering projectiles. Results are presented of Monte Carlo simulations in random solids which show excellent agreement with experiment without need of considering electronic disturbances induced by the projectiles.

Pronko *et al.*[1,2] have recently reported an unexpected enhancement in the near-surface yield of ~ 1-MeV light ions backscattered from polycrystalline and highly disordered solids within a very narrow angle close to 180° from the beam direction. This enhancement was found to be more conspicuous the narrower the acceptance angle of the detector, and the closer its angular position to 180°, and to increase with depth of penetration of the ions into the solid, pass through a maximum at depths of about 100 Å, and decrease for larger depths.

The purpose of this Letter is to provide an explanation of these surprising observations in terms of a correlation effect between inward and outward paths of the ions in the solid. The tool for this study was a specially developed Monte Carlo simulation technique; we have chosen the case of 1 MeV He on Pt as a working example.

The model for the target consists of a stack of $N_c$ square plane layers of side $L$ (~ 8 Å) separated by a distance $d$. The layers contain $N_a$ atoms distributed at random, but fixed for each trajectory history. The distance $d$ is set equal to $N^{-1/3}$, where $N$ is the number density of target atoms and $L$ and $N_a$ are chosen so that this density is preserved, on the average, over a sufficiently large volume. The projectiles are made to start their motion perpendicular to the first layer at a point with coordinates $x_p$ and $y_p$ chosen at random within a disk of radius $R = 1.5$ Å centered in the layer.

To calculate the trajectories at these high energies it is justifiable to use the small-angle approximation[3]

$$\alpha = C(s)/\epsilon p^s, \tag{1}$$

where we have used the power potential approximation to the Moliere interatomic potential. Here $\alpha$ is the scattering angle, $p$ the impact parameter, and the reduced energy $\epsilon$ and coefficient $C(s)$ are defined by Lindhard, Nielsen, and Scharff.[3]

The scheme of the calculation is the following. Let us assume that the projectile reaches the $i$th layer with coordinates $(x_p, y_p)_i$, and directional components $(\theta_x, \theta_y)_i$. The change in direction after leaving the plane is calculated as

$$\theta_{x,i+1} = \theta_{x,i} + \sum_{j=1}^{N_a} \alpha_j (x_{p,i} - x_{t,j,i})/p_j, \tag{2a}$$

$$\theta_{y,i+1} = \theta_{y,i} + \sum_{j=1}^{N_a} \alpha_j (y_{p,i} - y_{t,j,i})/p_j, \tag{2b}$$

where $\alpha_j$ is the scattering angle given by Eq. (1), and resulting from a collision with impact parameter $p_j$ with the $i$th target atom located with coordinates $x_{t,j,i}$ and $y_{t,j,i}$ in the $i$th layer. The projectile will then reach the $(i+1)$th layer at a point with coordinates

$$x_{p,i+1} = x_{p,i} + \theta_{x,i+1} d, \tag{3a}$$

$$y_{p,i+1} = y_{p,i} + \theta_{y,i+1} d. \tag{3b}$$

The stopping power of the projectiles in each layer, although small,[4] has been included in the simulation for completeness, and the small-angle approximation has also been used in Eqs. (2) and (3). In Eq. (1), we have chosen $s = 2$ since it is a good fit[3] for the screened Coulomb potential for the case under study.

When the last layer of interest at depth $z$ is reached, the projectile is sent back towards the surface with a direction randomly chosen within a cone of $\beta = 1°$ around a direction making an angle of 180° with respect to the direction of motion of the projectile before entering the solid. The trajectories are then followed to the surface in the same way as in the incoming path, and preserve the initial distribution of atoms in each layer. The calculations are then repeated many times with different starting conditions; one finally obtains distributions of projectiles backscattered from depth $z$ into an interval of solid

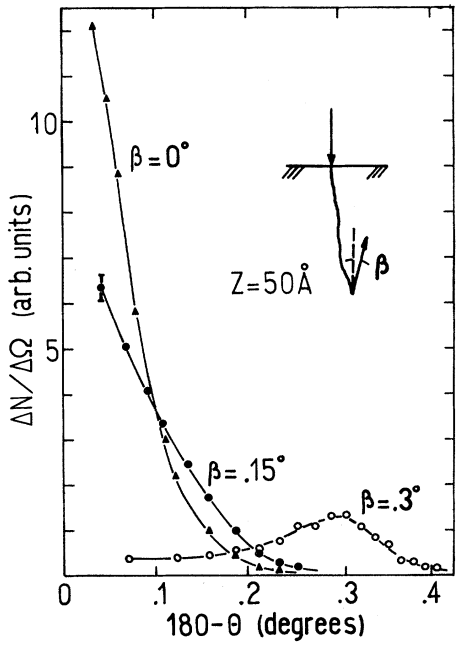


FIG. 1. Angular dependence of the flux of 1-MeV He backscattering from Pt at a depth $z$ = 50 Å and with initial angular distribution $f(\beta') = \delta(\beta - \beta')$. The exit direction is at 180°-$\theta$ from the incident-beam direction and backscattered particles are collected in constant-solid-angle intervals.

angle $\Delta\Omega$ centered at an angle 180°-$\theta$ from the incident direction.

To test for spurious effects we have made simulations increasing the parameters $L$, $R$, and $\beta$ until we were convinced that the specific choices did not affect the results within the inherent uncertainties of the simulation. In all cases a small correction based upon standard multiple-scattering theory was made to take into account contributions from angles larger than $\beta$.

Figure 1 shows angular distributions of particles which have emerged from the solid after undergoing a backscattering event at depth $z$ = 50 Å. In this particular case, the particles start their motion towards the surface within the initial hollow-cone distribution $\delta(\beta' - \beta)d\Omega'$. One can observe that the angular distributions for $\beta \neq 0$ "diffuse" preferentially into the $\theta$ = 0 direction, the more so, the smaller $\beta$ is. The reason for this is that multiple scattering on the way out is not random but it is determined by the particular atomic positions which have been sampled by the incoming ion, favoring outgoing trajectories similar to the incoming one. One must notice, in particular, that for $\beta$ = 0.15°, no

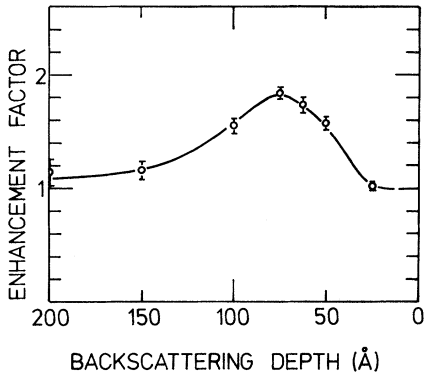


FIG. 2. Enhancement factor $F(\theta)$ averaged over $\theta < 0.2°$, as a function of backscattering depth, and for 1-MeV He on Pt. Bars represent standard deviations in the simulations.

indication of a maximum around $\theta$ = 0.15° is evident in the distribution of emerging particles.

Let us now define the enhancement factor $F(\theta)$ as the ratio of the yields for backscattering at 180° − $\theta$ to the backscattering yield at 180° − $\theta$ with $\theta > 1°$ where the effect shown in Fig. 1 is insignificant. Figure 2 shows $F(\theta)$, averaged over $\theta \leq 0.2°$, versus backscattering depth $z$; it can be observed that $F$ rises very slowly at small $z$ to a well-defined maximum around 75 Å, and then decreases slowly at larger depths. This can be interpreted in the light of the discussion around Fig. 1. $F$ rises slowly at small $z$ since particles at a given $\beta \neq 0$ need a certain number of scattering events to "diffuse" into the reversed incoming track, and then rises faster as the range of $\beta$ values contributing to the enhancement increases. As backscattering depth increases, however, fluctuations in the multiple collisions start to play a role; it will be increasingly more probable that collisions occur more violent than the typical ones, which remove the backscattered particles from the reversed incoming-track region.

The behavior of the enhancement factor with observation angle at $z$ = 75 Å, where $F(\theta)$ is maximum, is plotted in Fig. 3 together with the data of Pronko *et al.*[1] A very satisfactory agreement is found, specially considering that the experimental depth resolution is ~ 100–200 Å and so averages over depth regions where $F$ is below the maximum (Fig. 2). The behavior of $F(\theta)$ in Fig. 3 is just a consequence of integrating the "Green functions" of Fig. 1 over $\beta$.

The good agreement with experiment strongly indicates that the nonstochastic dependence of the incoming and outgoing paths accounts for the

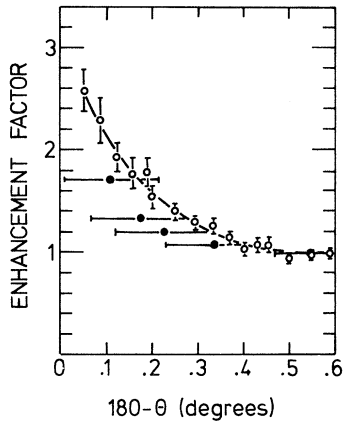


FIG. 3. Enhancement factor $F(\theta)$ as a function of observation angle for 1-MeV He backscattering from Pt at a depth $z = 75$ Å. Open circles, theory; full circles, data (Ref. 1) taken with ~ 100–200 Å depth resolution and representing maximum enhancement factors.

observations of enhanced yields in backscattering at 180° without need to consider neither particular distributions of atoms in the medium (those involving long- or short-range order), nor the electronic disturbances produced by the projectile in its incoming path.

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*Note added.*—After this manuscript was completed the authors were made aware of similar work by O. H. Crawford; see Phys. Rev. Lett. 44, 185 (1980).

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## Observation of Matthiessen's Rule in Strong Magnetic Fields

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Measurements of electrical resistivity as a function of temperature reveal that deviations from Matthiessen's rule (DMR) in aluminum can, under suitable conditions, be made to vanish in a strong magnetic field. Theories explaining DMR on the basis of anisotropic and inelastic scattering predict such behavior suggesting that such scattering is the source of DMR in dilute aluminum alloys at low temperatures.

In this Letter we present evidence for the existence in aluminum of a magnetic field and temperature range in which the electrical resistivity obeys Matthiessen's rule. We believe that is the only known domain in which this holds[1] and that its existence sheds light on the source of deviations from Matthiessen's rule (DMR) in metals.

The number of theories proposed over the years to explain DMR is huge. Bass,[2] in his review article, lists fourteen different *categories* of theories. At present, none of these theories is completely satisfactory for all temperatues and impurity concentrations. If we ignore those theories which invoke changes in the Fermi surface or other such gross effects (they cannot explain the DMR observed in very dilute alloys) the list of proposed low-temperature theories includes those which consider many-body effects,[3] low-temperature phonon drag,[3] interference between phonon and impurity scattering,[4] inelastic impurity scattering,[5] and small changes in the phonon spectrum (see Ref. 2 for a complete list of references). However, the most successful of the recent theories are those which take into account the anisotropy and energy dependence of the electron-phonon interaction.[6] These theories are the