ENHANCED BACKSCATTERING NEAR 180° FOR ENERGETIC IONS IN SOLIDS*

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Summary

A new ion scattering effect which enhances backscattering yields near 180° has been recently reported.¹ A computer program which simulates this scattering effect is discussed and the results compared with measurements. Both the angular distribution and depth profiles of the backscattered yield enhancements are compared. These comparisons verify the proposed explanation for the new scattering phenomena and a tentative explanation is offered for the small discrepancies which exist.

Introduction

Recent research activity at the accelerator facility of the Solid State Division, Oak Ridge National Laboratory resulted in the discovery of a new ion-scattering effect.^{1,2} During the course of experiments involving uniaxial double alignment,³ an anomalously large ion-scattering yield near 180° from the near-surface of solid targets was discovered. The small-acceptance-angle detection of backscattered ions near 180° concomitant to the uniaxial double alignment experimental geometry imposed the unique constraints necessary for the observation of the effect. In Fig. 1 backscattered spectra for 0.8 MeV $^4\text{He}^+$ ions incident upon polycrystalline Cu are shown for two detection geometries. It is immediately obvious that the near-surface scattering yield in the small-acceptance-angle detector near 180° is much enhanced over that of the large-acceptance-angle detector at 160°. Initially the effect was observed in only polycrystalline solids and single crystals that were continuously rotated during spectra acquisition, a procedure designed to simulate the random impact parameter distribution an ion beam encounters in a random solid. This prompted speculation^{1,2} that the effect might be due to some mechanism in crystalline solids which results in uncompensated backscattering yields from channeled ions. Lindhard⁴ in his "rule of angular averages" has shown that any physical process in a single crystal which depends linearly on the spatial distribution of the ion flux, when averaged over external angles, is identical to that of a random solid. Since this averaging is essentially accomplished by the random orientation of the crystallites in a polycrystal or in rotating a single crystal, the backscattered yield in such systems is not normally expected to deviate substantially from that of a disordered solid. However, the detected scattering yield in the uniaxial double alignment geometry, as required by Lindhard's⁴ "rule of reversibility," does not depend linearly upon the flux spatial distribution but rather as the square of the distribution. Therefore, compensation of the scattering yield outside the solid is no longer guaranteed; a circumstance that could account for the observed yield enhancement. Although it was felt that this explanation is qualitatively correct, the nature of the effect was found to be more general as seen in Fig. 2. This figure shows backscattering spectra from a Ge single crystal that was turned amorphous in the near-surface region through a graded-energy P ion implant. Comparison of the substrate aligned and rotating random spectra for both the large- and small-acceptance-angle detection geometries are seen. The spectra in Fig. 2a, which were normalized by current

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Figure 1. Backscattering spectra of 0.8 MeV $^4\text{He}^+$ ions incident upon polycrystalline Cu observed in a wide-acceptance-angle detector at 160° and a small-acceptance-angle detector at 180°.

integration techniques, clearly show that amorphousization of the near-surface was accomplished by the implantation. However, it is clear in Fig. 2b that

Figure 2. Comparison of spectra of 0.8 MeV $^4\text{He}^+$ ions incident upon P implanted Ge with the [100] substrate aligned and while continuously rotated in a (a) wide-acceptance-angle detector and a (b) small-acceptance-angle 180° detector.

the scattering yield in the 180° small-acceptance angle detector from the disordered region is still enhanced. The possibility of uncompensated channeling yields previously discussed is really a manifestation of a much more general mechanism in the ion-solid interaction-the reversibility of ion trajectories. Therefore, it was proposed by one of the present authors⁵ that the reversibility or near-reversibility of trajectories for ions backscattered near 180° introduced correlations between incoming and outgoing trajectories which would favor emergence from the solid, independent of lattice order, near 180°.

This work presents the results of measurements using both helium and hydrogen ions incident upon Pt. Determination of the magnitude and angular dependence of the effect for the various ion-solid combinations was accomplished through detailed angular detector-scans about 180°. Also, the results of computer simulation are presented along with comparisons with experimental data.

Experimental Arrangement

The present work was also done at the 2.5 MeV Van de Graaff accelerator facility of the Solid State Division, Oak Ridge National Laboratory. The experimental arrangement is shown in Fig. 3. As seen in the figure, angular scans were expedited through the use of multiple detectors which acquired spectra for different scattering angles simultaneously. The detectors, which were standard 7 mm² surface barrier detectors, were mounted on a manipulator along with a Faraday cup which was used to initially align the detector array. The detectors were angularly separated in the array by 0.214° and at the lowest vertical position, the angle between the center of the bottom detector and beam center at the target 0.082°.

To prevent carbon build-up on the samples during prolonged exposure to the beam, necessitated by the small acceptance angle of the detectors, various cryopumps were utilized. The beam line between the sample and detectors was pumped using a closed-cycle cryopump. A copper shield surrounded the target that was electrically isolated and cooled to LN₂ temperatures. When biased, this served the dual purpose of pumping the target area and providing electrical suppression for secondary electrons. The pumping maintained an ambient pressure in the target chamber of $\approx 5.0 \times 10^{-8}$ Torr. The sample was mounted on a two-axis goniometer from which it was electrically isolated thus allowing beam monitoring by direct integration from the electron suppressed sample. The spot diameter of the ion beam at the target was 2 mm and had an angular divergence of 0.026°.

Computer Simulation

A computer program was written which simulates the ion-solid interaction in a disordered solid. To allow for the possibility of reversible trajectories, a special feature was incorporated into the program which stores the locations of all atoms that interact with an ion on its incident trajectory. These stored locations are subsequently used as sites for atoms in determining the outgoing trajectory of an ion after backscattering. In determining the trajectories of the ions within the solid, the program treats successive atomic collisions suffered by an ion as independent, binary events. The scattering due to a single event is determined solely by the elastic part of the ion-atom interaction which is given in a Thomas-Fermi approximation by Lindhard⁴ as

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \left[1 - \left(1 + \frac{3a^2}{r^2} \right)^{-1/2} \right] \quad (1)$$

where r is the internuclear separation, $Z_1 e$ and $Z_2 e$ are the nuclear charge of the ion and atom respectively and a is the Thomas-Fermi screening length given by

$$a = 0.8853 a_0 Z_2^{-1/3} \quad (2)$$

where a_0 is the Bohr radius.

A random lattice is simulated in the program by placing all atoms at lattice sites in equally spaced parallel planes within which a two-dimensional square lattice is constructed. For each new incident trajectory the program stacks the planes at random using random number generators. The stacking sequence is repeated for outgoing trajectories to permit reversibility. Since the program computes only the scattering due to the nearest atom approached as an ion passes through a plane, great savings in computational time are realized if the interplanar separation is kept large. Therefore, for each backscattering depth, the program reconstructs the lattice with the interplanar separation maximized subject to the criteria that the lattice constant in the plane exceed ten times the atomic screening length. This construction is constrained such that the atomic density of the simulation solid equals that of the real solid. Although somewhat arbitrary it was felt that the criteria prevented the overlap in the planes within which significant scattering results. No significant variation in the scattering yields was observed using this lattice construction when compared to one in which the interplanar separation was fixed at the intraplanar lattice constant.

In the time elapsed between the passage of an atom

Figure 3. Experimental arrangement.

Figure 4. Calculated angular dependence of the normalized yield of 1.0 MeV ${}^4\text{He}^{++}$ ions backscattering near 180° from three scattering depths in disorder Pt.

in the solid by an ion on its incoming and outgoing trajectory, the atom is not stationary but is in motion as a result of thermal energy in the lattice, as well as recoil energy transferred by the ion during its initial passage. Such disturbances in the media can measurably affect the reversibility of an ion's trajectory. Estimates⁶ have shown nuclear recoil to be dominate. Therefore, to account for this effect, the recoil of an atom is added to its initial location before it is used to determine outgoing trajectories. In the program, the recoiling atom is displaced along the intersection of the scattering plane with the

Figure 5. Comparison of spectra of 0.5 MeV ${}^4\text{He}^+$ ions incident upon Pt backscattered at different angles.

plane within which the atom is located. If an ion is scattered through an angle γ in passing an atom and then travels a distance d before backscattering, the ion finds that the atom has been displaced from its original position a distance

$$d_0 = \frac{2x}{1-x} d\gamma \quad (3)$$

upon its return, where x is the mass ratio of the ion to the atom. As one might expect, the above equation shows that the effect of nuclear recoil increases in importance as the mass ratio x increases.

In Fig. 4 the angular distribution about 180° of the simulation backscattering yield for various scattering depths in platinum is shown. The scattering yields are averaged over a 0.07° angular range and normalized to the normal Rutherford yield (i.e., the yield if correlations between incoming and outgoing trajectories are ignored). The angular dependence of the scattering yield, as shown in the figure, is rather characteristic of the effect for all simulated ion-solid combinations. At shallow scattering depths the enhancement is small but extends over a large angular range. As the scattering depth increases, the yield enhancement increases markedly but the angular extent of the enhancement narrows. This continues up to some critical depth, $\approx 80 \text{ Å}$ in the present case, after which further increases in the scattering depth result in decreasing both the enhancement yields and angular width. Also, it is obvious in Fig. 4 that the yield of ions backscattered at 80 Å shows a deficit region at about $\psi = 0.5^\circ$ and extending beyond the range of the figure. Although statistical fluctuations are large compared to deviations from the normal yield in the region, the deficit seems large enough to compensate for the enhanced yields.

Results and Conclusions

Figure 5 show the backscattering spectra for 0.5 MeV ${}^4\text{He}^+$ ions incident upon polycrystalline platinum for two scattering angles. The influence upon backscattering yields at $\psi = 0.082^\circ$ due to the ion-scattering effect is striking as seen by the substantial difference between the two spectra, especially in the near surface ≈ 0.02 microns. As is evidenced in the figure by the spectrum at $\psi = 1.5^\circ$, spectra for $\psi > 1^\circ$ generally correspond to what is normally expected for backscattering from a thick, elemental target. Computer simulation further confirmed that scattering yields in this region do not deviate substantially from those determined when correlation is ignored. Therefore such spectra were used to

Figure 6. Comparison of the angular dependence of the maximum normalized yield of 1.0 MeV ${}^4\text{He}^+$ and 0.5 MeV ${}^1\text{H}^+$ incident on Pt.

Figure 7. Comparison of the angular dependence of the maximum normalized yield (determined after spectral convolution-see text) of 1.0 MeV $^4\text{He}^+$ ions on Pt with the maximum normalized yield of 0.5 MeV $^1\text{H}^+$ ions.

normalize the enhance spectra. The normalization procedure, which expresses the scattering yield at any given depth as a fractional part of the normal yield from the same depth, removes the details of the normal yield from the spectra leaving only the profile of the yield enhancement.

In Fig. 6, the angular distribution of the maximum normalized yields are shown for both 1.0 MeV $^4\text{He}^+$ and 0.5 MeV $^1\text{H}^+$ ions incident upon platinum. These yields correspond to the peak in the enhanced yield distribution for a given scattering angle. The angular distribution for a given scattering angle. The angular distributions illustrate the narrow angular interval over which the effect persists and how strongly peaked the effect is about $\psi = 0^\circ$ - exact 180° backscattering. As required by the Thomas-Fermi approximation, the elastic scattering of these ions within the solid should be identical since the ratio of the ionic charge-state inside the solid and the ion energy, Z^2/E , is essentially the same for both ions. It was therefore expected that the influence of the effect upon outgoing trajectories would be similar for these ions. However, the maximum enhanced yields are seen to be significantly lower for backscattered protons. Small variations might occur due to the finite mean free path for charge equilibration of

helium ions in Pt or nuclear recoil effects but these are not considered to be sufficient to account for the observed differences. Since the stopping power in the solid for the two ions are significantly different, it was felt that the resultant differences in the spectral depth resolution might be responsible. To test this idea, the depth profiles of the helium scattering data were degraded by convolution with a Gaussian function to reflect the same depth resolution as the proton spectra. The results after the convolution are shown in Fig. 7. It is clear that essentially all differences in the angular scans have vanished so that the expected Z^2/E behavior, consistent with the proposed enhancement mechanism, is verified.

Comparison between computer simulation and experimental results are shown in Fig. 8 for 1.0 MeV ^4He ions incident upon Pt. Figure 8a compares the angular distribution of the maximum normalized yield and Fig. 8b compares the scattering profile of the normalized yield for a fixed backscattering angle. The agreement is seen to be quite good and verifies the proposed explanation as the basic mechanism responsible for the effect without recourse to additional explanations. However it can be seen in the comparison of the depth profiles of the scattering yield that the rate of decay of the enhanced yields is consistently slower for the experimental results. Some preliminary results have shown significant differences in the scattering yields from disordered solids and single crystals continuously rotated. Enhanced yields from the rotated single crystal are generally larger and more persistent in scattering depth. This work may offer an explanation for the observed discrepancy between the present results from polycrystals and the simulation results from random solids.

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Figure 8. Comparison of the results of computer simulation and experiment for 1.0 MeV ^4He ions incident on Pt: (a) angular dependence of the maximum normalized yield and (b) depth profile of the normalized yield for scattering at $\psi = 0.082^\circ$.