Role of reversibility in enhanced ion backscattering near 180° scattering angle

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Computer simulations show that recently measured enhanced ion scattering near 180° originates in the reversibility property of ion trajectories. The simulation results explain the observed angular and depth dependence of the effect and predict a slight deficit in scattering at angles beyond the enhancement region that was not found experimentally. Collision-induced recoils of the target atoms and the depth resolution of the detector each produce sizable reductions in the effect, and their inclusion in the calculations is necessary for satisfactory agreement with experiment. The observed dependence on atomic number of the target is shown to be partly due to the nuclear charge and partly due to the dependence of target-atom recoils on mass. A calculation is also given of an enhancement to be expected under channeling conditions.

Enhanced ion-backscattering yields from the near surface region for scattering angles very near 180° have been reported recently by Pronko, Appleton, Holland, and Wilson.[1,2] The effect occurs in its simplest form for disordered, amorphous, or polycrystalline targets although it also occurs under channeling conditions in single crystals. It was proposed by one of the present authors[3] that this enhancement was a manifestation of the reversibility of ion trajectories in solids. We show that this is indeed the case. Computer simulation of ion trajectories has been used to explore the angular and depth variations of this phenomenon and the effects on it of ion charge and energy and of target-atom charge and mass. Included in our simulations are collision-induced recoils of the target atoms and the depth resolution of the detector, each of which produces a sizable reduction in the calculated values and is necessary for satisfactory agreement with measurements.

For a 1-MeV He ion backscattered from a depth of 10 nm in a solid, the time from entrance until exit is only about 3×10^{-15} sec. Reversibility of the ion trajectories may be interfered with during this very short time by slight motions due to nuclear recoils and thermal velocities of the lattice atoms and by other multiple-scattering effects. The balance between the reversibility and the perturbing scattering effects will determine whether or not the effect occurs and its dependence on the various experimental parameters. The possible influence of nuclear recoils and thermal velocities may be estimated very simply. Consider a 1-MeV He ion that passes within a distance b of a Pt target atom, travels 5 nm further through the solid, is backscattered by another Pt atom, and returns to the vicinity of the first target atom. The first atom will have recoiled a distance of about 0.005 nm for $b = 0.01$ nm and a distance of < 0.0005 nm for $b = 0.1$ nm. During the same period of time the thermal motion of a Pt atom would be $\lesssim 0.0003$ nm. From these estimates, we concluded that motion due to nuclear recoil was likely to be significant for close collisions and that thermal motion probably would not be significant. A second nuclear recoil effect which we believe is less important but which we also include is the kinematic energy loss of the ion in a large-angle-scattering event.

Although some of our work has been done using a computer program based on a random array of atoms, most of our calculations have been done using a simulation program designed primarily to study channeling phenomena.[4] The existing program was adapted to simulate disordered solids by: (i) choosing a suitably random beam direction, (ii) using a large thermal-displacement amplitude, and (iii) causing the backscattering events to occur completely at random in the solid. Individual trajectories were traced to a backscattering event, the exact positions of all atoms near the trajectory were stored, and the path of the ion was traced back out of the crystal using the stored atomic positions. The emerging trajectories were sorted into angular rings according to the angle $\psi = 180° - \Theta$ by which the scattering angle deviates from exact backscattering. In tracing the return path of a trajectory, each ion was started with a small random deviation from the incoming direction. These deviations were limited in magnitude to a few degrees. The results near the limit together with the Rutherford scattering law were used to estimate the contribution from beyond the limit; the contribution of this extrapolation procedure never amounted to more than a few percent. A calculation done using freshly selected random thermal displacements of the atoms in place of the stored positions in tracing the return path of the ion showed no enhancement or deficit of backscattering and confirmed that the program was adequately simulating a disordered solid.

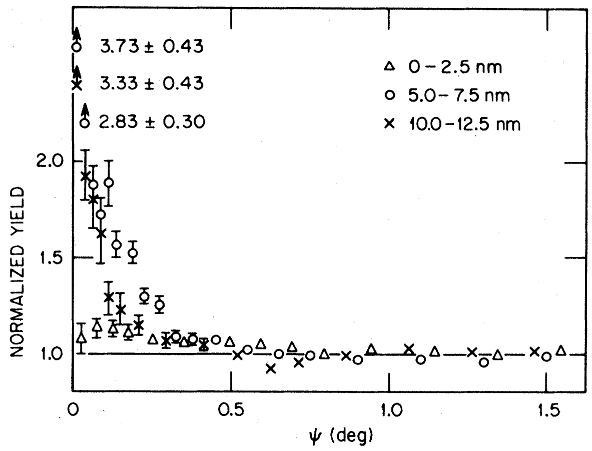

FIG. 1. Calculated angular dependence for three depth ranges of the normalized yield of 1-MeV He ions backscattered near 180° from disordered Pt.

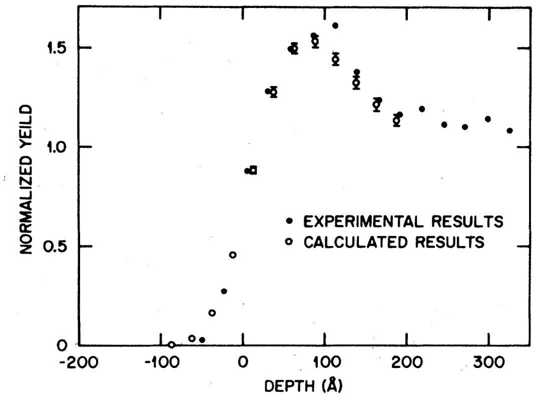

FIG. 2. Depth dependence of the normalized yield from a planar detector at $\psi = 0.11°$ for 1-MeV He ions backscattered from disordered Pt.

Figure 1 shows the backscattering yield calculated for Pt, the material for which we have the most experimental data. The yield is normalized to the Rutherford scattering cross section. The error bars in this and subsequent figures are estimated standard deviations for the statistical uncertainties of the simulation method. The results shown for the three depth ranges summarize the depth dependence of the calculated effect. For shallow depths, the enhancement is modest at even the smallest angles but has a broad extent, apparently beyond the range of the figure. The depth range 5–7.5 nm is the one that shows the maximum enhancement at small angles. Along with greater enhancement at small angles, the angular range of enhancement is narrower (out to $\sim 0.6°$), and there is a yield deficit of 1–2% at larger angles. For the range 10–12.5 nm, the enhancement at the smallest angles remains large, but the angular limit of the enhancement and the angular position of the yield deficit have both moved inward. At greater depths the angular range continues to contract and the peak enhancement falls.

Before making comparisons to the measured results, two features of the experiments were incorporated into the calculations. One was that the small planar detector used in the experiments was circular in shape and spanned a finite angular range. The overlap of this shape with the series of angular rings used to sort the emergent trajectories was calculated at each detector location. Contrary to our expectations the results obtained by incorporating this feature were found to be insensitive to the size assumed for the detector; incorporation of this feature primarily just reduced somewhat the statistical uncertainties at small angles. The second feature was a convolution of the simulation results with the depth resolution of the detector, which was taken to be a Gaussian with full width at half maximum of 8 nm. Principal results of adding this feature are a broadening of the depth range showing enhancement and a noticeable reduction in the maximum enhancement. As will be seen below, proper inclusion of the depth resolution has a sizable effect on the final results. For the detector position showing the maximum experimental enhancement, the agreement of the calculated and measured[2] results for the depth dependence of the enhancement is shown in Fig. 2.

Experimental measurements[1,2] were made at a series of angles, and Fig. 3 shows the angular depen-

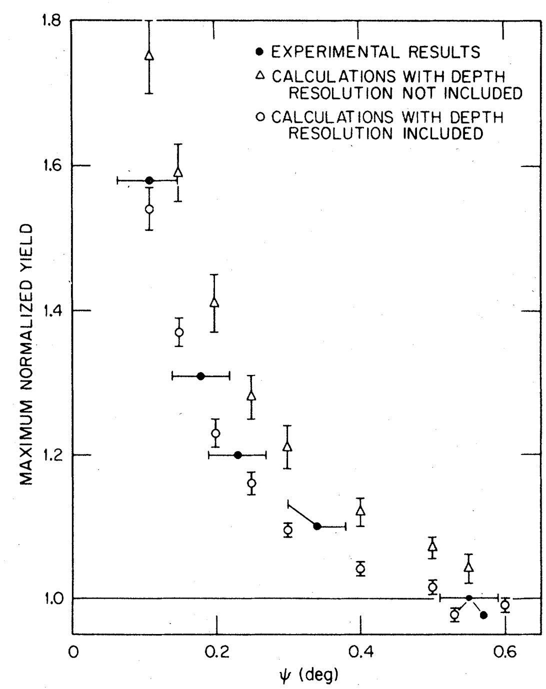

FIG. 3. Maximum normalized yields at various angles for 1-MeV He ions backscattered from disordered Pt.

dence of the experimental and calculated maximum enhancements. The horizontal bars associated with the experimental points are the $\pm 0.04°$ angular range that the planar detector subtends at a point on the target. The calculated values in Fig. 3 show the importance of including the depth resolution. The yield calculated at $\psi = 0.55°$ including depth resolution was 1.00 ± 0.01, confirming the normalization of the experimental data made in Ref. 1. No further normalization should be performed in making the comparison of experimental and calculated values.

We have also done calculations for Al to explore the target-charge dependence and further explore the influence of nuclear-recoil effects. Figure 4 shows the results for the depth range that gave the largest enhancement. The comparison in part (a) of the figure shows that the effect of nuclear recoil is quite large in this case. One expects that the region of enhanced yield must be compensated for by a region of yield deficit at larger angles. To test this in our results, part (b) of Fig. 4 shows a plot of the yield enhancement (or deficit) multiplied by $\sin\psi$, the appropriate weighting factor for the solid angle. The negative area corresponding to the deficit cannot be estimated accurately, but it appears very plausible that the region of yield deficit above 0.25° provides the expected compensation for the region of yield enhancement below 0.25°. It would be desirable to see this predicted region of deficit yield confirmed experimentally, but the observation of a 1–2% effect presents formidable difficulties. The area of the enhancement region in a plot such as Fig. 4(b) may be taken as a measure of the strength of the enhancement. For a plot like Fig. 4(b) for the Al results with nuclear recoil taken into account, the area of the enhancement region is 40–50% less than the area shown in Fig. 4(b). The corresponding reduction for 1-MeV He on Pt is 10–20%.

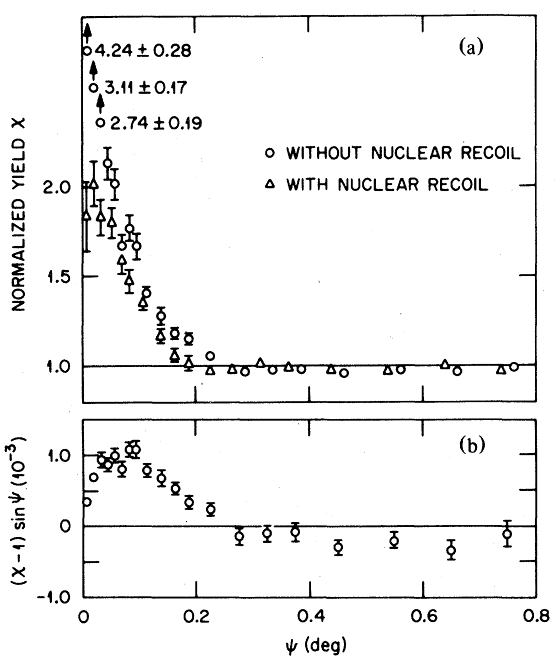

FIG. 4. Calculated angular dependence of the backscattering of 0.5-MeV He ions from depths of 8–12 nm in disordered Al: (a) normalized yield, (b) yield weighted by $\sin\psi$ to assess angular compensation.

For the annular detector used in the experiments,[1,2] which covered the range 0.05–0.20°, the maximum enhancement factor for 1-MeV He on Pt from Fig. 1 is 1.64 ± 0.04 while that for 0.5-MeV He on Al from Fig. 4 is 1.20 ± 0.02. The difference for these two cases is due in about equal parts to the greater influence of nuclear recoil on the Al results and a shrinkage of the angular range of the effect from Fig. 1 to Fig. 4. The different enhancements seen in the Pt and Al calculations are in reasonable agreement with the limited experimental results[2] available on Z_2 dependence.

Some insight into the enhancement effect may be obtained from the two-atom scattering model developed by Oen,[5] the two atoms being the one producing the backscattering and the atom back towards the surface which had the next most important interaction with the ion. This model provides a tolerance of path that allows the outgoing part of a trajectory to deviate slightly from the incoming part and yet emerge very near the beam axis. Also, there would seem to be a range of deficit yield at just about the positions seen in Figs. 1 and 4.

Other simulations have been done to assess the strength of this enhancement under channeling conditions, in particular for the double-alignment surface yield. Results were obtained for 1-MeV He ions incident on Au at room temperature along [110]. We found the single-alignment surface yield to be 2.176 ± 0.003 atoms/row and the uniaxial double-alignment yield to be as shown in Fig. 5. The

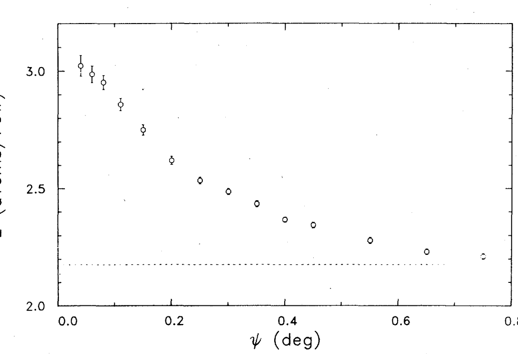

FIG. 5. Calculated uniaxial double-alignment surface yield as a function of deviation from 180° scattering angle for 1-MeV He on Au[011] at 298 K. The dashed line shows the single-alignment surface yield.

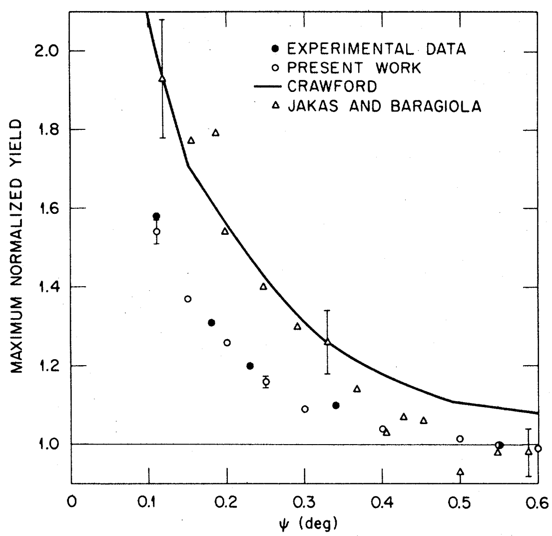

FIG. 6. Maximum normalized yields as a function of deviation from 180° scattering angle for 1-MeV He ions backscattered from disordered Pt.

enhanced surface yield in uniaxial double alignment is due to increased scattering by the atom layers just below the surface layer and hence by atoms that are sensitive to any atomic rearrangements in the surface region.

There have been two other calculations[6] based on the mechanism of Ref. 3. In each case, there was omission of both the effect of recoils of the target atoms due to the passage of the ions and the effect of the depth resolution of the detector. A comparison of all three sets of calculations with the experimental results is shown in Fig. 6. Crawford's results are from his Fig. 3 without the renormalization made in his Fig. 4. As pointed out above, this renormalization is unjustified; it gives a spurious appearance that his agreement with the measurements is better than it actually is. Crawford then goes on to say that his "quite good" agreement with experiment weighs against "invoking the disturbance of the medium by the ion." In Fig. 6, the other two calculations are generally a factor of 2 higher than either the observed enhancements or our calculated values, and the deviations would be even larger for most other ion-target combinations. Neither of the other papers gives any consideration to how the enhancement might depend on energy or atomic number and neither one found the region of deficit yield.

Our computer simulations have shown that the enhanced scattering yield near 180° is a manifestation of the reversibility of ion trajectories in solids. We have found that the calculated results show important dependences on the inclusion of nuclear-recoil effects and on the experimental depth resolution as well as on the ion energy and ion and target atomic numbers. Our calculations have been able to reproduce accurately the observed angular and depth dependences and to give the broad features of the variation with target atomic number. They also show that the effect will be seen under channeling conditions and may provide additional information from measurements of surface structure by ion backscattering.

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