are quoted between 17 and 22 MeV.[11] The bound exciton is 11 meV below the free exciton so that ϵ_{BX} lies between 28 and 33 meV. The binding energy of the hole with respect to the charged impurity can be extracted from Cohen and Sturge[7] as 34 meV. [In the case of an ideal band structure, it corresponds to the term $2\epsilon_{FX}$ of Eq. (1).] This gives, for the energy ϵ_{ei} needed to bind the electron, values between 1 and 6 meV. The calculated energies[12] ϵ_h and ϵ_{eh} for a hole gas and an EHP in pure GaP are shown in Fig. 2, as well as $\epsilon_h+\epsilon_{ion}+\epsilon_{pol}$. $\epsilon_h{}^i(h)$ is obtained by shifting this last curve by ϵ_{ei}. One can then obtain the energy $\epsilon^i(n)$ of an e-h system in the presence of impurities by interpolating between the curve $\epsilon_h{}^i(n)$ up to n_i and $\epsilon_{eh}(n)$. In Fig. 2 we have shown as an example the curve $\epsilon^i(n)$ for $r_i=1.5$ (effective Bohr radius 49 Å). We have used $\epsilon_{ei}=4$ meV and neglected the difference between $\epsilon_{eh}{}^i$ and ϵ_{eh} (r_i being much larger than d_0). Therefore, we conclude that for such an impurity density, the hole plasma is the stablest state and the phase diagram is that of Fig. 1(b).

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[8]The short-range potential V_0 attracts the electrons and so polarizes the EHP. This leads to a second-order correction $\sim U_0{}^2(d_0/r_i)^3\, mr^2/\hbar^2$.

[9]One remarks that, for semiconductors with isoelectronic impurities, the Fisher rule of thumb (M. E. Fisher, private communication) is verified, which says that in order to have two critical points, one needs to have two distinct forces—here the impurity attractive force and the Coulomb force. This was not the case for the Mott transition.

[10]In fact, the EHP density increases slightly above n_0 when n_i increases.

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Origin of the Anomalous Enhancement of 180° Backscattering Yields for Light Ions in Solid Targets

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The origin of the enhancement of the near-surface yield of backscattered projectiles at angles close to 180° for swift light ions in solid targets is shown to be a correlation between outgoing and incoming paths which occurs when an ion scatters by almost 180° in one of its collisions in a solid. The theory does not invoke the crystal structure, or the disturbance of the medium by the ion. Calculations agree with experiment for 1-MeV He^{++} in Pt.

Recent measurements of scattering of H and He ions in amorphous and polycrystalline materials[1,2] have revealed a surprising enhancement of the near-surface yield at angles close to 180°. With the assumption of the usual proportionality of depth to energy loss, the results indicate that the intensity of scattered ions as a function of scattering angle θ, for a fixed depth $\lesssim 700$ Å, has a peak a few tenths of a degree wide at 180°.

We will show that the effect has the following simple explanation. In a case (such as shown schematically in Fig. 1) where a swift light ion scatters from a heavy atom through an angle $180°-\alpha$ sufficiently close to 180° in a single collision, the outgoing path is, by time-reversal symmetry, nearly the same as the incoming one,[3] so that the

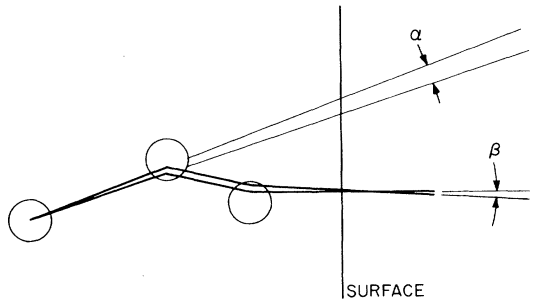

FIG. 1. Ion backscattering at nearly 180°. Schematic.

angle β between entry and exit paths is small, of the order of α. On the other hand, ions which backscatter with larger values of α have less correlation (or none) between their incoming and outgoing paths, and contribute intensity over a range of angles, extending to 180°. The net effect, after summing over α, is an enhancement at small β.

It simplifies the discussion and the calculations to consider an equivalent problem, in which pairs of outgoing trajectories are studied, each pair having a common origin and speed, but with an angle $\alpha < 90°$ between their initial velocity vectors. One such pair is illustrated schematically in Fig. 1, where the angles between the paths, the scattering angles, and the atomic sizes are all exaggerated for clarity. Consider an ensemble of such pairs, with intensity (number of pairs per unit time per solid relative angle) $I_0(\alpha)$. Let $f_l(\beta,\alpha)$ be the probability density of values of the angle β between the final velocities (after traveling a distance l) for a given α. (This probability density is an ensemble average over positions of atoms in the portion of the medium traversed between the origin of backscattering and the surface.) Then the intensity $I_l(\beta)$ of the pairs as a function of β is given by

$$I_l(\beta)=\frac{1}{\sin\beta}\int_0^{\pi/2} f_l(\beta,\alpha)I_0(\alpha)\sin\alpha\, d\alpha. \qquad (1)$$

Now, by time-reversal symmetry of the equations of motion, we may consider (either) one of the paths in each of the above pairs of trajectories as being an incoming path. (We are neglecting energy loss and vibration.) Therefore, if we take $I_0(\alpha)$ to be the number per unit time per unit solid scattering angle of ions scattering through the large angle 180°-α from atoms located at depths between l and $l+dl$, we may identify $I_l(\beta)$ as the corresponding intensity of scattering from the solid, at a scattering angle 180°-β from the incident beam.

Before proceeding, we present preliminary estimates of the magnitude of the enhancement, and of its angular width. Suppose the scattering angle is effectively independent of impact parameter for differences Δb in impact parameter up to r_0, the Thomas-Fermi screening length of the atoms of the medium, but not for $\Delta b > r_0$. Then $f_l(\beta,\alpha) = \delta(\beta-\alpha)$ for $\alpha < \alpha_c = r_0/l$, but the paired trajectories are not as highly correlated for $\alpha > \alpha_c$. Therefore, for small angles, $\beta < \alpha_c$, $I_l(\beta)$ receives a contribution equaling I_0 $[I_0 = I_0(0) \approx I_0(\alpha)]$ from the integration up to α_c in Eq. (1), plus a contribution, ranging from 0 at $l=0$ to I_0 at large l, from $\alpha > \alpha_c$. For angles $\beta > \alpha_c$, $I_l(\beta) \approx I_0$. This argument leads us to anticipate enhancements at $\beta = 0$ ranging from zero for $l=0$, to 100% for large l, with angular widths of about r_0/l. Although not as accurate as the theory presented below, these estimates provide a simple guide to the systematics of the effect.

To test the proposed mechanism, we have computed scattering intensities for 1-MeV He^{++} ions in Pt, evaluating Eq. (1) by a Monte Carlo method. Pronko *et al.*[1,2] went to pains to demonstrate that the enhancement is not associated with channeling or other crystal lattice effects. In the same spirit, we wish our results to be demonstrably free from crystal-structure effects, and even from effects of pairwise correlation of atomic positions in the medium. Therefore, the model used for Pt is a collection of atoms randomly distributed, independently of each other, with a uniform probability density, as in an ideal gas, with the experimental value of the density. The He^{++}-Pt interaction potential is taken to be twice the Moliére potential[4] for protons on Pt.

To simplify the computation, the medium was divided into 6.25-Å-thick layers parallel to the surface, and all the atoms in a given layer were treated as though they lay in the midplane of the layer. This was done so that changes in angle would be computed only every 6.25 Å along the trajectories. Since the mean free path for appreciable change in angle greatly exceeds 6.25 Å, this layering should not affect the results, and this was confirmed by comparing with some intensities calculated using four times the layer thickness.

Intensities $I_l(\beta)$ were computed from Eq. (1) with $I_0 = 1$, using a Monte Carlo method for the integration up to $\alpha = 2°$, and a method described

below for the contribution from $\alpha > 2°$. For the Monte Carlo calculations, a bin method was used, in which the range of β is divided into finite intervals or bins, and each pair of trajectories is assigned to a bin according to its value β_i of angle between the final velocities. The intensity $I_j(\beta)$, averaged over the jth interval, is approximated by the sum, over those trajectories falling in that interval, of $\alpha_{max} \sin\alpha_i / N w_j \sin\beta_i$ where N is the sample size, α_{max} is the upper limit of the Monte Carlo integration, 2°, w_j is the angular width of the jth bin, and α_i and β_i are the angles for the ith pair of trajectories. Except where noted, the bin widths are 0.05° for the first two bins ($\beta \leq 0.1°$), and 0.1° for the rest. The angles α_i are chosen randomly from a uniform distribution from 0 to 2°, and a different random solid is generated for each pair of trajectories. The statistical relative error (standard deviation) of the intensities is approximately 0.07 for the first two bins, and is ≤ 0.03 for the remaining bins.

The contribution from $\alpha > \alpha_{max} = 2°$ is approximated by $2P(\alpha_{max}) - P(\alpha_{max})^2$, where $P(\alpha_{max})$ is the fraction of single trajectories whose final and initial velocities have an angle between them of greater than α_{max}. The derivation of this last expression assumes that (i) $\alpha_{max}/\beta \gg 1$, (ii) two trajectories are not correlated in their scattering if the initial angle α between their velocities exceeds α_{max}, and (iii) $P(\alpha_{max}) \ll 1$. The derivation is based on the result that, in a pair of trajectories with a large α, if the trajectories become nearly parallel, it most likely occurs by one or the other of the trajectories bending by an angle $\approx \alpha$ toward the other one. Angular distributions obtained as a by-product of the Monte Carlo calculation give $P(\alpha_{max})$.

The correlation of trajectories is illustrated in a separate set of calculations for a single value, 0.1°, of α, for 1-MeV He^{++} from a depth of 100 Å. The bins are 0.02° wide. The resulting intensity is shown as the solid curve in Fig. 2. For comparison, the dashed curve shows intensities calculated in the same way, also for $\alpha = 0.1°$, but with no correlation between the scattering processes in the two trajectories of each pair. The chosen value of α, 0.1°, is somewhat greater than the critical value $\alpha_c = r_0/l$ discussed above, which is 0.06°.

As anticipated, we see from Fig. 2 that the in-

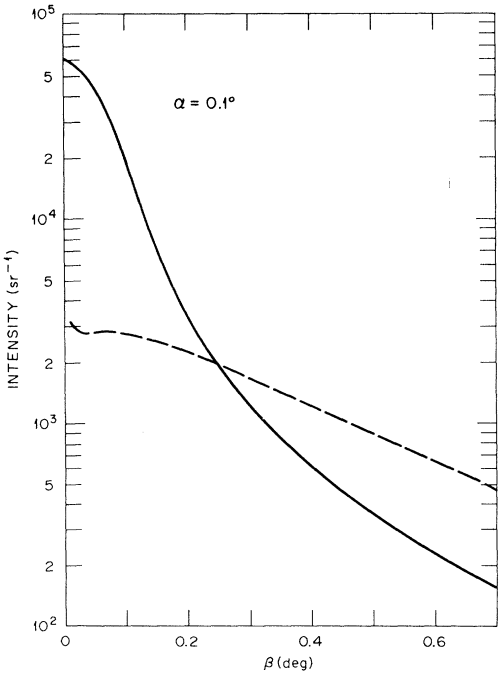

FIG. 2. Calculated backscattered intensity of 1-MeV He^{++} from Pt, arising from scattering by 179.9° at a depth of 100 Å. Solid line, correlated trajectories; dashed line, uncorrelated trajectories.

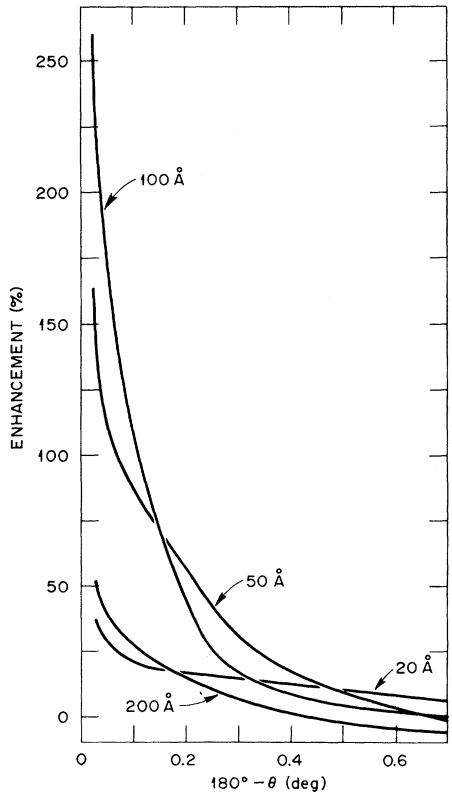

FIG. 3. Enhancement of intensity of scattered 1-MeV He^{++} from Pt, calculated for four different depths.

tensity at small angles is much greater than would be the case for uncorrelated collisions. Moreover, the intensity at $\beta = 0$ is three times that at $\beta = \alpha$. This extra intensity for $\beta < \alpha$ is due to collisional focusing of trajectories. How it occurs is illustrated in Fig. 1, where, in the first collision after leaving the origin, the path with the smaller impact parameter is bent by a larger angle than the other one, sufficiently so to make them parallel. (This is a special case where the focal length for the collision equals the distance from the origin of the trajectories to the atom in question.) This focusing can also be achieved as a cumulative effect of collisions with more than one atom, with path length less than the focal length. The focal length depends on the velocity and the impact parameter. Its value, for a pair of trajectories at impact parameters b and $b+db$, is $(d\theta/db)^{-1}$ where θ is the scattering angle.

The main computed results, the enhancements, given by $I_t(\beta)/I_0 - 1$, are shown in Fig. 3. The angular widths at half-height decrease with depth for 20, 50, and 100 Å, and correspond roughly to the predicted critical values, r_0/l. The 200-Å results appear at first to violate the trend. However, there presumably is a sharp peak of half-width $\approx r_0/l = 0.03°$, which is not resolved in this computation because it is narrower than the width, 0.05°, of the first bin.

We note that the calculated enhancements for 50 and 100 Å for $\beta < 0.1°$ exceed the preliminary estimate (100%) of the maximum enhancement for $\beta = 0$. The discrepancy is due to focusing, which is not incorporated in that estimate.

In Fig. 4 is plotted as a solid line the calculated maximum enhancement, defined as $I_{max}(\beta)/I_{max}(0.55°) - 1$, where $I_{max}(\beta)$ is the value, obtained from the previous figure, of the intensity from whichever depth gives the largest intensity at the given β. The circles are the corresponding experimental results of Pronko *et al.*[1] The agreement between this theory and the experiment is quite good, and supports the proposed explanation for the origin of the effect. The enhancement is therefore seen to originate in the correlation between incoming and outgoing trajectories without invoking the disturbance of the medium by the ion, the crystal structure, or even the atomic pair distribution function of the medium.

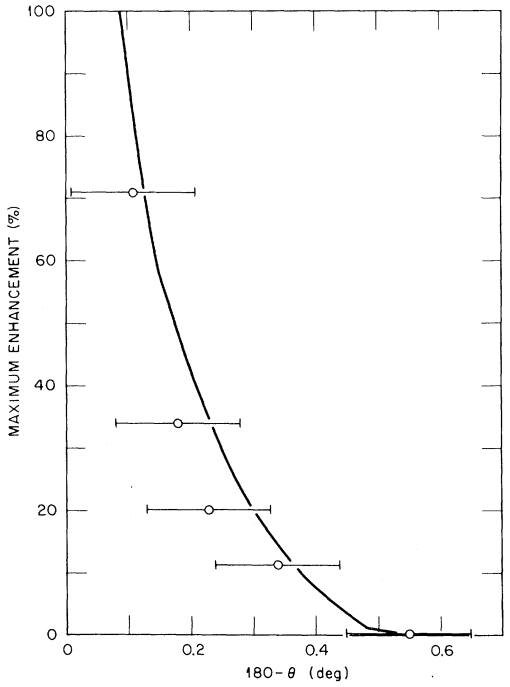

FIG. 4. Maximum enhancement of intensity of scattered 1-MeV He^{++} from Pt, as compared with the maximum intensity at 179.45°. The solid curve is the present theory, while the circles are experimental (Ref. 1) results.

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