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STUDIES OF DEFECTS AND SURFACES BY CHANNELING

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STUDIES OF DEFECTS AND SURFACES BY CHANNELING

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ABSTRACT

Uses of channeling to study defects and surfaces are reviewed briefly with emphasis on ways in which they are currently evolving. Consideration is first given to normalization of yields for channeling directions to the yield for a random direction, this normalization being important to the accuracy of both defect and surface studies. The discussion of atom location concentrates on the use that can be made of quantitative calculations of flux peaking. The treatment of surfaces includes accurate determination of the area of the surface peak as well as basic ways of extracting from experiments information on the positions of surface atoms.

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1. Introduction

When an ion beam impinges on a crystalline solid in a direction parallel to a major row or plane of atoms in the solid, the ions tend to be steered by the rows or planes into the regions between the atoms. This steering effect results in a reduced probability of interaction of the ions with the lattice atoms and has been given the name channeling. Some recent reviews^{1,2)} give general discussions of the field. Since shortly after its discovery, channeling has been used to locate the positions of atoms in solids, and several reviews³⁻⁵⁾ cover this particular application also. More recently, channeling has been used for determining the location of surface atoms⁶⁻¹⁰⁾; most of this work is so new that it is not covered by any review. The present paper will deal with some of the ways in which theory has been used to give quantitative interpretations of experiments on atom location and on surfaces. Channeling theory may be placed in analytical, semianalytical, or computer simulation categories. Completely analytical treatments are extremely difficult to do for realistic models. However, the theory has been developed in a number of cases as far as possible by analytical methods and then carried to completion by numerical methods; several examples of this semianalytical approach are being presented at this Conference¹¹⁾. The computer simulation method^{12,13)} follows a large number of ion trajectories from atom to atom through the solid and is able to extract much the same type of information as is measured experimentally. Although the simulation method involves large computers, complex programs, and large amounts of running time, it is able to incorporate more features of the physical situation than can other methods; consequently it gives the most reliable results. This paper will deal almost entirely with the simulation technique.

2. Normalization to a Random Direction

Before dealing with atom location or surface studies, some consideration will be given to how one normalizes to a random direction, a problem common to both types of study as well as to many other uses of channeling. Since it is extremely difficult to determine absolute yields of large angle Coulomb scattering, nuclear reactions, or other close nuclear encounter processes, it has become customary to express such yields relative to yields measured for a random, or completely unchanneled, direction in the solid. However, because there are so many axial and planar channels in a crystal, it is very difficult to be sure that one is away from the vicinity of all of them. Consequently the question of how one finds a random direction or how one normalizes is important. The complexity involved is illustrated by Fig. 1, which shows some simulation results¹⁴⁾ giving the variation of yield with beam direction. (Simulation calculations can be normalized to a random direction with no difficulty.) The results of Fig. 1 can be adapted with reasonable accuracy to the [011] direction of any face-centered cubic material at any energy by adjusting the angular scales by the factor $(Z_1 Z_2 / E)^{1/2}$ for the other case relative to that factor in Fig. 1 where Z_1 and Z_2 are the atomic numbers of the ions and the target atoms and E is the ion energy. For other directions or other crystal structures, Fig. 1 may serve as a qualitative guide. In the figure, contours for a yield of 1.0 are all in regions where the yield is very sensitive to the exact beam direction. The regions that are not direction sensitive all have yields in the range 1.1 to 1.3. Hence, it is not practicable to select a single satisfactory direction for which the yield is exactly 1. One approach to dealing with the complexities of the situation is to use the yield averaged around the axis at a fixed angle to the axis; such an average¹⁴⁾ is shown in Fig. 2. At angles several times the width of

the dip, the angular-averaged yield is very close to 1; the values of $\bar{P}(\theta)$ at $\theta = 4^\circ$ and 6° are 1.012 ± 0.005 and 1.018 ± 0.003 . This technique for randomization to normal has been used experimentally¹⁵⁾ with ϕ averaged from 0° to 360° and is the best method generally available. Another normalization method is illustrated in Fig. 3, where a series of measurements is compared to a corresponding series of computer simulations. In a previous work⁷⁾, the experimental results shown were normalized to the simulations for the TFM potential, which denotes the fit to the Thomas-Fermi potential made by Molière¹⁶⁾. Normalization was performed by using average values in the range between 1.0° and 1.5° . The normalization methods illustrated in Figs. 2 and 3 are comparable in accuracy. The 360° rotation method has the advantage of not requiring use of a computer simulation program, while the comparison method shown in Fig. 3 is easier to do if such a program is available. This discussion of normalization has been concerned with the beam direction, but the detector direction also deserves consideration. Ideally, the detector would be maintained at a fixed orientation with respect to the crystal. For a limited angular scan such as used in Fig. 3, such an arrangement is feasible, although it was not done in that particular case. For the 360° rotation method, such an arrangement is probably not possible. When the detector direction is not fixed relative to the crystal for either of the methods, some correlated average over beam and detector directions occurs. The effect of such a correlated averaging process is uncertain but one hopes that it is small.

One detail in which the computer simulation with the TFM potential does not agree well with the measurements in Fig. 3 is the width of the (200) planar dip. At the time of the earlier work, it was felt that this did not significantly affect the normalization procedure. More recently, some further simulations have been done to see how details of the electron multiple

scattering and/or ion-atom potential might affect the width. From these new simulation results it appears that use of an alternate electron scattering calculation does not affect the width significantly but that use of an alternate potential does. Figure 3 shows calculations, labelled HFR, in the vicinity of the (200) channel using a fit to the Hartree-Fock potential (excluding exchange effects) made for gold by Robinson¹⁷). Although still not completely satisfactory, the agreement with experiment in the figure is much better for the HFR potential than for the TFM potential. A calculation with the HFR potential in the vicinity of $\psi = 1.5^\circ$ gave a result about $2.0 \pm 1.0\%$ lower than with the TFM potential. Hence, it appears that the choice of potential affects the normalization procedure only to a minor extent. However, the widths of channeling dips seem much more sensitive to the choice of potential, and careful comparisons of measurements and calculations would appear to offer a rather sensitive test of the suitability of a potential for use in doing atomic collision calculations.

3. Atom Location

Positions of impurities in solids can be determined by a careful comparison of the channeling dip seen for backscattering from the impurity to the dip seen for backscattering from the host lattice. The discovery of flux peaking^{18,19}), the phenomenon of a higher flux of channeled ions at the channel center than at channel edges, added the possibilities of more features to be observed than had been realized before. Most position determinations are made by using just qualitative features of the dips, but some have used quantitative features as well. The features observed are the depth and width of the impurity dip compared to that for the host dip and also the possible presence of a peak at the center of the impurity dip or symmetrical

pairs of off-center peaks. One caution with regard to using qualitative features alone is that what appeared to be a classic application of this technique by Picraux and Vook²⁰⁾ to determine the positions of D in W and Cr was later modified by Picraux²¹⁾ as a result of quantitative calculations.

One recent application of channeling to atom location was by Swanson *et al.*^{22,23)} who observed what happened to the Mn atoms in an Al-0.09 at. % Hg alloy which was irradiated at 35-40 K. By making observations for various axial and planar channels, they were able to show that a substantial fraction of the Mn atoms had trapped migrating interstitials and formed mixed Al-Mn dumbbell interstitials. One quantity that could not be determined accurately by them, however, was the displacement of the Mn atom from its lattice site when it had trapped an interstitial. So it was of interest to apply computer simulation to the evaluation of this quantity, and a series of calculations has been done²⁴⁾ to correspond as closely as possible to the experimental conditions for an angular scan through the [011] direction. The main features of this scan of normalized yield vs. angle were a peak at the axis, a valley about 0.5° either side of the axis and a level region beyond about 2°-3° from the axis; these features will be termed the peak, valley, and shoulder regions, respectively. The significant results from the computer simulations are shown in Table 1, which gives the peak-to-valley and valley-to-shoulder ratios as functions of the interstitial fraction and the displacement of the Mn atoms. In the table, it can be seen that the peak-to-valley ratio is a function of the displacement only with no dependence on the interstitial fraction, while the valley-to-shoulder ratio is primarily a function of the interstitial fraction with only a weak dependence on the displacement. This decoupling of the effect of the two parameters greatly eases the problem of determining the displacement and the interstitial fraction from the experimental observations.

In addition to the values shown in Table 1, additional peak-to-valley ratios were calculated for displacements of 1.45 and 1.50 Å and an interstitial fraction of 0.6. From all of the calculated peak-to-valley ratios together with an experimental value of 1.38 from Ref. 23, one may infer a displacement from its lattice site of 1.43 ± 0.05 Å for a Mn atom that has trapped an interstitial. This value for the Mn displacement is much more precise than the value that Swanson *et al.*^{22,23} were able to estimate on the basis of an analytical theory of flux peaking. It is of interest to note that this very large displacement of the Mn atom in the dumbbell is very similar to the situation observed for ^{57}Co in Al by Vogl *et al.*²⁵ using the Mössbauer effect. In Table 1, it may be noted that there is no peak at the center of the impurity dip for a displacement $\lesssim 1.2$ Å. For Ag and Zn in Al in small amounts, experiments^{23,26} show no peak at the center of the impurity dip, which allows an upper limit of about 1.2 Å to be set on the displacement of the Ag and Zn atoms when they trap interstitials.

From the results in the lower part of Table 1, it would seem that one could estimate the interstitial fraction. However, there is a problem with doing that since the calculated values in the shoulder region (2° - 3° from [011]) are 15-20% higher than the experimental ones. The reason for this difference is not known, but one factor might be that the scan plane used for both experiment and theory is within a few degrees of the (422) channel; as can be seen in Fig. 1, this makes the yield in the shoulder region very sensitive to uncertainties in orientation. No attempt will be made to estimate the interstitial fraction, but the present calculations are in reasonable agreement with the value of 0.6 estimated by Swanson *et al.* Absolute values of the interstitial fraction are probably not of as much interest as

absolute values of the displacement; however, changes in this fraction - which are of more interest - can be measured with considerable accuracy.

Virtually all of the work on locating atoms in solids has involved impurity atoms. Impurities appreciably heavier than the host can be studied by large angle Coulomb scattering, and those lighter than the host can be studied by nuclear reactions when suitable reactions are available. One study^{27,28}), however, has been made of self-interstitials in silicon. When looking at a self-defect, no technique can distinguish the defects from the other atoms in the crystal since all atoms are identical to each other. The only feasible method of seeing self-interstitials appears to be double alignment, an arrangement in which the incoming beam is aligned with one channeling axis and the detector with another channeling axis. Alignment of the beam with an axis increases the sensitivity of the measurement to atoms out in the channel relative to the sensitivity to atoms on lattice sites by almost two orders of magnitude, and the detector alignment results in a similar increase. By using both types of alignment together, an experiment should be sensitive to a defect concentration as low as 10^{-3} . Computer simulations have been done for silicon by Morita²⁷) and experiments done by Morita and Carstanjen²⁸) on a silicon sample that had been irradiated with $\sim 10^{17}$ 2 MeV He^+ ions/cm² at random incidence and at room temperature. Their measurements indicated a fractional interstitial concentration of about 5×10^{-3} with the interstitial atoms being about equally divided between hexahedral sites and bond centered sites, the type of site perhaps depending on the charge state of the interstitial. Both the calculations and the experiments involve an extra degree of difficulty for the double alignment configuration, but the results are certainly of great enough importance to justify the effort.

4. Surfaces

Channeling reduces the probability for close encounters of ions with lattice atoms much more in the bulk of the crystal than at the surface so that channeling can be used for surface studies. This relative enhancement of the surface interactions comes about because the steering effect that constitutes channeling requires some depth to make itself felt, which means that the interaction with atoms in the first few angstroms is little affected while interactions deep in the crystal are reduced by as much as two orders of magnitude for a good axial channeling direction. Studies using this effect require very good depth resolution, which means very good energy resolution, in order that the surface peak in the yield versus depth function may be measured accurately. Some of the factors involved in making precise measurements are illustrated by the computer simulation results shown in Fig. 4. The choice of ion, energy, and target was made to correspond to a particular experimental situation of interest^{29,30}). The simulation results as originally calculated drop to very small values 20-30 Å behind the surface peak so that it is easy to separate the surface yield from the subsurface yield. This separation was made before folding in the depth resolution appropriate to the experiments so that the figure shows the total yield curve along with the surface and subsurface contributions to it, all after having the depth resolution folded in. The experimental results resemble the total yield curve, and some technique must be devised to estimate the surface contribution alone. One such technique used by Appleton *et al.*⁷) involves reflecting (or folding over) the left hand side of the surface peak across the depth position of the maximum of this peak; the resulting curve is included in the figure. The scattering from the surface region can be conveniently expressed as being equivalent to a certain number of atoms per row acting as random

scatterers; this quantity can be converted readily to atoms/unit area, effective number of monolayers, or any other units desired. For the particular example in Fig. 4, the fold-over method gives 1.612 atoms/row whereas the exact value is 1.545, an error of 4.4%. Another method that has been used in Refs. 29, 30 and elsewhere is to subtract off a background that is given by a straight line running from zero yield at the position of the surface maximum up to be tangent to the yield curve at a depth just beyond the minimum behind the surface peak ($\sim 200 \text{ \AA}$ for the example in Fig. 4). This method of background subtraction gives a surface peak of 1.561 or an error of 1.1%. For each of these methods of finding the surface peak, only one specific example has been considered, and the size of the error may be different for other experimental conditions. For this one example, the error in each case is reasonably small, particularly so for the background subtraction method.

The main example that will be given here of the use of channeling to study surfaces will be experiments such as those of Davies *et al.*⁸⁾ to measure the relaxation of the surface layer of atoms. In this type of measurement, the beam is aligned with or near a major row direction and the detector is in a random direction. Figure 5 illustrates the principle of the method used. Part (a) of the figure shows a static lattice with all layers spaced the same. For a beam coming in along any row direction, the first atom of that row (which may not be a surface atom) shields all other atoms in the row for many layers below it within its shadow cone. Consequently, scattering from the surface region of the crystal is the scattering from one atom per row. Part (b) of Fig. 5 shows a static lattice with the surface layer having a spacing from the second layer which is different from the bulk interlayer spacing. For a beam incident along the surface normal, the

surface layer would shield all the atoms below as discussed for part (a). However, for incidence along other major row directions, whether or not the other atoms in the row are shielded depends on the energy of the beam; this latter situation is the one depicted in (b). The influence of the energy occurs through its regulation of the size of the shadow cones that the surface atoms cast in the beam of particles. At a low enough energy, the second atom will lie within the shadow cone and there will be scattering from one atom per row. At a high enough energy, the second atom will lie outside the shadow cone and there will be scattering from two (or more) atoms per row. The idea behind an experiment of this type is to seek a critical energy for which the second atom is just on the surface of the cone. Implementation of this idea, however, is complicated by two factors. The first is that the atoms of a solid are not static but are vibrating. The random motion of the atoms is superimposed on the offset produced by the shift Δd in the position of the surface atoms so that there is no unique size of shadow cone that has the second atom on its surface but a distribution of sizes. As a result, there is no energy at which there is a sudden jump of N , the number of atoms per row contributing to the scattering, but rather a smooth rise of N over some range of energies. The second complicating factor is the presence of a shoulder on the outer side of the shadow cone; that is, just beyond the region behind an atom from which ions are excluded by Rutherford scattering, there is a higher probability per unit solid angle for finding an ion than there is at larger angles³¹). The effect of this shoulder when combined with the effect of the thermal vibrations is to shift the energy range over which N rises from 1 to 2 towards lower energies. In the analysis of their experiments, Davies *et al.* assumed that there is no appreciable shift of the sort just mentioned and that the smearing effect of thermal vibrations is to

transform the critical energy from the energy at which a sudden jump occurs into the energy at which $N = 1.5$. By this method of analysis, they arrived at a value of $\Delta d = 0.31 \pm 0.05 \text{ \AA}$.

Simulation calculations were done to correspond to the experiments of Davies and co-workers. A Debye temperature of 236 K was used; at 40 K, this gives $\rho = \langle x^2 + y^2 \rangle^{1/2} = 0.043 \text{ \AA}$. Figure 6 shows the simulation results for incidence along [011] together with the experimental results for this direction. Also shown in the figure are the simulation results for just the first two atoms in the row along with a two-atom calculation done by Oen³²⁾ using the same method as in his earlier calculation of a blocking pattern³¹⁾. The two-atom calculations are accurate up to values of N ranging from about 1.25 on the $\Delta d = 0$ curve to about 2.0 on the $\Delta d = 0.3$ curve. Two-atom calculations could be used to interpret the experimental results if only two of the three experimental points are used; the results are essentially the same as those obtained by using all three experimental points and the simulation results. Davies *et al.* used only the point at 0.5 MeV in determining Δd . From that point and the simulation results, one would deduce a value of 0.25 for Δd . Using the full simulation results, the other two points also yield a value for the relaxation. From all three points together, it may be estimated that $\Delta d = 0.22 \pm 0.03 \text{ \AA}$. The error limit assigned here is based primarily on the scatter that the experimental points would have about a $\Delta d = 0.22$ curve. It is also possible²⁴⁾ to use the experimental results for beam incidence along [112] to make an estimate of Δd , but it is less accurate than the [011] estimate.

There are two aspects of the lattice vibrations that have not been incorporated into the present calculations. These are the larger vibrational amplitude that surface atoms have in comparison to bulk atoms (the Debye

temperature used was the bulk value) and the correlations that exist between the vibrations of neighboring atoms. The effect of including larger surface vibrations would be to shift the curves in Fig. 6 somewhat to the left together with some changes of shape. The effect of the correlations would be to shift the curves in the opposite sense. These two effects will have competing influences on Δd , but the surface vibrations will probably predominate. Hence, the estimate given above may be a few hundredths of an angstrom too large. Exact calculations of these effects would be very worthwhile.

This value of Δd deduced for the (111) surface of Pt is in disagreement with the results of low energy electron diffraction measurements³³⁾, which indicate that $\Delta d \lesssim 0.1 \text{ \AA}$. Davies *et al.* have determined that they have oxygen adsorbed on their surface and have speculated that this may be the source of the difference. Additional measurements under conditions where the oxygen is not present, as they are planning to do, are clearly highly desirable.

Double alignment has been applied to measurements of surface relaxations by Turkenburg *et al.*^{9,10)}. Although no double alignment simulations have been done, single alignment simulations can tell us something about the method used to interpret the double alignment experiments. The method used by Turkenburg and co-workers assumes that the atom at the end of a row is the only atom in that row which contributes to scattering from the near surface region. The experiment makes an angular scan of the detector across one major row direction while the incoming beam is aligned with another major row direction. The position of the center of the blocking dip seen in the detector scan is used to infer the value of Δd . When more than just the first atom is contributing to the scattering, the analysis is more complex. Single alignment simulation calculations can indicate the contribution to be expected for atoms in the row other than the first. Double alignment measurements have

been made for Cu and for Ni. In the Cu results^{9,10}), the surface layer seems to be positioned exactly in accord with the bulk spacing. In a case such as this with $\Delta d = 0$, scattering from more than one atom in the row should not affect the interpretation. Hence, it is of more interest to consider the case of Ni, for which Δd was found to be non-zero¹⁰). Calculations for this case²⁴) are shown in Table 2; a Debye temperature of 389 K was used, giving $\rho = 0.101$ Å at 289 K and 0.080 Å at 173 K. The two axes for which results are given in Table 2 are the two directions along which the incoming beam was channeled in different parts of the experiments. In the experiments, the energies used were 165 and 200 KeV, and the temperature was 298 K. For the experiments with the beam incident along a $\langle 314 \rangle$ direction, the contribution from atoms in the row other than the first appears to be near the threshold for causing concern about the interpretation of the experiments. This concern could be removed by using a lower energy or a lower temperature. For the experiments with the beam along $\langle 011 \rangle$, the contributions from atoms beyond the first cause serious concern about the method of interpretation. It appears that both a lower energy and a lower temperature would be needed to remove this concern. The situation may be further complicated, just as it is in the single alignment case, by the effects of surface vibrations and by correlations. Clearly, care needs to be exercised in choosing the experimental conditions if the analysis of the double alignment experiments is to be sound.

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References

- 1) D. S. Gemmell, Rev. Mod. Phys. 46 (1974) 129.
- 2) D. V. Morgan (editor), *Channeling* (Wiley, N.Y., 1973).
- 3) J. A. Davies, Chap. 13 in Ref. 2.
- 4) S. T. Picraux, *New Uses of Ion Accelerators*, (ed. J. F. Ziegler; Plenum, New York, 1975) Chap. 4.
- 5) H. D. Carstanjen, Proc. 2nd Int. Conf. on *Ion Beam Surface Layer Analysis*, Karlsruhe, 1975 (eds. O. Meyer, G. Linker, and F. Käppeler; Plenum Press, New York, 1976) v. 2, p. 497.
- 6) E. Bugh, Chap. 15 in Ref. 2.
- 7) B. R. Appleton, D. M. Zehner, T. S. Noggle, J. W. Miller, O. E. Schow, III, L. H. Jenkins, and J. H. Barrett, Proc. 2nd Int. Conf. on *Ion Beam Surface Layer Analysis*, Karlsruhe, 1975 (eds. O. Meyer, G. Linker, and F. Käppeler; Plenum Press, New York, 1976) v. 2, p. 607.
- 8) J. A. Davies, D. P. Jackson, J. B. Mitchell, P. R. Norton, and R. L. Tapping, Phys. Lett. 54A (1975) 239, and Nucl. Instr. and Meth. 132 (1976) 609.
- 9) W. C. Turkenburg, W. Soszka, F. W. Saris, H. H. Kersten, and B. G. Colenbrander, Nucl. Instr. and Meth. 132 (1976) 587.
- 10) W. C. Turkenburg, thesis, University of Amsterdam, 1976 (unpublished).
- 11) See the papers by J. A. Ellison and S. T. Picraux; H. H. Ohtsuki, T. Omura, and U. Tanaka; and N. Matsunami, T. Goto, and N. Itoh.
- 12) J. H. Barrett, Phys. Rev. B 3 (1971) 1527.
- 13) D. V. Morgan, Chap. 3 in Ref. 2.
- 14) T. S. Noggle and J. H. Barrett, phys. stat. sol. 36 (1969) 761.
- 15) For instance, see the paper by P. Blood, L. C. Feldman, and G. L. Miller at this Conference.

- 16) G. Molière, Z. Naturforsch. 2a (1947) 133.
- 17) M. T. Robinson, Phys. Rev. B 4 (1971) 1461.
- 18) B. Domeij, G. Fladda, and N. G. E. Johansson, Rad. Eff. 6 (1970) 155.
- 19) J. U. Andersen, O. Andreasen, J. A. Davies, and E. Uggerhøj, Rad. Eff. 7 (1971) 25.
- 20) S. T. Picraux and F. L. Vook, Phys. Rev. Lett. 33 (1974) 1216.
- 21) S. T. Picraux, Proc. 2nd Int. Conf. on *Ion Beam Surface Layer Analysis*, Karlsruhe, 1975 (eds. O. Meyer, G. Linker, and F. Käppeler; Plenum Press, New York, 1976) v. 2, p. 527.
- 22) M. L. Swanson, F. Maury, and A. F. Quenneville, Phys. Rev. Lett. 31 (1973) 1057.
- 23) M. L. Swanson and F. Maury, Can. J. Phys. 53 (1975) 1117.
- 24) J. H. Barrett, Proc. 4th Conf. on *Scientific and Industrial Applications of Small Accelerators*, Denton, Texas, 1976 (eds. J. L. Duggan and I. L. Morgan; IEEE Conf. Record #76CH1175-9 NPS, 1976) p. 571.
- 25) G. Vogl, W. Mansel, and P. H. Dederichs, Phys. Rev. Lett. 36 (1976) 1497.
- 26) M. L. Swanson, F. Maury, and A. F. Quenneville, Proc. Int. Conf. on *Applications of Ion Beams to Metals*, Albuquerque, N.M., 1973 (eds. S. T. Picraux, E. P. EerNisse, and F. L. Vook; Plenum Press, New York, 1974) p. 393; M. L. Swanson, L. M. Howe, and A. F. Quenneville, phys. stat. sol. (a) 31 (1975) 675.
- 27) Kenji Morita, Rad. Eff. 28 (1976) 65.
- 28) K. Morita and H. D. Carstanjen, Rad. Eff. 28 (1976) 97.
- 29) R. A. Zuhr, L. C. Feldman, R. L. Kauffman, and P. J. Silverman, paper given at this Conference.
- 30) L. C. Feldman, R. L. Kauffman, P. J. Silverman, R. A. Zuhr, and J. H. Barrett, Phys. Rev. Lett. 39 (1977) 38.

31) O. S. Oen, Phys. Lett. 19 (1965) 358.

32) O. S. Oen, private communication.

33) L. L. Kesmodel and G. A. Somorjai, Phys. Rev. B 11 (1975) 630.

Table 1

Computer simulation results for the backscattering of 1 MeV He ions from Mn in Al-Mn interstitials at 40 K.

	Interstitial Fraction	Displacement (Å)			
		1.2	1.4	1.6	1.8
<u>Peak</u> Valley	0.4	.98	1.34	1.50	1.94
	0.6	.98	1.34	1.50	1.95
	0.8	.98	1.34	1.50	1.96
<u>Valley</u> Shoulder	0.4	.38	.38	.40	.40
	0.6	.60	.61	.64	.65
	0.8	.86	.87	.92	.97

Table 2

Computer simulation results for the probability P_n of H ions interacting with the n-th atom in a row when channeled along row directions in Ni. All results are accurate to within 0.01 or less.

$\langle hkl \rangle$	T (K)	E (keV)	P_1	P_2	P_3	$P_{\geq 4}$
$\langle 314 \rangle$	298	200	1.00	0.18	0.01	0
		100	1.00	0.05	0	0
		50	1.00	0.02	0	0
	173	200	1.00	0.05	0	0
		100	1.00	0.01	0	0
		50	1.00	0	0	0
	298	200	1.00	0.63	0.25	0.08
		100	1.00	0.38	0.06	0.01
		50	1.00	0.15	0	0
$\langle 011 \rangle$	173	200	1.00	0.45	0.09	0.01
		100	1.00	0.19	0.01	0
		50	1.00	0.04	0	0

FIGURE CAPTIONS

- Fig. 1. Contour plot of the yield of radiation damage relative to the yield in a random direction for 60 MeV I ions in Au. [011] and several important planes containing it are shown. (Taken from Ref. 14.)
- Fig. 2. Plot of $\bar{P}(\theta)$, the average damage rate relative to a random direction, as a function of θ , the angle from [011]. The average performed was over ϕ from 0° to 90° in Fig. 1. (Taken from Ref. 14.)
- Fig. 3. Comparison over a range of orientations of measured yields with yields from computer simulations. The range of orientations is shown in the insert in the lower right hand corner; ψ is the angle from the (200) channel. The measured values have been normalized to those from the simulations in the manner explained in the text.
- Fig. 4. Computer simulation yield curves with a gaussian depth resolution of $130 \text{ \AA}$ FWHM for 2.0 MeV He ions incident along [001] onto W.
- Fig. 5. Schematic illustration in two dimensions of the effect of relaxation of the surface layer of atoms in a static lattice on the near-surface scattering of ions incident along a major row direction.
- Fig. 6. Effective number of atoms per row contributing to backscattering of He ions incident along [011] onto a Pt (111) surface at 40 K; experimental values are from Ref. 8.

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Fig. 2

Fig. 3

Yield curves for 2.0 MeV He on W [001]
with a depth resolution of 130 Å FWHM

Fig. 4

Fig. 5

Effective Number of Atoms per Row Contributing to Backscattering of ^4He Ions Incident Along [011] onto a (111) Pt Surface at 40 K ($\rho = \langle x^2 + y^2 \rangle^{1/2} = 0.043 \text{ \AA}$).

Fig. 6