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NOTES

Dynamics of ion channeling at low energies: Nonnormal incidence

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In a recent paper[1] we described our initial investigations of ion channeling in an energy regime which is sufficiently low that the conventional dynamical picture of such a process is of questionable validity. Indeed, our calculations tend to support the experimental findings of Panitz,[2] who obtained a noticeably structured penetration depth profile, as opposed to the strongly bimodal but otherwise featureless result predicted by Lindhard's[3] analysis (which is known to reflect well the ion dynamics at higher energies). Furthermore, we have suggested experiments which might elucidate the particulars of the ion–solid interactions, forces which are in general rather poorly understood at the present.

As an extention of that initial study[1] (hereafter I), an examination has also been made of the extent to which the calculated distribution of ion penetration depths and backscattered ion energy spectra are altered by small rotations of the angle of incidence of the ion beam away from the surface normal. One should certainly still expect to see a significant number of channeled ion trajectories just on the basis of the fact that at high temperatures the critical acceptance angles are known to be inversely proportional to the ion's velocity. Thus, acceptance angles of 10° or so would hardly be surprising. What is not clear is the extent to which the more detailed characteristics of the channeling process, e.g., the analyses indicated above, display an incidence angle dependence. If such a dependence should be very strong even for the gross features of the various distributions, then one may find practical limits placed on experimental measurements, with the uncertainties being related to the beam collimation errors.

The present calculations were performed in essentially the same manner as were those described in I. In fact, the only change made was in the way in which the initial x and y coordinates of the ions were chosen. Instead of the regular grid of points selected previously, we this time chose coordinates which were randomly distributed over the surface unit cell. Again our system consisted of 80 eV deuterons impinging upon a (110) tungsten crystal face, the adjustable potential parameters being taken as $K_{el} = 0.7$ and $K_{inel} = 0.135$ (eV)$^{1/2}$/Å. Inasmuch as we saw in I that the gross features of the penetration depth profile and the backscattered ion energy spectrum were given quite accurately using a rather modest potential summation, such a truncated direct summation method was used again in this study. The angles of incidence investigated here were (2°, 0°), (4°, 0°), (6°, 0°), (8°, 0°), (4°, 30°), (4°, 60°), and (4°, 90°). [The angle notation used throughout refers to the pair of angles (θ, ϕ), where θ represents a rotation away from the surface normal in the y–z plane and ϕ represents an azimuthal rotation in the x–y plane.] For each set of angles a total of 400 trajectories were generated.

In Table I we have listed the mean ion penetration depths and standard deviations for the sets of trajectories described above. [The displayed results for

TABLE I. Parametrization of the penetration depth distribution.

θ	ϕ	$\langle z \rangle^{a}$	σ
2°	0°	16.3	9.2
4°	0°	15.5	9.0
6°	0°	14.6	7.9
8°	0°	14.0	7.6
4°	30°	15.5	8.3
4°	60°	15.7	8.3
4°	90°	15.9	8.9
0°	0°	18.1[b]	9.6

[a]Units correspond to a W(110) interlayer spacing.
[b]Results calculated in I (adjusted as indicated in the text).

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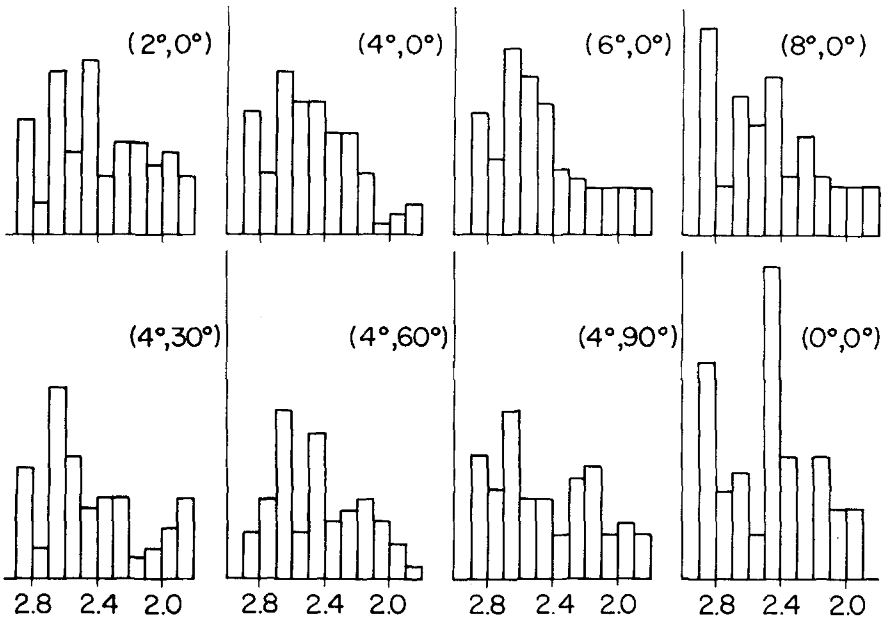

FIG. 1. High-energy portions of backscattered ion energy spectra for given incidence angles (θ, ϕ). Energies shown are in hartrees (1 hartree ≅ 27.2 eV), while the intensities are normalized such that the total backscattered ion flux is a constant.

(0°, 0°) are for the distribution obtained in I except that the trajectories directed precisely along the [110] channel axis have been removed. It is clear that since these particular points of incidence are associated with much longer range penetration than are other points on the lattice cell, and that since there is a vanishingly small probability that these special points will be chosen in a random selection of initial conditions, their penetration ranges must be subtracted from the results obtained with a regular point grid in order that a realistic comparison may be made.] Note that one observes a modest yet definite trend toward smaller mean penetrations as the angle θ is increased. Such an effect is not seen, however, upon making an azimuthal rotation. Overall, one is led to conclude that it is well within the capability of experiment to yield adequate depth profiles (and hence values of K_{e1}) as long as only the gross features are of real interest.

A greater sensitivity to changes in the angle of incidence may be seen in the backscattered ion energy spectra, the high-energy portions of which are given in Fig. 1. (The spectra have been normalized to a constant total backscattered flux for comparison purposes.) Most notably, one finds an apparent lack of structure in the nonnormal incidence spectra as compared with the one for normal incidence. Such a result is really not surprising when one remembers that normally incident ions on the average spend less time (i.e., they have shorter path lengths) in the vicinity of the surface than do those at nonzero incidence angles. Thus, these latter ions are more likely to yield a broadened, "washed-out" backscattered energy spectrum. One consequently must, it seems, do a very good job of ion beam collimation if experimental energy spectra are to be of much value as an analytic probe of ion–solid interactions.

Hence, the conclusions of this note are twofold. First, channeling *per se* is much less sensitive to the angle of incidence of the ions at these low energies than it is in the high-energy regime; a plot of mean penetration versus θ should consist of a series of broad peaks with maxima occurring at those angles corresponding to alignment with a major crystallographic axis rather than sharp spikes. The second point, however, is that the backscattered ions do display a significantly greater sensitivity to the incidence angle, thereby suggesting that their energy spectrum may be somewhat harder to characterize experimentally than is a depth profile. With these comments in mind, one can now proceed to an investigation of the analytic uses of ion channeling in surface and adsorbate structure problems as was suggested in I.

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