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Influence of electronic energy losses on atom ejection processes

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Two independent computer simulations models establish that when ions bombard solid targets, electronic energy losses by atoms within the collision cascade have greater influence on the ejected atom yield than the ion's electronic losses. This conclusion is independent of the ion's mass or energy, or the mass ratio.

The ejection of atoms from metal surfaces by ion bombardment has been studied in great detail, both theoretically[1] and by computer simulation,[2] but relatively less attention has been paid to the effects of "inelastic energy losses," energy removed from atoms of the collision cascade by electronic processes as described by the electronic stopping power, S_e, in Lindhard-Scharff-Schiott theory.[3] Robinson and Torrens[4] were aware of the importance of the cumulative effect of small electronic energy losses by atoms, but Robinson's study of the self-sputtering of U (Ref. 5), which also contains an examination of inelastic effects, did not distinguish the effect reported here because the ions and atoms are identical.

The theory of the quantitative influence of S_e on the total atom yield has not been worked out in detail.[6] Andersen and Bay[7] voice the consensus among many workers in the field that these processes will significantly reduce the atom yield for light bombarding ions, and show that existing experimental data can be interpreted in this way. This does not preclude the possibility that the experimental data will support alternative conclusions.

To the extent that it exists at all, the analytic theory has been worked out on the assumption that the inelastic losses of the atoms can be neglected.[6] This conclusion is not well justified, because the relative magnitude of S_e vs S_n, the nuclear stopping power, at low atom energies has not been studied in detail.[6]

Even the direction of the inelastic loss contribution has not been determined. For light ions and moderate ion energies, inelastic effects have been presumed to decrease the atom yield.[1,7] On the other hand, the suggestion has been made that atom associated inelastic effects might increase the atom yield at intermediate ion energies because such losses would decrease the velocity of primary knock-on atoms, thereby increasing the total energy deposited in the surface region of the target. The problem is further compounded because all experimental data may contain contributions from inelastic effects.

Simulations can make a useful contribution in this situation because inelastic effects can be added, or suppressed, in a computer model. Results of a simulation study of the inelastic energy-loss dependence of atom ejection are reported here. The simulations establish that electronic energy losses by the low-energy atoms of the cascade have greater influence on the atom yield than electonic losses by the ions. This conclusion is independent of the ion's mass, the mass ratio, or the ion's energy.

Four cases are compared: (a) No inelastic losses, designated (0,0); (b) inelastic loss terms are included for both the ions and atoms, designated (1,1) (this case is closest to the experimental situation); (c) only inelastic terms for the atoms are included, designated (0,1); and (d) only inelastic terms for the ions are included, designated (1,0).

A simulated Cu(111) target was bombarded with 3.0-keV inert gas (He, Ne, Ar, and Xe) and B ions. Standard Moliere ion-atom potential functions were used,[8] and a compound Moliere-Morse function was used for atom-atom interactions.[2] The Lindhard-Scharff inelastic loss model[3] was assumed because it is easy to implement and produces a large effect. In it

$$\frac{dE}{dx} = -Kv = -NS_e \ ,$$

with

$$S_e = 8\pi e^2 a_0 (Z_1^{7/6} Z_2 / Z)(v/v_0) = (K/N)v \ ,$$

and

$$Z = (Z_1^{2/3} + Z_2^{2/3})^{3/2} \ .$$

The symbols have their usual meanings. Even if this electronic stopping power model does not correctly describe all aspects of the inelastic process, the conclusions of this study are representative of any loss model having losses proportional to the particle velocity.

The four cases for each system were run on ODYN, the Naval Postgraduate School continuous-time–multiple-interaction simulation program, and on a discrete-event simulation, TRIM.SP, the TRIM version adapted to follow the motion of recoil atoms.[9] Results are presented as sputtering yield ratios

$$R(i,j) = Y(i,j)/Y(0,0) \ ,$$

where the $Y(i,j)$ are the computed yields for cases described above.

Figure 1 shows the sputtering yield ratios as functions of the ion/atom mass ratio. For these systems, one immediately sees that inelastic losses affect the yield ratio for a wide range of systems, not only light ions. Detailed examination of the completed output in each case indicates that other characteristic results are practically indistinguishable with and without losses. In all systems, except He, the (1,0) ratio is around 0.7–0.8; that is, inelastic effects reduce the computed yield by approximately 20%. The other two curves show that the atom losses, (0,1), contribute almost all of the change, while the ion loss contribution, (1,0), to the change is much smaller. The effect is almost independent of the mass ratio, and does not depend on the simulation model chosen.

The variations of the yield ratios with K are shown in Fig. 2. This figure also indicates the yield-ratio variation with the electronic stopping power S_e, because, once the velocity

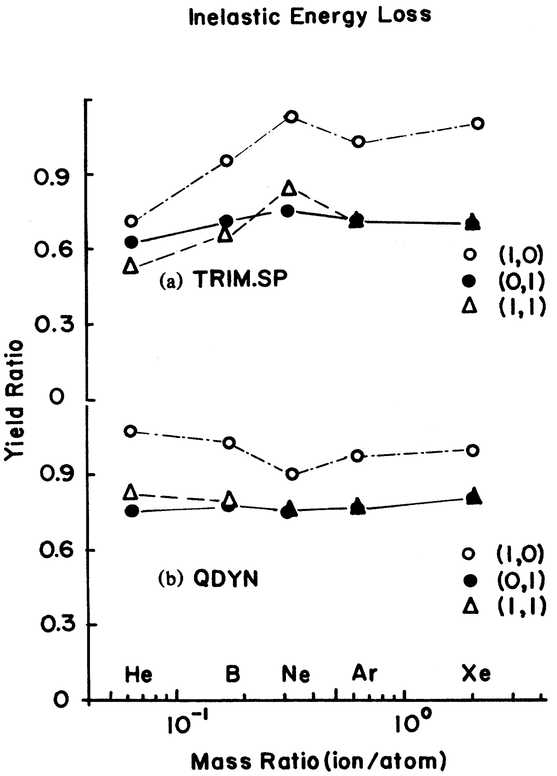

FIG. 1. (a) The yield ratios obtained from the QDYN simulation. The ratios calculated including inelastic energy losses for the atoms (0,1) and for ions and atoms (1,1) are very similar, while those calculated with ion losses alone differ little from the lossless results. (b) The same calculations done with TRIM.SP. Except for He ions, the dependence is similar in the two simulation models.

dependence is segregated, $K \propto S_e$. This is a further indication of the relative importance of ion versus atom inelastic losses. QDYN produces similar results, but because the QDYN computation requires a thin target, which might influence the outcome, only the TRIM.SP results are shown. Although the range in K values is not large, these curves seem to indicate that a direct relation may exist between $1/S_e$ and the ejected atom yields.

Results are reported here for intermediate energy ions,

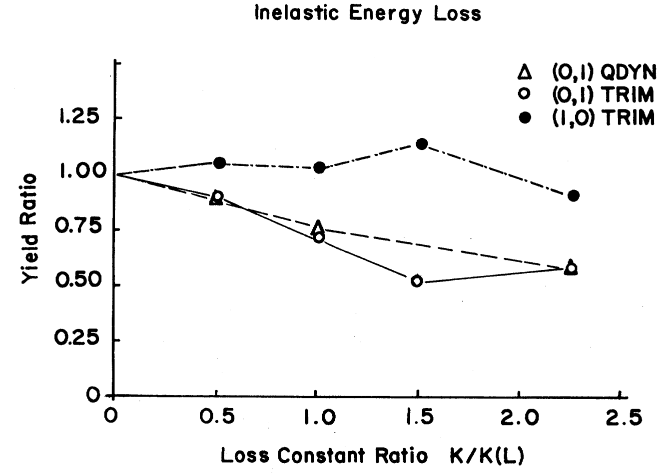

FIG. 2. Dependence of some TRIM.SP and QDYN ratios on K, the inelastic energy-loss constant. The ion-loss case (1.0) values remain near 1.0 over a range of K/K(Lindhard) values which spans the plausible K values. In both simulations, the atom loss ratios (0,1) decrease monotonically as K/K(Lindhard) increases, indicating that the effect exists, no matter how the value of k is chosen.

3.0 keV, but runs at higher energies show that the effect is universal. Tests with other ion-atom systems are similar. The findings are not an artifact of the single-crystal targets used in QDYN, because the TRIM.SP results are computed for amorphous targets. All QDYN runs of this series were made on face-centered-cubic target materials, but past experience indicates that the effect will not be sensitive to the target geometry.

To summarize, the results of this study do not support the assumptions on which existing theoretical analyses are based, or the conclusions reached by Andersen and Bay; in particular, see Fig. 4.39 of Ref. 7.

A forthcoming paper reinterprets the experimental data, and discusses the implications of these findings for collision cascade theory.

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