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Computer simulation of back sputtering and ion penetration into polycrystalline targets

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Abstract. In the present work computer simultations of the back sputtering of low energy neon ions with low impact parameter and the penetration of the same for higher values of the impact parameter have been performed. Initial ion energies in the range 100 to 500 eV and impact parameters in the range $0 < p \leq 0{\cdot}61$ Å have been used. Assuming a binary collision model and for the interatomic potential the Leibfried-Oen matching potential, we compute the complete collision cascade. For Ne^+–Cu interaction, the sputtering threshold energy is found to be 125 eV and the sputtering yield increases with the ion energy. The sputtering yield versus ion energy is plotted and is found to agree well with experiment. It is seen that the back scattering is confined to small impact parameters justifying the use of the binary collision model.

Keywords. Computer simulation; back sputtering; ion penetration.

1. Introduction

When a solid surface is bombarded with energetic ions or atoms, some of the atoms from the surface of the target are ejected or ' sputtered ' out. This is known as ' back sputtering ' by the ion beam. Back-sputtering is generally observed for low impact parameters of the incoming ion when greater part of its energy is transferred to the struck atom resulting in back scattering leading to back sputtering of the atom from the surface of the target. For higher values of the impact parameter, the incident ion retains a greater part of its energy after the first collision and penetrates into the target undergoing a cascade of collisions. Sputtering does not occur until the energy of the incoming ion is sufficiently great as to displace the atoms in the surface layer of the target. Displacement requires that a certain energy E_d called the displacement energy be transferred to a lattice atom during a collision. We consider the detailed progress of the incoming ion through a solid. After the first collision of the incoming ion with the target atom, one gets two moving particles. After the Nth collision 2^N particles are generated. The history of all the particles in the collision cascade which received an energy greater than E_d, the displacement threshold are followed up. If the energy of the ion falls below E_d, then it is considered to have stopped. When an atom reaches the surface with an energy greater than the surface binding energy, it is sputtered out.

Sputtering studies have recently become important in connection with the sputtering of the first wall in a nuclear fusion reactor contributing to the sputtered impurities in the plasma. The estimation of the wall sputtering for different wall materials can be

easily done by means of computer simulation based on a convenient mathematical model of the physical experiment.

The sputtering effect at a solid surface is determined by the sputtering yield S, i.e. the average number of target atoms leaving the bombarded surface per incident ion. Section 2 deals with the simulation of the sputtering process and gives a brief outline of the mathematical model employed here. The next section gives the results and discussions.

2. Simulation of the sputtering process and the mathematical model

We consider low energy neon ions in the energy range 100 to 500 eV with impact parameters in the range. $0{\cdot}0 < p \leqslant 0{\cdot}61$ Å incident on polycrystalline copper target. In this energy range only elastic collisions take place.

In the simulation the incident neon ion undergoes collisions with the target atom and is then back sputtered or undergoes further collisions with the target atom and is then back sputtered or penetrates into the target. The following assumptions have been made:

(i) A random distribution of target atoms
(ii) Only two-body elastic collisions are considered
(iii) A target atom can only be knocked out if the energy transfer is greater than E_d, the displacement threshold energy. For copper E_d is 25 eV.
(iv) A target atom which has reached the surface can leave the target only if it has sufficient energy to overcome the surface potential. The surface potential E_d is assumed to be 5 eV.

For the interaction potential we use the Böhr potential

$$V(r) = \frac{E_B a_B}{2r} \exp(-r/a_B) \tag{1}$$

where

$$E_B = \frac{2Z_1 Z_2 e^2}{a_B}, \quad a_B = \frac{a_0}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}} \tag{2}$$

and

$a_0 = 0{\cdot}529$ Å, radius of the first Böhr orbit in a hydrogen atom.

For a head-on-collision the distance of closest approach R_0 is given by

$$V(R_0) = E_R \tag{3}$$

where E_R is the energy of relative motion.

$$E_R = \left(\frac{A}{1+A}\right) E \text{ and } A = \frac{M_2}{M_1},$$

M_1 and M_2 being the masses of the primary and struck particles respectively and E the primary energy. We have

$$R_0 = 2R = \frac{ka_0}{(Z_1^{2/3}+Z_2^{2/3})^{1/2}} \log \frac{Z_1 Z_2 e^2}{2R\, E_R} \tag{4}$$

where R is the hard sphere radius and k is an adjustable parameter.

The displacement mean free path λ_d in the hard sphere approximation is given by

$$\lambda_d = \frac{1}{n\pi (2R)^2} \tag{5}$$

where n is the number of target atoms per unit volume.

The range (Holmes and Leibfried 1960) of the incident energetic particle may be easily estimated in terms of the mean free paths and scattering angles:

$$\text{Range} = \lambda_d + \lambda_1 \cos\phi + \lambda_2 \cos\phi \cos\phi' + \ldots \tag{6}$$

where the λ's are the mean free paths and ϕ, ϕ', etc., are the scattering angles of the incident particle at each collision. Similarly the projected range for any of the struck atoms along the direction of the normally incident particle may be easily estimated.

Range=Initial depth of the particle from the target surface+the projected range. When the range thus estimated is equal to zero or is equal to the thickness of the target, we consider the energy of the atom. If it is equal to or greater than the surface binding energy, the atom is sputtered. The sputtering yield, that is the number of atoms sputtered per incident ion, is computed.

In this analysis we compute the impact parameter of the incident ion or any of the struck atoms at each collision while tracing the cascade of collisions. This is done as follows:—

The real potential is the Böhr potential as given by (1). One method of obtaining simple analytical expression for the impact parameter is to replace the real potential $V(r)$ extending to infinity by an approximate cut off potential $V_m(r)$ which matches V as well as possible. We use a truncated matching potential of Leibfried and Oen (1962):

$$V_m (r < C) = B\,(C/r - 1)$$
$$V_m (r \geqslant C) = 0 \tag{7}$$

B and C are constants which may be easily found by matching the potential given by (7) to the real potential (1).

When the primary is projected at the target atom, under the influence of the interatomic potential, it is deflected from its trajectory through a centre of mass angle θ which can be shown to be

$$\theta = \pi - 2 \int_{R_0}^{\infty} \frac{p\,dr}{r^2 f(r)} \tag{8}$$

where $f(r) = \left(1 - \frac{p^2}{r^2} - \frac{V(r)}{E_R}\right)^{1/2}$

and R_0 is the distance of closest approach of the composite particle to the centre of force defined by $f(R_0) = 0$.

$$f(R_0) = \left(1 - \frac{p^2}{R_0^2} - \frac{V(R_0)}{E_R}\right)^{1/2} = 0. \tag{9}$$

For any given p

$$R_0 = p\left(\frac{E_R}{E_R - V(R_0)}\right)^{1/2}. \tag{10}$$

The matching between the potential given by (7) to the real potential is done at R_0. For this potential the constants B, C and the impact parameter p' are given by (Leibfried and Oen 1962):

$$B = -[V(R_0) + R_0 V'(R_0)] \tag{11}$$

$$C = R_0\left(1 + \frac{V(R_0)}{R_0 V'(R_0)}\right)^{-1} \tag{12}$$

$$p'^2(T) = \left(\frac{BC}{2E_R}\right)^2 \frac{\left(1 - \frac{T}{T_m}\right)}{\left(1 + \frac{B}{E_R}\right)\left(\frac{T}{T_m}\right) + \left(\frac{B}{2E_R}\right)^2} \tag{13}$$

where T is the energy transfer and T_m is the maximum energy transfer.
The expression for θ can be rewritten as

$$\theta = \pi - 4p_0 \int_0^1 \frac{du}{\left\{p^2(2-u^2) + \frac{R_0^2}{Eu^2}[V(R_0) - V(u)]\right\}^{1/2}} \tag{14}$$

where $r = R_0 / (1 - u^2)$.
Scattering angle ϕ in the laboratory system is given by

$$\tan\phi = A \sin\theta / (1 + \cos\theta). \tag{15}$$

Recoil angle ψ is given by

$$\psi = \frac{\pi}{2} - \frac{\theta}{2}. \tag{16}$$

The energy transferred to the struck atom is given by

$$T = (1 - \alpha) E \sin^2\left(\frac{\theta}{2}\right) = T_m \sin^2\left(\frac{\theta}{2}\right) \tag{17}$$

where $\alpha = [(A-1)/(A+1)]^2$ and T_m is the maximum energy transfer. The energy retained by the primary in a collision of deflection angle θ is thus

$$E' = E - T = E\,\alpha \sin^2 \frac{\theta}{2}. \tag{18}$$

3. Results and discussion

We study the collision cascade development of Ne^+—Cu interaction in the energy range 100–500 eV. We find that the sputtering threshold energy is 125 eV. For low impact parameters in the range 0·04 to 0·19 Å back-sputtering is observed. For higher impact parameters the ion penetrates into the target creating a cascade of collisions. Figures 1 and 2 show the collision cascade generated by 200 eV and 500 eV neon ions for $p = 0{\cdot}13$ Å. Back sputtering is observed in both the cases. For 500 eV ion the cascade of collisions generated is more widespread than for the 200 eV ion. Figures 3 and 4 show the collision cascade for 200 eV and 500 eV ions for $p = 0{\cdot}55$ Å. In this case there is no back-sputtering. The incident ion penetrates somewhat deeper into the target and the collision cascade is wider for 500 eV than for 200 eV incident ion energy.

For 500 eV neon ions incident normally on copper target with different impact parameters, the scattering and recoil energy after the first collision are plotted versus the impact parameter in figure 5. Large scattering angles and recoil energies are observed for low impact parameters resulting in back sputtering after two or three collisions. This also justifies the use of a binary collision model. In figure 6 the sputtering yield is plotted versus the incident ion energy for Ne^+—Cu. The experimental points are due to Wehner *et al* (1961). The agreement between theory and

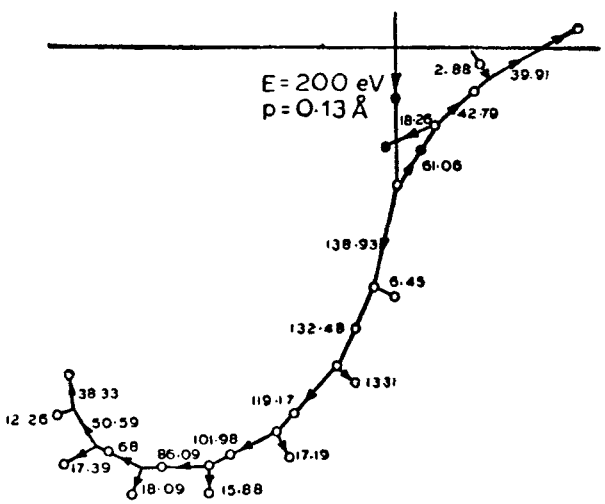

Figure 1. Collision cascade for 200 eV neon ions incident on copper target for the impact parameter $p = 0{\cdot}13$ Å. Open circles represent the target atoms and closed circles the incident ion and the numbers their energies in eV.

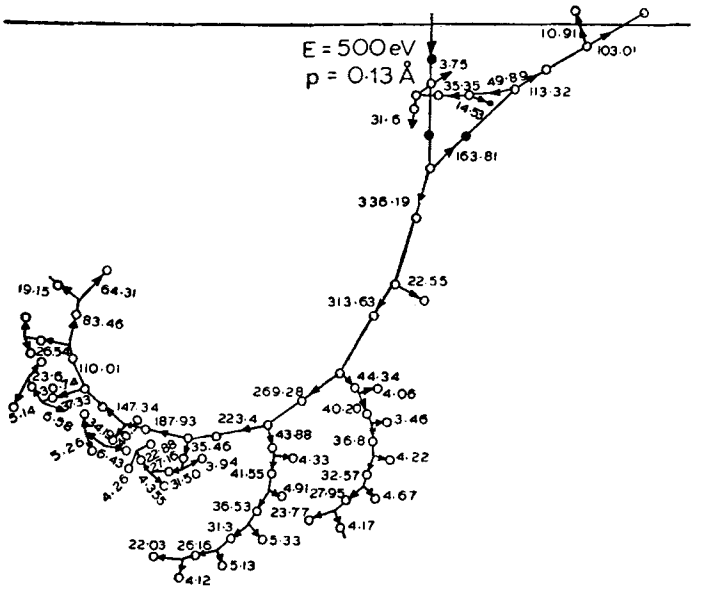

Figure 2. Collision cascade for 500 eV neon ions incident on copper target for the impact parameter $p=0{\cdot}13$ Å. Details as in figure 1.

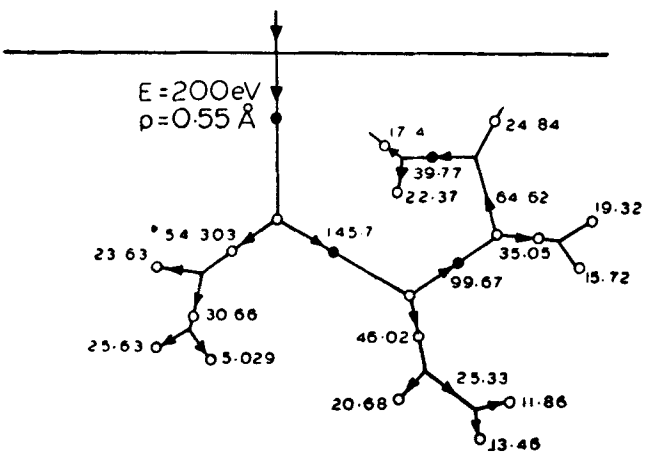

Figure 3. Collision cascade for 200 eV neon ions incident on copper target for the impact parameter $p=0{\cdot}55$ Å. Details as in figure 1.

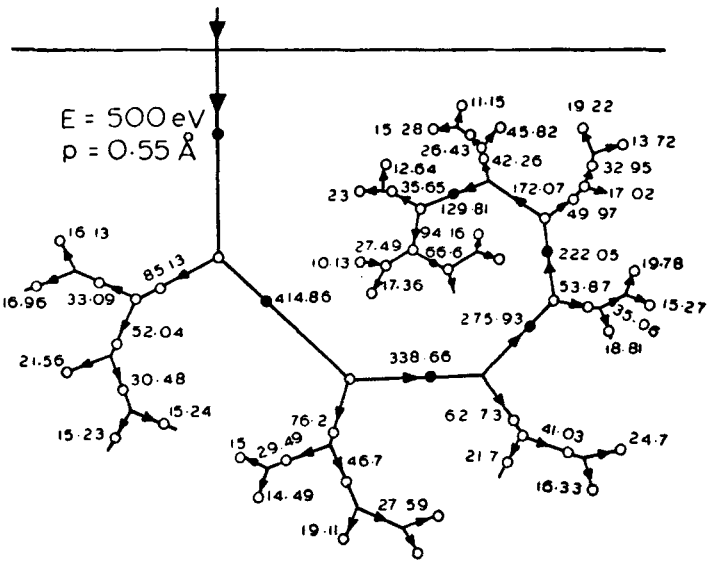

Figure 4. Collision casade for 500 eV neon ions incident on copper target for the impact parameter $p = 0{\cdot}55$ Å. Details as in figure 1.

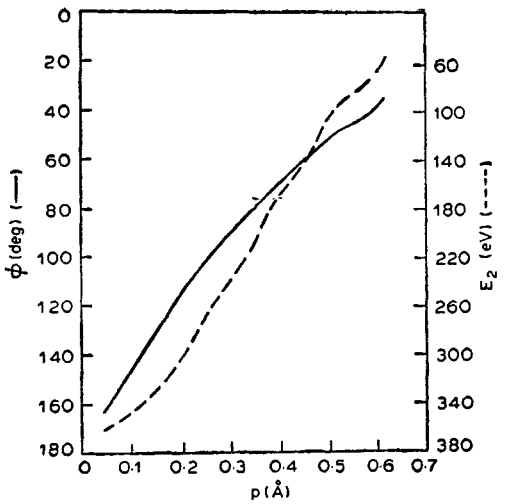

Figure 5. Scattering angles and recoil energies after first collision vs impact parameter for 500 eV neon ions incident on copper target. Solid line represents the scattering angle vs impact parameter and dashed line represents the recoil energies vs impact parameter.

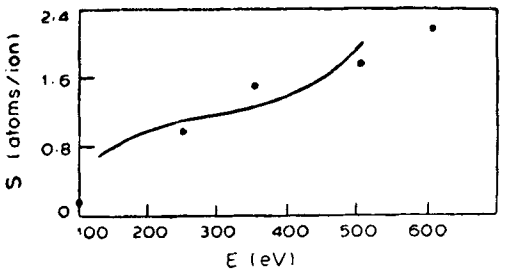

Figure 6. Sputtering yield vs ion energy for neon ions incident on copper target. The dots and the smooth line represent the experimental and the theoretical results respectively.

experiment is quite good considering the fact that no parameter fitting has been done in this analysis.

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