

NUMERICAL SIMULATIONS OF THE BACKSCATTERING FROM A CRYSTALLINE LATTICE

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The backscattering of 100, 300, and 500 eV Ar atoms from the {100} and {110} planes of a Al crystalline target is investigated with a computer code based on the Molecular Dynamics(MD) method. The interactions between particles are described by a screened Coulomb type potential. The angular (both azimuthal and radial) distribution of the backscattered particles together with the distribution of the energy and of the energy loss of scattered particles are calculated using the Lindhard-Scharff parameterization. The azimuthal distribution shows high peaks for 300 and 500 eV incident energies and a quasi-continuum for 100 eV incident energy in the case of {100} plane, and a single peak for the {110} plane. The radial distribution of backscattered particles evidences the symmetry properties of the crystal. The relative energy loss decrease when increasing incident energy, and is compatible with the backscattered energy distribution. The results do not agree with the Binary Collision Approximation(BCA).

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1. Introduction

When an energetic atom collides with the surface of a solid, it experiences forces of interaction with the atoms of the solid, which determines its trajectory. There will be a certain probability, for any incident atom type and energy and target atom species and geometry (i.e. crystal orientation and type) that the atom will be so deflected as to be reflected from the solid surface, while there will be another probability for the atom to penetrate beyond the surface into the solid lattice. When the impact parameter is small, the force is almost wholly repulsive. Because of the screening effect of the atomic electrons, the potential cannot be simply described by a Coulomb form. Therefore, we adopt a screened Coulomb type potential, as described in [1].

2. Model

The model used to describe the backscattering process is based on the MD method and is described in [2]. The energy loss is parameterized using the Lindhard-Scharff model [3], in which the inelastic energy loss is considered to be proportional to the velocity of an atom moving through an electron gas of constant density. Using the Thomas-Fermi [4] treatment for the variation of the stopping cross section per atom, the expression for the energy loss becomes:

$$\Delta E_{LS} = L_m N S_L(E), \quad S_L = k_L E^{1/2} \quad (1)$$

with:

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$$k_L = \frac{1.21Z_1^{7/6}Z_2}{(Z_1^{2/3} + Z_2^{2/3})^{3/2}M_1^{1/2}} \quad (2)$$

where L_m is the distance between collisions, M_1 the atomic mass of the target and N the target density.

The incident beam is formed by 4096 Ar atoms, normally incident on a cube of side 32.58 Å containing 3888 Al atoms in a cfc crystalline configuration. Fig. 1 displays the pair distribution function for Al atoms. The peaks show the periodicity of the crystal lattice.

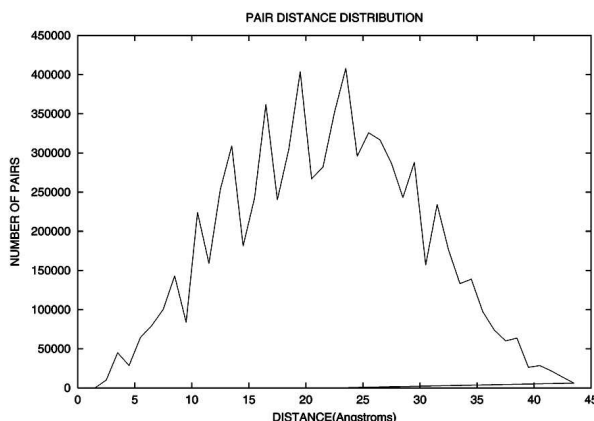


Fig. 1. Pair distribution function for Al atoms.

Only the interactions between Ar atoms and Al atoms in a sphere of 4 Å radius were considered at each time step, following the trajectory of Ar atoms. The time step was calculated using the formula:

$$\Delta t = 0.05d\sqrt{M_{Ar}/2E_c} \quad (3)$$

as the fastest knock-on atom does not move more than 5% of the interatomic distance in one time step.

3. Results and discussion

Fig. 2a presents the azimuthal distribution of backscattered particles for normal incidence on the {100} plane (ϑ is the angle between the Ar atom trajectory and the normal) for 100, 300, and 500 eV incident energies. The channel width is $\Delta\vartheta = 0.05$.

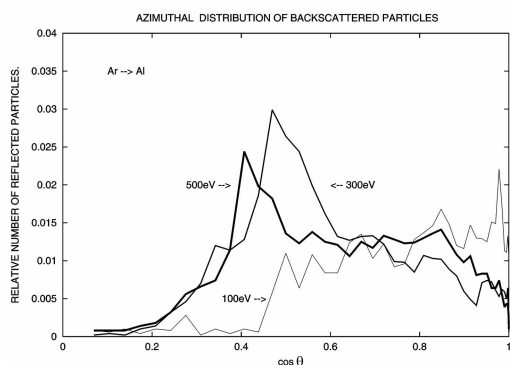


Fig. 2a. Azimuthal distribution of backscattered particles for {100} plane.

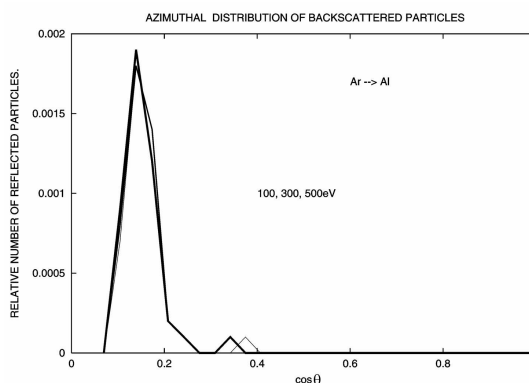
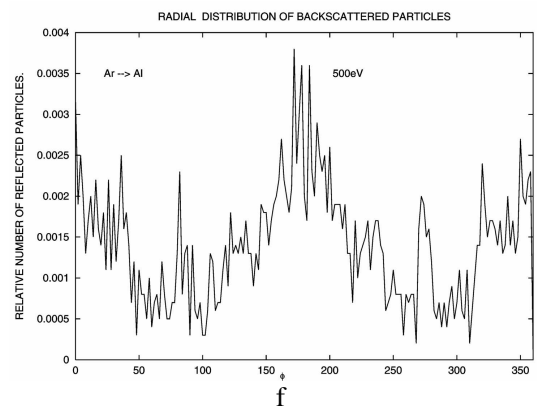
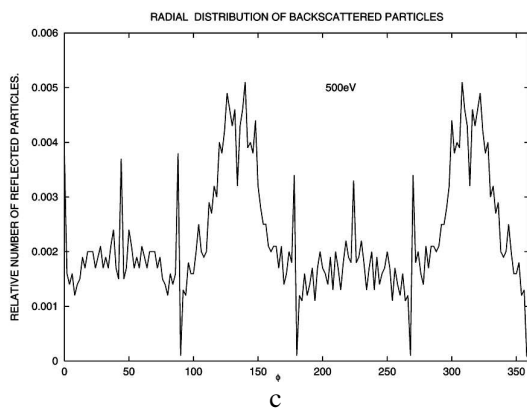
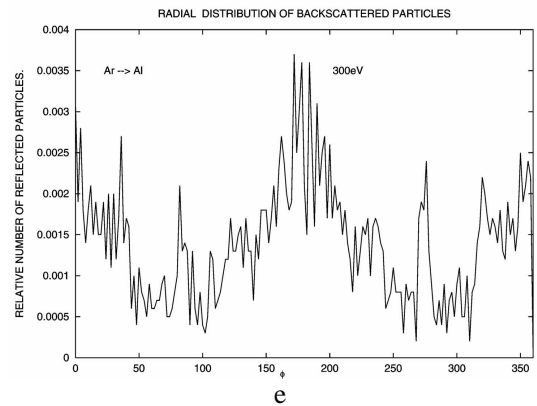
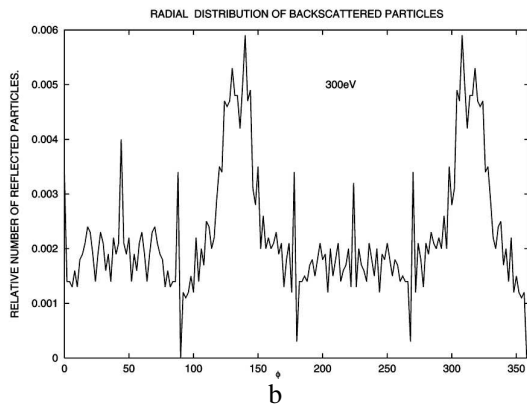
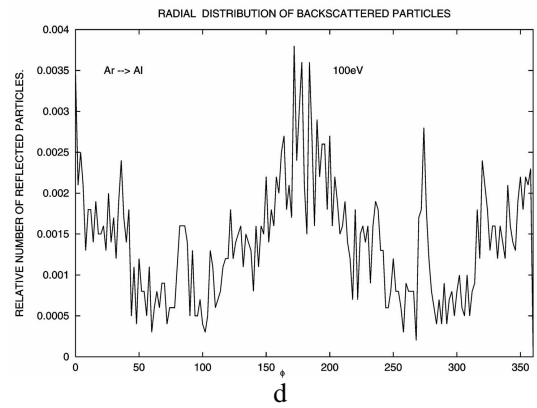
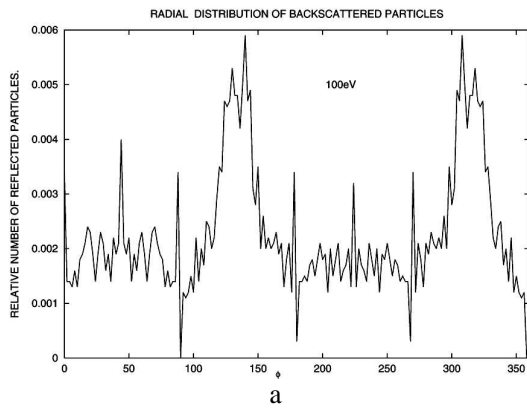


Fig. 2b. Azimuthal distribution of backscattered particles for {110} plane.

We see that almost all the particles are scattered at angles $\vartheta < 60^\circ$. The quasi-continuous spectrum for 100 eV incident energy may be associated with dislodged Al atoms of the surface. For 300 and 500 eV peaks at $\vartheta = 65^\circ$ and $\vartheta = 60^\circ$, which disagree with the BCA do appear. The rest part of the graphs may correspond to dislodged atoms too.

In Fig. 2b we present the same for $\{110\}$ plane. We can see that the graphs corresponding to 100, 300, and 500 eV superpose, having a peak at $\cos\vartheta = 0.15$, indicating the validity of the BCA.

The radial distribution of backscattered particles is presented in Figs. 3a-c (Φ is the radial angle of spherical coordinates) for the $\{100\}$ plane and in Figs. 3d-f for the $\{110\}$ plane.



Figs. 3a-c. Radial distribution of backscattered particles for $\{100\}$ plane at: a. 100 eV; b. 300 eV; c. 500 eV.

Figs. 3d-f. Radial distribution of backscattered particles for $\{110\}$ plane at: d. 100 eV; e. 300 eV; f. 500 eV.

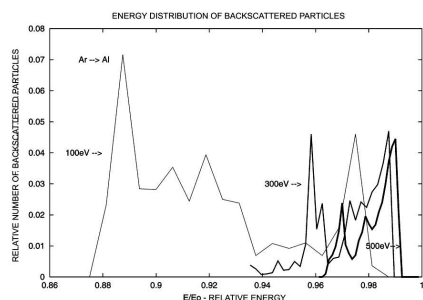


Fig. 4a. Energy distribution of backscattered particles for {100} plane.

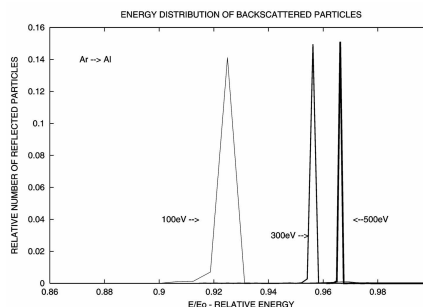


Fig. 4b. Energy distribution of backscattered particles for {110} plane.

Accordingly, the energy loss distribution (Figs. 5 a,b) shows two peaks for each incident energy in the case of {100} plane (Fig. 5a) and a single peak for each incident energy in the case of the {110} plane. The quasi-continuum between peaks in both graphs from Figs. 4a and 5a corresponds to dislodged atoms from the crystal surface.

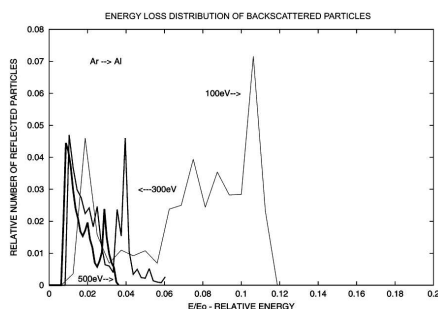


Fig. 5a. Energy loss distribution of backscattered particles for {100} plane.

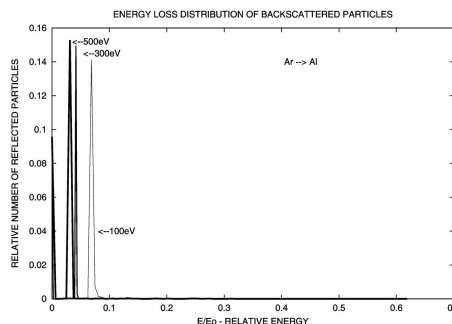


Fig. 5b. Energy loss distribution of backscattered particles for {110} plane.

In order to explain this difference, we can invoke the interplanar distances they are “sawn” by the incident particles. For the {110} plane the interplanar distance is larger than for the {100} plane, which fact leads to a more pronounced channeling effect.

Further studies will consider the {111} plane as well as other arbitrarily oriented incidence versus crystalline planes, aiming to evidence the possible correlation. The results will be published elsewhere.

4. Conclusions

We have simulated the backscattering of Ar atoms from a crystalline Al target, for 100, 300, and 500 eV incident energies, normal incident on two planes, namely {100} and {110}. We have evidenced the symmetry properties of the crystal lattice in the radial distribution of scattered particles for both planes of incidence. Due to the small number of the target atoms, a maximum number of two collisions is present in the case of {100} plane. The energy and the energy loss distribution allow for distinguishing between particles which suffered one or two collisions for this plane. The Lindhard-Scharff model for the inelastic energy loss was used. The computer time for this configuration was about 100 hrs on a Pentium II at 300 MHz. Further research will be focused on other energy interval and other energy loss parameterizations.

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