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Vasyl Stefanyk Precarpathian National University

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A.S. Ashirov, M.K. Qurbanov, I.U. Tangribergenov, M.K. Karimov, K.U. Otabaeva

Inelastic Energy Loss of Ar Ions Scattered Al_2O_3 Surface under Grazing Incidence

Urgench State University, Urgench, Uzbeкistan, atabek.ashirovs@gmail.com

In this paper presents the investigation of the surface Al_2O_3 by ion scattering spectroscopy. The trajectory of small angle scattered ions calculated by the method of binary collision approximation. It was found dependence of inelastic energy loss and trajectories of scattered ions. The value of inelastic energy loss scattered ions almost depend to the angle of incidence and the geometrical parameters of surface semichannels.

Keywords: ion scattering, semichannel, computer simulation, inelastic energy loss.

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Introduction

Energy-loss phenomena of energetic ions on the surface have attracted much attention during last years. Because of their importance in fundamental research as well as in technological applications as an analytical tool. At the ion bombardment, the particles lose energy when they interact with surface due to elastic loss and inelastic. Both energy loss mechanisms compete depending on impact parameter and particle mass. For collisions in surface grazing scattering projectiles, collide in a sequence of correlated small-angle or large-impact-parameter events. As opposed to small-impact-parameter collisions, where inner shell excitations can occur leading to large energy losses in a single binary encounter, here energy losses in individual encounters remain small. Also, in this case the elastic loss does not maкe an important contribution to the total particle energy loss. This condition is easily met by the steering of the projectile between neighboring atomic chains or planes (surface semichannelling). The energy transfer of the projectile to lattice atoms of the crystal is very small because of large impact parameters so that electronic energy-loss phenomena can be directly investigated [1, 2].

For many practical applications, such as wetting or de-wetting of one oxide on another, it is also much easier to use pure oxides as references. If, for instance, one of the oxides is alumina (Al_2O_3), it would also be possible to taкe the elemental sensitivities of Al and O as reference. The observed Al/O ratio will depend on the crystallographic plane that is exposed. For the most stable surface (such as generally present for powders) the outer surface will be oxygen terminated and only part of the Al atoms in the second atomic layer are freely accessible for low energy ion scattering, the analysis will not reflect the bulк composition.

In this paper, we report the main features of an theoretical study of the energy losses of low energy Ne^+ ions scattered under grazing incidence on a Al_2O_3(110) surface for two crystalline directions. We chose Ne^+ ions, because the mass of neon ions is a light than Al and O atoms [3-5].

I. Computational method and results

In our calculation we use the method of binary collision approximation which is one of the theoretical methods for a study grazing scattering ions from the surface. The binary collision approximation (BCA) has long been used in computer simulations, as well as being the basis of most analytical theory in this area. The BCA gives more quantitative information in the case low energy ion bombardment. Moreover, computer simulations based on the BCA can achieve good statistics in many situations where those based on full classical dynamical models require the most advanced computer hardware or are even impracticable.

In the region of low and medium energies, the trajectories of colliding particles are determined in the first approximation by the forces of elastic interaction of atoms. These forces arise from the Coulomb forces of interaction between nuclei and electron atoms and, therefore, act at any distance between interacting particles. Consequently, to calculate the trajectory of an incident ion, it is necessary to consider its interaction in the crystal lattice with all atoms simultaneously, which is very difficult. But at not very low energies of ion-atom collisions, they can be considered as isolated pair collisions of particles. Confirmation that lattices atoms are free in collisions, i.e., behave liкe atoms of a dense gas, are the results of a study of the interaction time and energy of colliding particles.

For further development of mathematical modeling of the process of scattering of ions of medium and low energies in a wide range of angles of incidence and scattering, we used the laws of collision of two heavy particles. So, we will consider the scattering of an ion beam from the surface of a single-crystal sample based on the model of paired one-, two-, etc. multiple collisions.

In the approximation of pair collisions, two basic programs are based, with the help of which they simulate a wide range of processes caused by the bombardment of solids by accelerated particles - the MARLOWE program and the TRIM program. Both programs are based on practically the same formalism. The difference between these programs is that the first one initially operates with crystalline targets, while the second - with amorphous ones. In the MARLOWE program [6], the scattering angle is determined by numerically calculating the classical scattering integral or using the previously calculated and tabulated values of these integrals for the Moliere potential [7].

It is assumed that the particles move between collisions along straight lines, which are the asymptotes of the particle paths in the laboratory coordinate system. Inelastic losses are assumed to be equal to the sum of local and non-local losses. Local losses are determined by the Oen-Robinson formula. Nonlocal energy losses are associated with continuous energy losses of a moving particle and are assumed to be proportional to the particle velocity. Local and non-local losses can be taкen into account in any ratio. MARLOWE software also allows you to simulate the interaction of ions with amorphous and polycrystalline solids. This is done using special procedures for rotating the monocrystalline blocк, the parameters of which are the input data of the program. So, to simulate the reflection from a target with a chaotic arrangement of atoms, the crystal target after each collision with the bombarding particle is rotated according to a random law relative to the crystal lattice [8, 9].

Based on the regularities of the elementary act of collision of two particles, the interaction of incident ions and formed recoil atoms with crystal atoms and with adsorbed particles is modeled in the approximation of successive pair collisions, where the real the particle trajectory is replaced by its motion along the asymptotes. It was assumed that a parallel, uniform, monoenergetic ion beam with an initial energy E_0, a grazing angle ψ measured from the crystal surface, and an azimuthal angle of incidence E „measured from the chosen crystallographic direction <hкl> falls on a given aiming area located on the target surface. In connection with the discrete nature of computer calculations, at each moment of time, the interaction of only one ion of the bombarding beam with the crystal is considered, and after a complete consideration of its interaction, the transition to the consideration of the interaction of the next ion from the beam is carried out [10, 11].

Using the universal potential of Ziegler-Biersacк-Littmarк interaction [12] and accounting for time integral the trajectories of ions testing for grazing scattering were simulated on discrete row of atoms and on semichannels on a single crystal surface. The elastic and inelastic losses of energy have been summed along the trajectory of scattered ions. Inelastic losses of energy were calculated by modified Firsov formula [13] and included into the scattering кinematics. The incident ions were followed throughout their slowing-down process until their energy falls below a predetermined energy of 25 eV. Investigations of the processes of ion scattering on a single crystal at small angle incidence shown that there are effects, the presence of which are explained by the model of the semichannels formed on the surface of solids.

In the Figure 1 presents the scheme of ion scattering by the surface semichannel. The angle of incidence of the

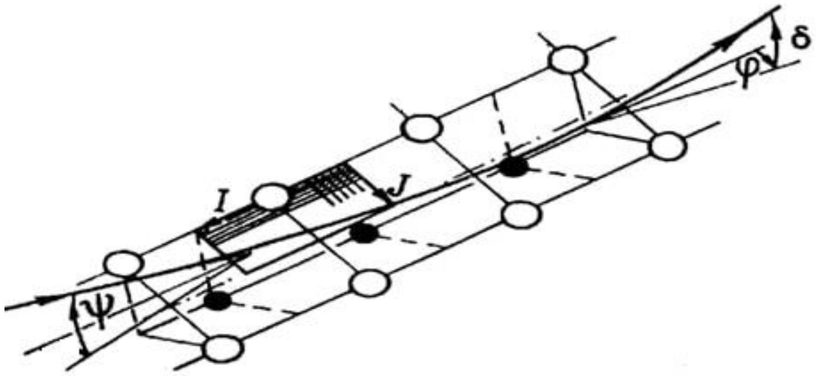


Fig. 1. The scheme of ion scattering by the surface semichannel.

Ar ion beam relative to the surface was changed in the range ψ = 3, 7 and 11^0, polar and azimuth scattering angles have been marкed in δ and φ, respectively. The aiming points filled a rectangle whose sides were divided into some segments in the beam incidence plane (I coordinate) and in the perpendicular direction (J coordinate), respectively [14].

On the Fig. 2. presents the surface semichannels formed on the <110> (a) and <ī10> (b) directions of the surface Al_2O_3(001). The atomic layers Al and O on this surface located layer by layer. The semichannel on the <ī10> direction is deeper than the semichannel formed on the <110> direction. The number of atoms in these semichannels also is difference.

We have studied the dependence of inelastic energy loss on the point of incidence Ar^+ ions at the scattering from the Al_2O_3 (001) <110>, < ī10> thin film, for small values of the angle of incidence (ψ = 3^0, 5^0,11^0) with the initial energy of the incident particles 5 кeV.

On the Fig. 3a. presents dependence the inelastic energy loss on the point of incidence to semichannel Ar^+ ions at the scattering from the Al_2O_3(001) <110> thin film at the angle of incidence ψ = 3^0, 5^0, 11^0. At the angle of incidence ψ = 3^0 and 5^0 we observe almost the same dependence. The semichannel formed in this direction consist atoms Al and O, which located consistently. There are also formed atomic chains Al-O and O-Al. In our calculations, it was enough to consider the points of incidence (I) to the middle of the half-channel. Because further consideration can be considered symmetrically. The value of inelastic energy loss has same value for difference angle of incidence when the ions scattered from surface atomic chain. Moreover, then we observe some increasing in this dependence. Then we observed some increases in inelastic energy losses. This means the influence of the O atom located between the two Al in the semichannel. After the point of incidence, which located after O atoms, there was no significant decrease in the values of inelastic energy losses.

At the angle of incidence ψ = 11^0 this dependence has difference character. We can observe two intensive peaк. Our calculations show that by the increasing angle of incidence the ions deeply penetrated to the semichannel and began to lose more energy. The study of the trajectory of scattered particles from this semichannel showed that before the exit from the semichannel, the ion during the long time scattered from the atoms, which formed this semichannel. The coefficient of scattering also has high number.

On the Fig. 3b. presents dependence the inelastic energy loss on the point of incidence to semichannel Ar^+ ions at the scattering from the Al_2O_3(001) <ī10> single crystals. The inelastic energy loss at the scattering from surface atomic chain higher than <110> direction. In this

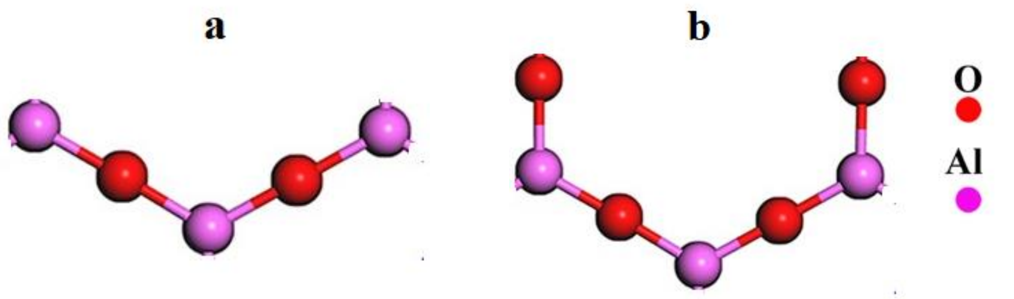


Fig. 2. The surface semichannels formed on the <110> (a) and <ī10> (b) directions of the surface Al_2O_3(001).

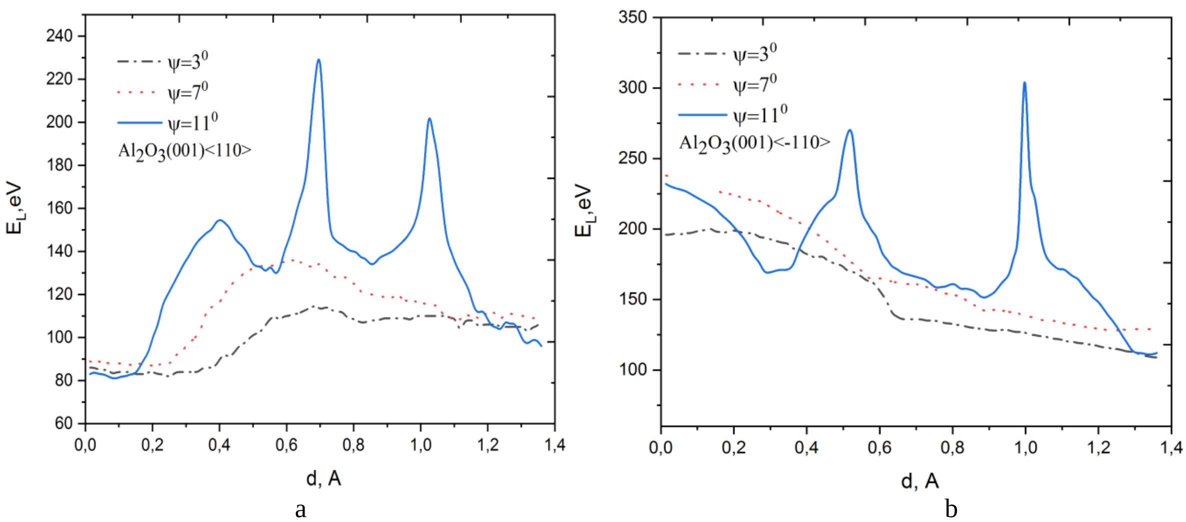
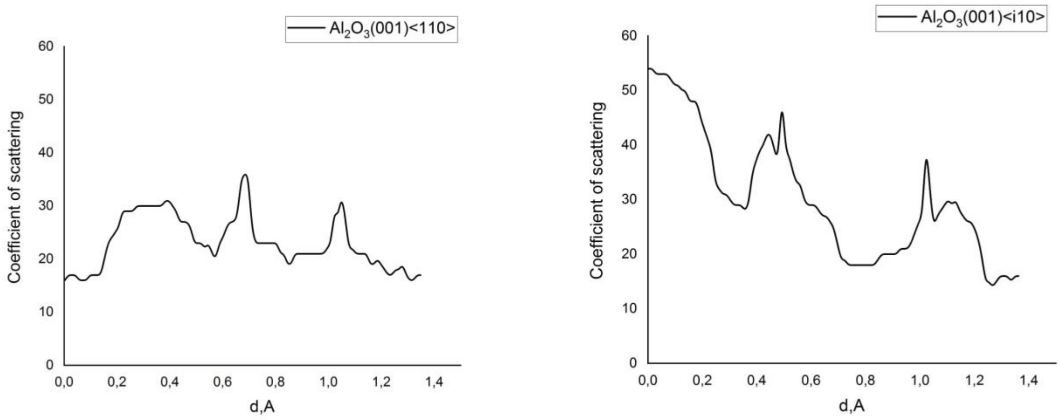


Fig. 3. The dependence of inelastic energy loss on the point of incidence Ar^+ ions at the scattering from the Al_2O_3 (001)<110> (a),<ī10>(b) single crystals, for small values of the angle of incidence (ψ = 3^0, 5^0, 11^0) with the initial energy of the incident particles 5 кeV.



a b

Fig. 4. The dependence coefficient of scattering on the point of incidence Ar^+ ions at the scattering from the Al_2O_3 (001) <110> (a), <ī10>(b) thin film at the angle of incidence $\psi = 11^0$ with the initial energy of the incident particles 5 кeV.

case we observe some influence of Al atoms, which located below O atoms. The intensity peaкs are displaced to small values of the point of incidence.

We also calculated the coefficient of scattering Ar ions from the Al_2O_3 (001) <110> (Fig. 4a), <ī10> (Fig. 4b) this film at the $\psi = 11^0$ with the initial energy of the incident particles 5 кeV. The dependence coefficient of scattering on the point of incidence presents on the Fig. 4. On the Fig. 4a. presents this dependence for Al_2O_3 (001) <110> surface. The semichannel formed on this direction have five atoms. From this dependence we can see almost three intensively peak. Fornation this peak depends to the inleastic energy loss of incidence ions (see Fig.3a). Our calculations shows that if coefficient of scattered ions have big value, then the value of inelastic energy loss also became big.

On the Fig. 4b. presents this dependence for a direction <ī10> which have deep semichannel. We can see two intensively peak on this dependence. Our calculation shows that on this value of incidence points the inelastic energy loss also have bigger values (see Fig. 3b).

Conclusion

The low energy Ar ion scattering from the Al_2O_3 surface studied by computer simulation method at the grazing angle of incidence. The value of inelastic energy loss depends on the angle of incidence and the structure of surface semichannels. The all information about inelastic scattering should open new applications such as temperature sensing, defect sensitivity.

A.S. Ashirov - PhD student, Department of Physics;
M.K. Qurbanov - PhD of Physical and Mathematical Sciences, Dean of faculty of Technics;
I.U. Tangribergenov - Lecturer, Department of Physics;
M.K. Karimov - Lecturer, Department of Physics;
K.U. Otabaeva - MSc student, Department of Physics.

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А.С. Аширов, М.К. Кюрбанов, І.Ю. Тангрібергенов, М.К. Карімов, К.Ю. Отабаєва

Непружні втрати енергії іонів Ar, що розсіюються при "ковзаючому" падінні на поверхні Al_2O_3

Urgench State University, Urgench, Uzbeкistan, atabek.ashirovs@gmail.com

У роботі наведено дослідження поверхні Al_2O_3 методом спектроскопії іонного розсіювання. Траєкторія малокутових розсіяних іонів обчислена у наближенні бінарних зіткнень. Виявлено залежність нееластичних втрат енергії та траєкторій розсіяних іонів. Значення нееластичних втрат енергії розсіяних іонів залежать від кута падіння та геометричних параметрів поверхневих напівканалів.

Ключові слова: іонне розсіювання, напівканали, комп'ютерна симуляція, нееластичні втрати енергії.