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The Characteristic Trajectories of Scattering Ions from the Ice Thin Films

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***Abstract*— The characteristic trajectories of scattering Ne and Ar ions have been calculated by the computer simulation method. In this calculation was used the method of binary collision approximation. The dependence of visible surface layers by coordinate of aiming point have been received. The trajectories of scattering ions have several refocusing points and they moved between channels in the monocrystal.**

Keywords—computer simulation; channeling; ion scattering spectroscopy;

I. INTRODUCTION

Ion scattering spectroscopy (ISS) is a technique in which a beam of ions is scattered by a surface. The kinetic energy of scattered ions is measured; peaks are observed corresponding to elastic scattering of ions from atoms at the surface of the sample. Each element at the sample surface produces a peak at a different measured kinetic energy, caused by the momentum transfer between the incident ion and atom. The scattered ion and the scattering atom are normally of different masses, but the total momentum of the atom and ion is conserved. Therefore, as the initially "stationary" atom recoils, some kinetic energy is lost from the scattered ion, and the quantity of lost energy depends on the relative masses of the atom and ion[1].

An ion scattering spectrum typically contains one peak for each element in the sample, with their separation in energy relating to the relative atomic masses of those elements. In some cases, different isotopes of the same element can be resolved, although this usually requires a primary ion heavier than He^+. Strong scattering signals are limited to the topmost layer of atoms, so ISS is extremely surface-sensitive. Therefore, the sample must be clean, and even a small quantity of surface contaminant can significantly influence the ion scattering spectrum[2].

In this paper, we present binary collision approximation simulations aimed at obtaining such a microscopic picture of characteristic trajectory and dependence of coefficient of scattering by the angle of incidence.

We believe that the model presented here provides the basis for understanding of the ion-atom collision processes leading to the scattering ions from thin films.

II. COMPUTATIONAL METHOD

The numerical code used in this work is based on the consequence binary collision approximation [3]. Using the universal potential of Ziegler-Biersack-Littmark interaction [4] 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[5]. The simulations were run with the crystal atoms initially stationary at equilibrium lattice sites because in the conditions of grazing incidence the influence of the thermal vibrations of lattice atoms at room temperature on ion scattering results is insignificant. 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 and included into the scattering kinematics. The incident ions were followed throughout their slowing-down process until their energy falls below a predetermined energy of 25 eV. Details of the present code have been described in [6].

Fig.1 shows schematically a surface semichannel and the target area on it, and identifies the angles used in the computation. The aiming points filled a rectangle whose sides were divided into 50 and 200 segments in the beam incidence plane (I coordinate) and in the perpendicular direction (J coordinate), respectively. Thus, the number of incident ions is $2x10^4$. The angle of incidence of the ion beam relative to the surface was changed in the range ψ = 5 - 20^0, on azimu-thal angle of incidence the ion beam was directed along the axis of surface semichannel or atomic row, polar and azimuth scattering angles have been marked in δ and φ, respectively (Fig.1).

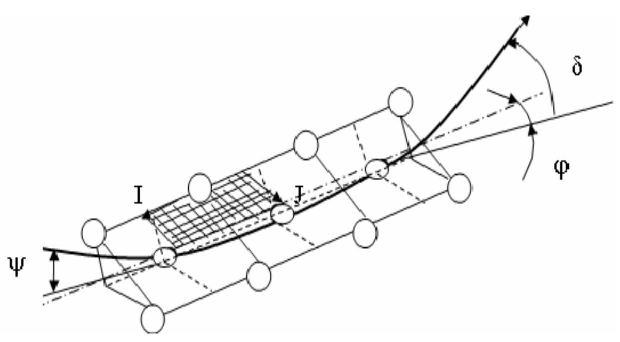

Figure 1. Schematically a surface semichannel and the target area on it.

III. COMPUTER RESULTS AND DISCUSSIONS

On the Fig.2a presents the dependence of visible surface layers by coordinate of aiming point -N(J) at the scattering Ne^+ ions from the ice film <ī10> by E_o= 5 keV and ψ= 6^0 .

In this direction are formed a wide semichannel by H and O atoms. The H atoms located on the surface atomic chain and the atoms O located on the second layer. The bottom of semichannel are formed by H atoms which located on third layer. The width this semichannel is d= 2,27Å, the depth h=1,6 Å, distance between atoms a=4,02 Å.

At the N(J) dependence we choose some points (A,B,C) and we will consider the trajectory on this points. On the Fig.2b presents the consequently trajectory scattering ions on the point A (J=0.114Å). It is seen that ion at the beginning initially feels the collisions with surface atomic rows (atoms H) and the following collision has come of two atomic chains H, located in the first and third layer. Then the ion is enthralled in semichannel. At the scattering from semichannel, the ion felt the influence fourth layer (the atomic chain H). Follows to note that ion in this case not to got into the other channels i.e. process of the scattering has occurred in one semichannel only. The coefficient of the collision for this trajectory is 34, the no elastic energy losses -100eV.

On the Fig.3. presents the trajectory in flat type (a) and three-dimensional type (b) of ion on the point B(J=0,68Å). In this point ion path look more complex. Follows to note that ion are penetrated into monocrystal until 5-layer. We can see that the ion occurred to the channel which formed under surface semichannel. The flat snapshot (fig.2b) enables in more detail to study the form to paths in crystal.

The coefficient of the collision for this trajectory is 91, the no elastic energy losses -314eV.

On the Fig 4. presents a trajectory scattered ion on the point C (J=1.47Å). We can observe that the ion occurred to the one semichannel. The coefficient of

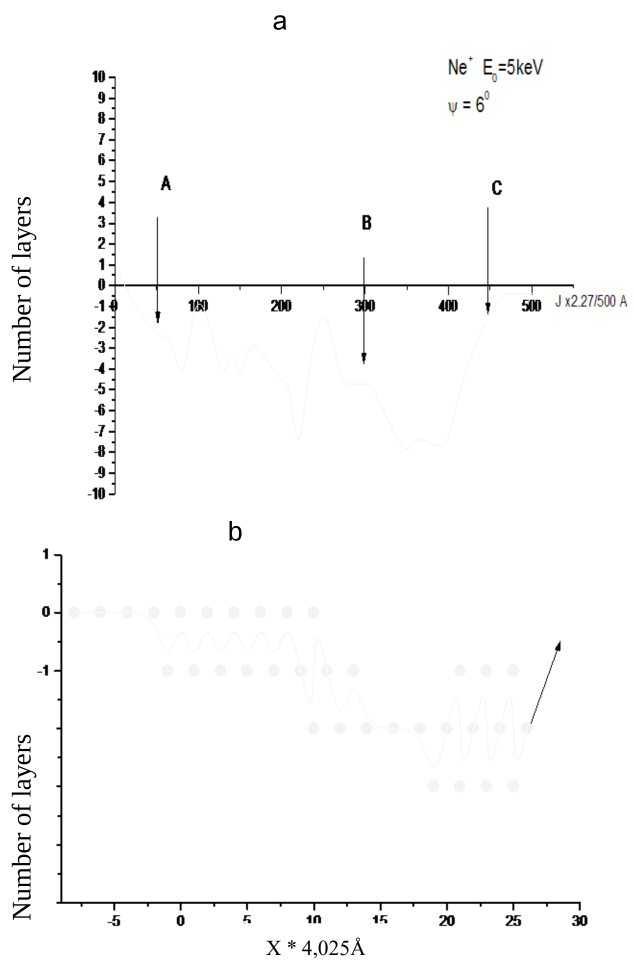

Figure.2. The dependence of visible surface layers by coordinate of aiming point -N(J) at the scattering Ne^+ ions from the ice film <ī10> by E_o= 5 keV and ψ= 6^0 (a) and the trajectory ion at the J= 1.114Å (b)

the collision for this trajectory is 23, the no elastic energy losses – 140eV.

We also observed the dependence coefficient of scattering to the angle of incidence- $K_p(\psi)$ for the Ne^+ and Ar^+ ions scattered from the ice film surface by E_0=1кeV(fig.5).

The dependence $K_p(\psi)$ have double peak structure. The Ne^+ ions started to penetrate to the ice film at the ψ= $3,31^0$, the ions Ar^+ at the ψ= $3,93^0$.

The line pertains to the ion Ne^+, the dotted line to the Ar^+. The peak which formed at the ψ= $6,9^0$ and ψ= $7,5^0$ pertain to focused ion for Ne^+ and Ar^+ consequently.

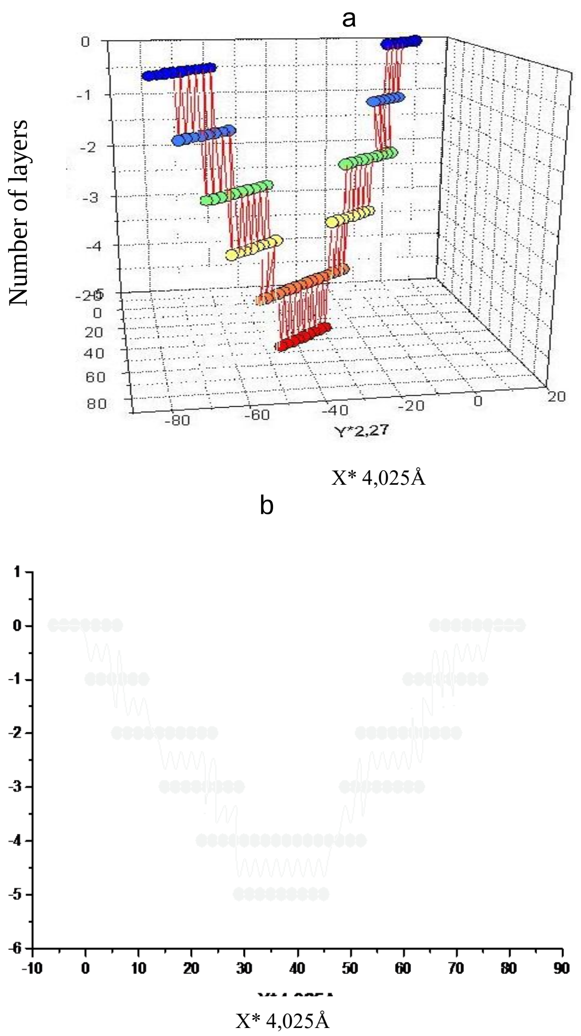

Figure.3. Trajectory in flat type (a) and three-dimensional type (b) of ion on the point B (J=0,68Å).

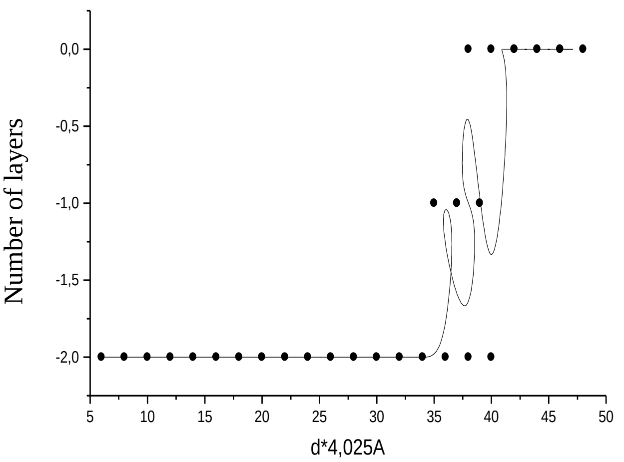

Figure.4. The trajectory of scattered ion on the point C (J=1.47Å).

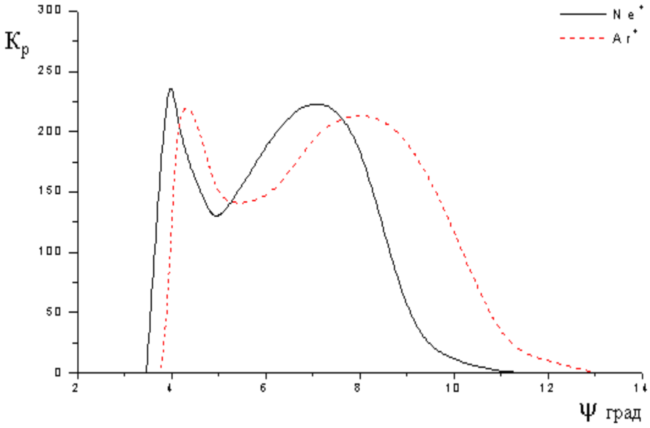

Figure.5. The dependence coefficient of scattering to the angle of incidence- $K_p(\psi)$ for the Ne^+ and Ar^+ ions scattered from the ice film surface by E_0=1кeV

By this dependency we can observe the angle of the penetration of the ion to semichannel is $3{,}93^0$. This is indicative of that that with increase of importance of the initial energy importance angle of the penetration of the ion in semichannel moves aside small importance.

IV. Conclusions

We observe the characteristic trajectories of scattering ions from the ice thin films on the three aimed points, which incidence ion will strike on the surface of semichannel. Trajectory of scattered ions, almost have complex style. The ion moved from one channel to another and we can observe the effect channeling and dechanneling. Also the energy loss, coefficient of scattering ions has been calculated by computer simulation method.

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