Computer Simulation of Ne^+ Ions Scattering from Cu(100) Surface at the Grazing Incidence

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***Abstract*—The scattering Ne^+ ions from the Cu(100) and GaP(100) surfaces at grazing incidence has been simulated by the method of binary collision approximation. The peculiarities of trajectory scattered ions from the multi-component mono-crystals has been by the computer code. The shapes of trajectories of refocused particles have been carefully studied for the different surface semichannels. The received results may be interesting at the analyzing of surface structure.**

Keywords—computer simulation; ion scattering spectroscopy; ion refocusing;

I. Introduction

Grazing-incidence ion scattering can be used to probe the structure of clean and defected surfaces. .At grazing angles, incident particles can travel along distance parallel to the surface, while not penetrating very deep into the sample. The projectile trajectories are highly sensitive to both short-and long-range lateral surface structure. Consequently, grazing incident scattering is potentially a good technique for monitoring the modification of surfaces in real-time. An example of a possible application is as a probe of the interaction of plasma with surfaces. We have built an instrument to study plasma-treated surfaces in real time and in-situ by means of grazing incidence ion scattering. The desire to better understand and interpret the experimental data produced prompted us to undertake a complementary program of simulations

If ions are scattered from ordered crystals at grazing incidence, the particle motion is to a great extent determined by the mutual position of the surface atomic layers of the irradiated target. Currently there are some experimental and theoretical results concerning ions scattering from surface atomic rows and semichannels at grazing incidence of the beam on the one-component crystal surface [1, 2]. In particular, the ion focusing effect of scattered particles [3-6] observed in the regime of surface semichanneling, the ion refocusing [7] observed at very small grazing angles of incidence have been investigated in detail.

Ion bombardment of a solid surface leads to radiation-induced vacancy defects, atomic steps and their clusters, as well as surface roughness. The concentration and the type of the radiation defects being formed depends upon the experimental conditions and significantly influences the trajectories, angular and energy distributions, as well as the number of the scattered particles. Moreover, there is a correlation between the defect type, the blocking angles of the reflected beam and the energy distributions of the scattered particles, that allows a determination of the defect type and its surface concentration [8-10]. Thus the detection of scattered ions provides a powerful tool for surface analysis that is exclusively sensitive to the outermost atomic layers.

The aim of present work is to study by both computer simulation and analytical approaches on the refocusing effect of particles reflected from the surface semichannels versus the shape of semichannels.

II. Computational Method

Ion beam techniques are well suited for a quantitative analysis of the surface and near-surface composition of a sample because the energy spectrum of scattered particles shows mass dispersion, and the scattering process has a well-defined cross-section at high energies.

The surface under study is hit with a low energy beam of noble gas ions, usually helium. The collisions that take place can be considered as elastic, in the sense that both the energy and the momentum are conserved. We can also consider that, except in some special cases, the collision is matrix independent, that is the atoms in the solid behave as free atoms.

In practice, working at a fixed angle, low energy ion scattering spectroscopy (LEIS) can be used as a probe of the surface composition. Owing to the high probability of neutralization of the ions that penetrate below the first atomic plane, LEIS has the characteristic of being sensitive only to the outermost surface composition, a capability which is unique among surface analytical techniques.

The numerical code which used in this work based on the consequence binary collision approximation [2]. Using the universal potential of Ziegler-Biersack-Littmark interaction [11] 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. For consideration of possible simultaneous collisions of ion with several target atoms, the procedure proposed by Robinson and Torrens [12] was used. 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 [2] 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 [2, Chapter 2].

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 azimuthal 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).

We have found an analytical approach for a describing effect of ion refocusing at the bombardment of monocrystals by noble gases at the grazing incidence[13]. The trajectories of scattered Ne^+ ions have been received by using computer program.

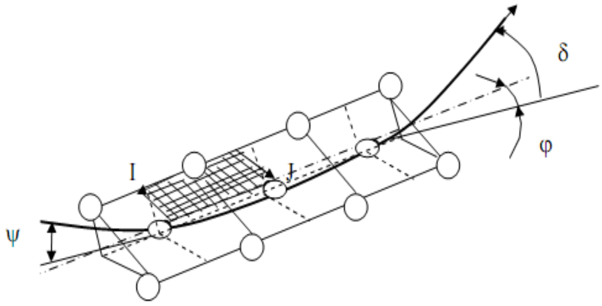

Figure 1. The scheme of ion scattering by the surface semichannel

III. Computer Result and Discussion

In Fig.2(a) the dependence φ (J) for refocusing part of 5 keV Ne^+ ions scattered from the *Cu*(100) <110> surface at $\psi = 6^0$ was presented. It is seen, that the magnitudes of φ are less than $\pm1^0$ in large range of coordinate J.

For presentation of influence of impact point coordinate J on the shape of trajectories of refocused ions the some of such trajectories are shown in Fig.2(b).

For J = 0.936 Å (impact point A, Fig.2(a)) the ion trajectory is symmetric relative to the incidence plane of primary beam passing through a semichannel axis (the case A, Fig.2(b)). At incidence on the surface the ion interacts with atomic row 1, changes its trajectory to the side of neighbor atomic row. Penetrating inside of semichannel the ion interacts with neighbor atomic row. Under influence of the semichannel wall formed by atomic rows 2 and 3 the ion moves to the atomic row 3 and it is reflected by this row. It is seen that the “reflected part” of its trajectory is symmetric relative to the “incident part” of ones. Thus, the ion trajectories are focussed at first by surface rows with the focus point lying near the surface, then are diverged and again are focussed (i.e. refocussed) by semichannel walls with the focus point lying inside of semichannel.

In this case the number of collisions of ion with target atoms is 83, a length of ion trajectory is 74.2 Å (35.8Å corresponds to the movement inside of semichannel), the elastic and inelastic energy losses are 19 and 502 eV, respectively.

For comparison the analogous data for ions scattered by the ridge of surface atomic row (J = 0) are given: in this case the number of collisions is 13, a length of ion trajectory is 31.1 Å, the elastic and inelastic energy losses are 10 and 106 eV, respectively.

At approaching of coordinate J to the center of the semichannel the shape of ion trajectories has some change (the cases B-D, Fig.2(b)). "Incident" and "reflected" parts of the trajectory are near the axis of a semichannel and it becomes parallel to the incident plane at J=1.28 Å (center of semichannel). In the range 0.936 Å < J < 1.6 Å the characteristics (the number of collisions, retained energy, length of a trajectory) of all incident ions, undergoing the refocusing in the surface semichannels, are similar.

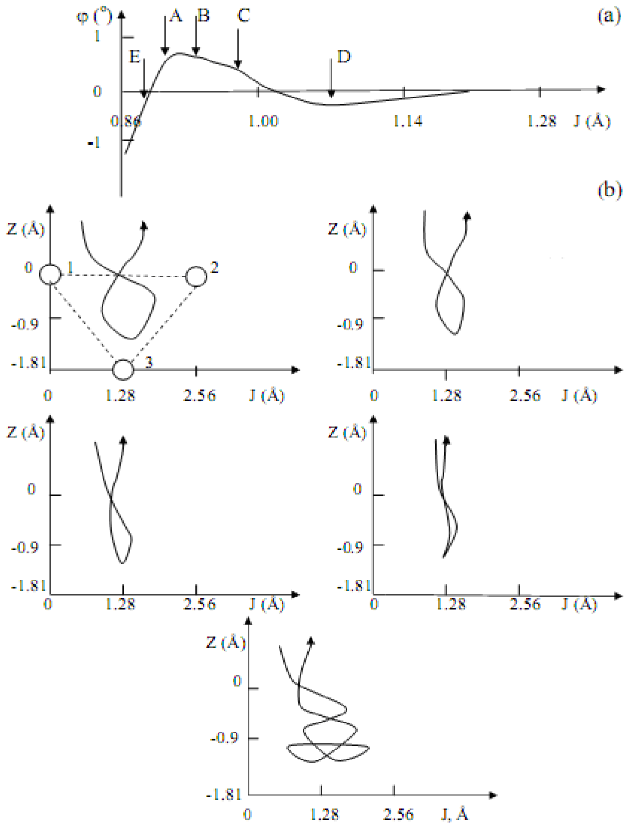

Figure 2. The dependence φ (J) for refocusing part of 5 keV Ne^+ ions scattered from the *Cu*(100) <110> surface at $\psi = 6^0$ (a) and the some refocusing ion trajectories projected in transverse plane of the semichannel (b).

At coordinates of impact point, which are outside of range 0.936 Å < J < 1.6 Å, the refocusing of ions is not observed. In Fig.2(b) (the case E) the projection of one of such trajectories is shown corresponding to J = 0.90 Å (point E in Fig.2(a)). It seen that in this case the shape of the trajectory is more complex. The parameters of such trajectory are sharply different in comparison with corresponding parameters of refocusing ions trajectory. In this case the number of collisions is 157, the total length of ion trajectory is 148.5 Å (93.4 Å corresponds to the movement inside of semichannel), the energy losses 1056 eV. Besides both the shape of the trajectory and the characteristics of scattered ions are not stable in relation to the change of coordinate J.

IV. Conclusions

The refocusing effect of particles reflected from the surface semichannels of single crystals have been investigated by the method of computer simulations. The analytical expressions of refocusing energy for the different surface semichannels have been obtained. The peculiarities of 5 keV Ne^+ ion trajectories refocused by semichannels on the Cu(100) surface have been carefully studied. The received results show that the trajectory of refocusing ions has two focuses. The received results may be interesting at the analyzing of surface structure.

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