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Investigation Of The Effect Ion Refocusing: A Computer Simulation

Kutliev Uchkun Otoboyevich
dept. General Engineering Science
Urgench State University,
Urgench, Uzbekistan
e-mail: uchkunk@mail.ru
Turaev Nazar Yuldashevich
Head of educational centre “FANUM” Academy of Science,Tashkent, Uzbekistan
e-mail: uchkunk@mail.ru
Otabaeva Kamola Uchqun qizi
“Tagan” professional college of the service
Yangiarik district, Uzbekistan
e-mail: uchkunk@mail.ru

Abdukarimov Xidoyat Egamberganovich
dept. Physics, Urgench State University
Urgench, Uzbekistan
e-mail: abdukarimov.azamat@rambler.ru
Qurbonov Davron Shavkatovich
dept. Physics Urgench State University
Urgench, Uzbekistan
e-mail: davronoka@mail.ru

***Abstract*—The scattering of Ne^+ ions from the GaP(100) monocrystal surface at the grazing incidence with the initial energy E_0 = 1 keV was studied by the method of computer simulation. As a result of investigation has been obtained the dependence of the scattering of ions on the incidence angle ψ. In simulations was used the model of binary collision approximation. The analytical expression for the refocusing ions was found. This calculation more interesting for a study of surface processes.**

Keywords—ion scattering; computer simulation; ion refocusing

I. Introduction

Low-energy ion scattering (LEIS) is an analytical tool that provides information on the atomic composition of the outer surface, when noble gas ions are used as projectiles. In fact, quantitative composition analysis is currently done on a huge variety of materials, including catalysts and organic materials. The information on the surface composition is contained in the signal of backscattered ions (typically 1–3 keV He^+,Ne^+). In order to translate the LEIS signal to an elemental surface concentration all factors determining the LEIS signal must be known. These are in particular the scattering cross section and the ion fraction of the backscattered particles. The scattering cross section, which is due to the screened electrostatic potential between target atom and projectile, is well-known for the prevailing conditions of LEIS. It is an intriguing fact that, despite the large quantity of successful applications, the charge exchange processes in LEIS are not yet fully understood. It is e.g. not known why in LEIS for a given atomic species on the surface the signal usually does not depend on which other species are present (absence of matrix effects). Significant progress has recently been made in the understanding of the underlying charge exchange processes[1-2].

II. COMPUTER SIMULATION AND RESULTS

The simulation program which used at the present work based on the binary collision approximation. This program described in [3-4]. For the particles interaction description the Biersack-Ziegler-Littmark (BZL) potential [5] with regard to the time integral was used. The BZL approximation for the screening function in the Thomas-Fermi potential takes into account the exchange and correlation energies and the so-called “universal” potential, obtained in this way shows good agreement with experiment over a wide range of interatomic separations. Elastic and inelastic energy losses have been summed along trajectories of scattered ions. The inelastic energy losses have been calculated on the basis of Firsov and this model modified by Kishinevsky [6].

Investigation of ion scattering by the single crystal at grazing incidence particles have shown that there is an effect, which are explained model semichannels formed on the surface of solids.

In this paper presents the scattering of Ne^+ ions from the surfaces of monocrystal of GaP (100) at the grazing incidence with the initial energy E_0 = 1 keV. As a result has been obtained the dependence of the scattering of ions on the grazing angle ψ.

It should be noted that the penetration of ions into the semichannels depend on its form and size. It is known that when $\psi = 0^0$ ions scattered from atomic chains formed on the surface layers. With increasing angle of incidence, the ions can move in semichannels with different geometrical parameters depending on the direction of single crystals.

Fig.1 shows the dependence of the scattering coefficient (K_p) of the Ne^+ ions from the surface of GaP(100) <110> direction (solid line) and $<\bar{1}10>$ (dashed line) with E_0 = 1 keV from the angle of incidence ψ. It should be noted that the width of these semichannels formed on this directions are identical, and the depth in the direction of <ī10> two times greater than in the direction of <110>. From the dependence is clearly seen that this dependence has the two-peak structure. The first intensive peak refers to refocusing ions in the surface semichannels(effect refocusing). This effect is manifested in the fact that the ions begin to penetrate inside the semichannel and scattered by atoms of semichannel. These refocusing ions can not penetrate to the other semichannel, because the values are very small angle of incidence charged particles.

This relationship shows that Ne^+ ions begin to penetrate inside semichannel at the $\psi = 3{,}20^0$ in the <110> direction, and when $\psi = 3{,}80^0$ in the direction <ī10>. On the dependence we can see the intensive peaks corresponding torefocusing ions.

The our calculations shows that the angles of incidence at which the ions started to penetrate inside semichanel mainly depend on its geometrical parameters (the width semichannel and the distance between atoms) and varieties of atoms at the surface layers. Note that these directions are not only semichannels geometrical parameters, but also a form that affects the magnitude of the incidence angle at which the ions begin to penetrate inside the solid.

By increasing values of incidence angle scattering coefficient Ne^+ ions is decreased, reflecting the impact of lower layers of semichennels on the incidence particles.

The following peaks are formed at $\psi= 10{,}41^0$ in the <110> direction (solid line), when $\psi = 12{,}44^0$ in the direction <ī10> (dotted line) are corresponded to focused ions. At these values, the incidence angle is observed ion focusing effect which is manifested in the increase in the intensity and half-width reduction of the spatial distribution of scattered flux at certain orientations of the target with respect to the incident beam. This effect observed when ions passing between two rows of atomic surfaces and are focused at the bottom semichannel.

Studies refocus the ion trajectory shown that ion collisions occur first on the one wall and the bottom of semichannel, and then the other wall and a bottom of semichannel. Current projection trajectory scattered ion of semichannel has two foci one of which is inside of semichannel and the second near the surface layer. Each path can be determined path length (distance of scattered ion), the coefficient of collision, energy of the scattered ion, values of inelastic and elastic energy losses.

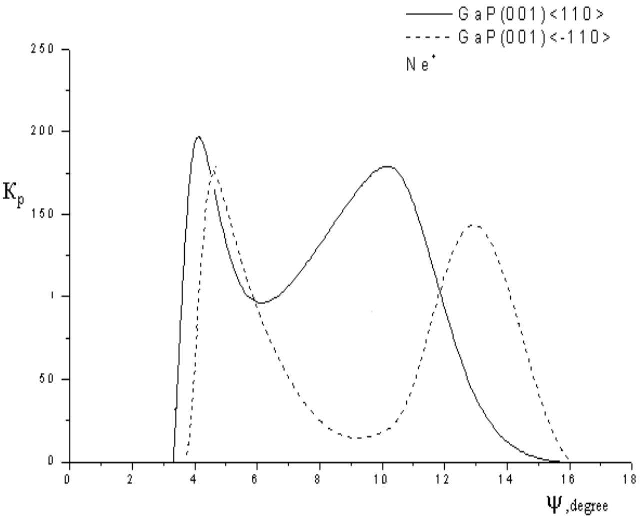

Figure 1. The dependence of the scattering coefficient (Kp) Ne^+ ions to the surface of GaP (100) <110> direction (solid line) and <ī10> (dashed line) with E0 = 1 keV from the slip angle ψ.

We have also found the analytical expressions for determining the energy of the scattered particles refocusing for two component monocrystals. At small grazing angles, depending on the angle of the scattering coefficient of sliding two-peak structure is observed. It is found in [6] for one-component target. It is proved that the effect of ion focusing and refocusing observed for small values of the angle of incidence of the incident particles. It should be noted that the peak refocus particles are formed at low bombardment angles than the peak ion focusing.

Refocusing effect manifests itself when the transverse energy of the incident particle energy $E_\perp = E_0 \sin^2 \psi$ exceeds the limit surface semichanneling. In this case, the bombarding particles may overcome the potential barrier which is formed by atomic rows of the surface.

We found an analytical expression for determining the energy refocusing E_{rf}. As noted in [7] reflection of particles from the surface at the grazing incidence ions is determined by the combined effect of the surface atomic rows. Therefore, the falling particles can penetrate the surface semichannels if the following conditions are met:

$$E > E_{rf} = \sum U(r_i) \qquad (1)$$

where, U (r_i) - potential between two atomic rows of semichannel created by first atoms nearby, located at a distance r_i from the middle of the two surface atomic rows in a continuous approximation. Since the effect of refocusing, semichannels observed on the surface of the target, we can not ignore the impact of the lower layers.

In all of our calculations, we used the BZL potential and expression (1) for semichannels consisting of three atomic rows and thus surface atomic rows are composed of atoms and the bottom semichannel atoms. In this case, expression (1) has the form:

$$E_{rf} = \begin{cases} C_A \sum_{i=1}^{4} \alpha_i K_0(\beta_i h / a^{a}{}_{s}) + C_B \sum_{i=1}^{4} \alpha_i K_0(\beta_i h / a^{b}{}_{s}) \text{....ïðè ..} \dfrac{a}{h} \geq \dfrac{\sqrt{2}}{2} \\ C_A \sum_{i=1}^{4} \alpha_i K_0(\beta_i h / a^{a}{}_{s}) \text{...ïðè ...} \dfrac{a}{h} < \dfrac{\sqrt{2}}{2} \end{cases}$$

where $K_0(x)$ - modified Bessel function of the second kind of zero order, and - half-width of semichannel, h - depth of semichannel, d is the distance between the atomic rows, $C=2(2Z_1Z_xe^2/d)$, , X-grade surface atoms of the substrate, (α_i = {0.1818; 0.5099; 0.2802; 0,02817}, β_i = {3,2; 0.9423; 0.2016; 0,2016}, $a_s= 0,4685/(Z_1^{0,23}+Z_2^{0,23})$. Such semichannels formed in the direction <110> and <100> on GaP (100) surface.

In the direction of <ī10> on GaP (100) surface formed a semichannel which consist five atomic rows. For this semichannel expression to determine the energy refocusing will obtained by:

$$E_{rf} = C_A \sum_{i=1}^{4} \alpha_i K_0(\beta_i h / a^{a}{}_{s}) + C_B \sum_{i=1}^{4} \alpha_i K_0(\beta_i b / a^{b}{}_{s}) + C_A \sum_{i=1}^{4} \alpha_i K_0(\beta_i h / a^{a}{}_{s})$$

We have carried out the calculation of energy refocusing at the bombarded with Ar^+ ions on the Cu (100) surface in the direction of <110>, and it was E_{rf} = 136eV. This value agrees well with the experimental value E_{rf} = 160 ± 30 eV in [7].

III. Conclusion

By computer simulation we calculated grazing incidence ions and the effect of refocusing for two component materials and the corresponding values of refocusing energy was found. Our calculations show that the particles that penetrated inside the crystal are also subject to multiple refocusing and these calculations are useful in the study of ion implantation and channeling processes.

It should be noted that the effect of ion refocusing is a first step for explaining a process of multiple refocusing, which is observed in the surface region of the target to the total reflection of the incident particles.

IV. References

[1] H.Brongersma, M. Draxler, M.de Ridder, P.Bauer. Surface composition analysis by low-energy ion scattering// Surface Science Reports, Vol 62, 2007, P 63–109.

[2] H. Winter Collisions of atoms and ions with surfaces under grazing incidence// Physics Reports, Vol 367, 2002, P. 387–582.

[3] Dzhurakhalov A.A., Kutliev U.O., Umarov F.F. Low energy ion scattering by atomic steps on the single crystal surface// Radiation Effects & Defects in Solids. London,2004, -Vol. 159.-P.293-299.

[4] W.Eckstein. Computer simulation of ion-solid interaction. Springer. Heidelberg, 1991

[5] J.F.Ziegler, J.P.Biersack, U Littmark. The Stopping and ranges of ions in solids. Pergamon Press, New York, 1985.

[6] A.A.Dzhurakhalov, U.O.Kutliev, B.S.Kalandarov, M.Kurbonov, H. Dreysse Study of ion scattering and dechanneling from surface defect structure by computer simulation//Computational materials science –Amsterdam.2002,24.-P.111-116.

[7] E.Mashkova, V.B.Flerov. Reflection of ions from the monocrystals at the grazing incidence// Poverkhnost, Moskow,1983,№3.P.41-46.