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# INVESTIGATION OF DEFECT INP(001) SURFACE BY THE METHOD OF LOW ENERGY ION SCATTERING

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Бошланғич энергияси 3 кэВ бўлган $Ar^+$ ва $Xe^+$ ионларининг нуқсонли InP(001) сиртидан сочилиш жараёни тадқиқ қилинди. Компьютерда моделлаштириш жараёнида сонли таҳлилга асосланган кетма-кет тўқнашувлар усулидан фойдаланилди. Шу нарса аниқландики, сочилган ионларнинг энергетик тақсимоти сиртдаги нуқсонларга боғлиқ бўлар экан ва шу нуқсонларга мос келувчи чўққилар энергетик тақсимотининг кичик энергияли қисмида кузатилар экан.

Исследовано малоугловое рассеяние ионов $Ar^+$ и $Xe^+$ с начальной энергией 3 кэВ дефектной поверхностью InP(001). Компьютерное моделирование на основе приближения бинарных столкновений позволяет проводить количественный анализ данных. Установлено, что энергетические распределения рассеянных ионов напрямую зависят от дефектной структуры верхнего поверхностного слоя, и эти дефекты образуют пики в малоэнергетической части спектра.

Investigation of grazing scattering of 3 keV $Ar^+$ and $Xe^+$ ions from the defect surface InP(001) are reported. Computer simulations based on the binary collision approximation permit one to carry out a quantitative analysis of data. It is determined that energy distributions of reflected ions directly depend on the defect structure of the topmost surface layer, and these defects form some peaks in low energy part of energy distribution.

## I. INTRODUCTION

The interaction of the low energy ions with atoms in solids is of fundamental importance for knowledge of the surface defect structure as well as for development of analysis technique [1-3].

Understanding of the theory of particles traveling through matter began with the work of Bohr [4]. As the energetic ion (or atom) moves through a solid, it interacts and collides with lattice atoms. This interaction is due to the force of repulsion between the two nuclei and between the two electron clouds, and attraction between nuclei and electrons. It is usually described in terms of an interatomic potential, the precise form of which depends on the degree of nuclei penetration through the electron screen. Scattering can be described in terms of simple binary collisions or sequences of such collisions. However in addition to energy loss via such collisions the incident particle loses energy directly to the electrons in the solid, and particularly at scattering high energy light ions, the latter is the dominant process. As a simple rule of thumb, when the energy (in keV) is less than the ion mass (in amu) ($E < M$) then elastic energy loss dominates. When the energy is greater than the ion mass ($E > M$), inelastic energy loss dominates [5].

In this work we present the low energy ion scattering (LEIS) investigations on the point defect of InP(001) surface. Unique properties of InP have attracted enormous research interest. It is being widely applied in high speed electronic and opto-electronic

devices due to its attractive electronic properties as well as its excellent lattice match with low band gap alloys like GaInAs, GaInAsP, AlGaInAs, etc. GaInAsP/InP-based photo-diodes operate in low loss window of silica bers with high quantum efficiency and fast response time. Due to its excellent physical properties, like high thermal conductivity, high peak velocities for electrons and holes, InP is considered an important semiconductor material and it is being prominently utilized in the devices for high electron mobility transistors, high efficiency and high speed quantum well lasers, photodetectors, photonic integrated circuits, etc. InP is also preferred, over GaAs based devices, for millimeter-wave sources and amplifiers due to its low noise and higher efficiency operations in high frequency regime [6].

## II. COMPUTER SIMULATION AND RESULTS

For a study process of ion scattering we use a computational model which is based on approximation of pair collisions. In the approximation of pair collisions, two basic programs are used to simulate a wide range of processes caused by the bombardment of solids by accelerated particles – the program MARLOWE and program TRIM. The basis of both programs is almost the same formalism. The difference between these programs is that the first one initially operates on crystalline targets, while the second one – on amorphous ones [7].

The simplest approach applied to describe collisions of particles is to treat each interaction as a binary collision. This approximation is valid due to the limited range of interaction of the nuclei, and hence other nuclei will not be involved. Total energy will be conserved, so the energy lost by the incident ion will be gained by the target atom [8].

It is a convenient approximation to describe the interacting particles as point masses, which is reasonable in view of the nucleus size. There are forces of attraction between nuclei and electrons, and repulsion between nuclei and between electrons. The interaction is governed by the potential between the two particles, which is the sum of the potentials of interaction for each individual electron and the nuclei from the two particles. A useful simplification is to treat the potential for interaction as simply the potential between the two nuclei, with the electrons serving only to screen the positive nuclear charges from each other hence reducing the effective positive charges.

For small atomic separations $r$ ($0<r<<a_0$), where $a_0$ is the radius of the Bohr orbit in hydrogen (=0.53 Å) there are no electrons between nuclei, and the potential is purely repulsive and can be described by a Coulomb potential.

Using the hard sphere model a collision between an energetic ion and a stationary target atom is illustrated in Fig. 1. The incident ion (mass $M_1$) moves towards the target atom (mass $M_2$) with some perpendicular distance between the line of the centre of the

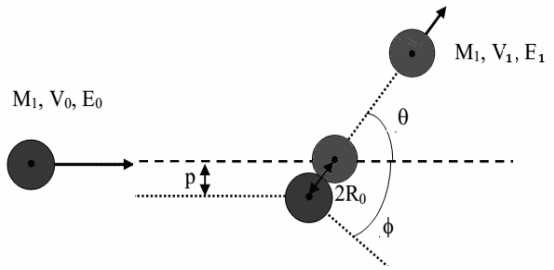



**Figure 1.** Scattering geometry for two colliding particles.

particles, $p$, called the impact parameter. The centre of the incident ion will approach the centre of the target atom to a distance equal the sum of the radii of two spheres, $2R_0$, where a collision takes place. The incident ion will be scattered and energy will be imparted to the target ion causing its recoil. Because there are no external constraints the total energy and momentum are conserved [9].

Figure 1 presents the scattering geometry for two colliding particles. A particle of mass $M_1$ strikes with a velocity $v_0$ the target atom which is initially at rest and who's mass $M_2$. If there were no interaction between the incidence particle and the target atom, the particle would pass at a distance $p$ from the target atom. As a result of the interaction the particle is scattered through an angle θ relative to the direction of its initial motion. As regard the target atom, after the collision it moves in a direction that makes an angle ϕ with the direction of the initial motion of the incidence particle.

This atom called a recoil atom. If the collision is elastic, i.e. if it is not accompanied by changing a charge in the internal state of the particles, then from the laws of conservation kinetic energy and momentum we obtain expressions both for the energy of the particle scattered through an angle θ. Using the universal potential of Ziegler-Biersack-Littmark interaction [10] 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.

$$E_1 = E_0\left(\frac{M_1}{M_1+M_2}\right)^2\left[\left(\cos\theta_1 \pm (M_2/M_1)^2 - \sin^2\theta_1\right)^{1/2}\right]^2.$$

For consideration of possible simultaneous collisions of ion with several target atoms, the procedure proposed by Robinson and Torrens [11] 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 [12] and included into the scattering kinematics. The incident ions 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 is explained by the model of the semichannels formed on the surface of solids.

We have studied the processes of scattering of $Xe^+$ ions from the defect surfaces of InP(001)<110>, (001)<ĭ10> single crystals, for small values of the angle incidence (ψ = 3º, 5º, 7º) with the initial energy of the incident particles equal to 3 keV (Fig. 2). At the bombardment of the surface InP(001)<110> by Xe ions in mentioned angle of incidences the energy distribution have double peaks which formed by surface atoms and semichannel (Figure 2a.).

From the energy distribution which presents on Figure 2b we can see several peaks. It is necessary to note that the geometric parameters (depth and widely) surface semichannel formed in <ĭ10> direction large than in direction <110>.

In the energy distribution we see two peaks with more high energies which are related to particles scattered from surface atoms and semichannel. But also we can see low intensively peaks on the energy spectrum. That low energy peaks formed by the ions scattered from point defects. In this two case, peaks presented in the energy spectrum

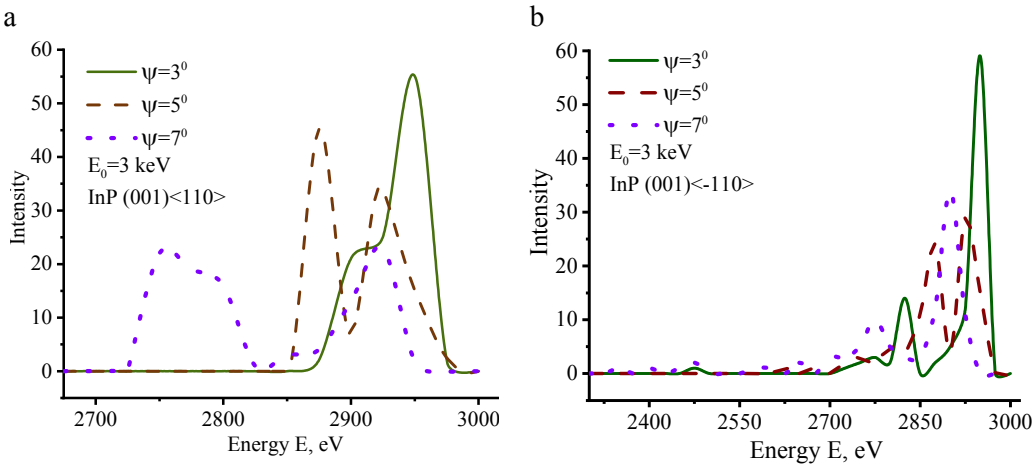



**Figure 2.** Energy distributions of Xe ions from the defect structure InP(001)<110> (a), InP(001)<ĭ10> (b) with the initial energy 3 keV and ψ = 3º, 5º, 7º.

resulting from collisions of $Xe^+$ with In (surface atomic chains) and P (semichannels) surface atoms are clearly visible. The scattered ion energies are observed to be slightly below those for purely elastic scattering, presumably due to inelastic processes during the collision event.

We can note from this distribution that in low energy part of energy spectrum some peaks are observed formed by scattered ions from point defects.

The energy distributions of scattered of $Ar^+$ ions with the initial energy $E_0$= 3 keV from the defect surfaces of InP(001)<110>, InP(001)<ĭ10> monocrystals are presented in Fig. 3 at the incidence angle of ψ = 3º, 5º, 7º.

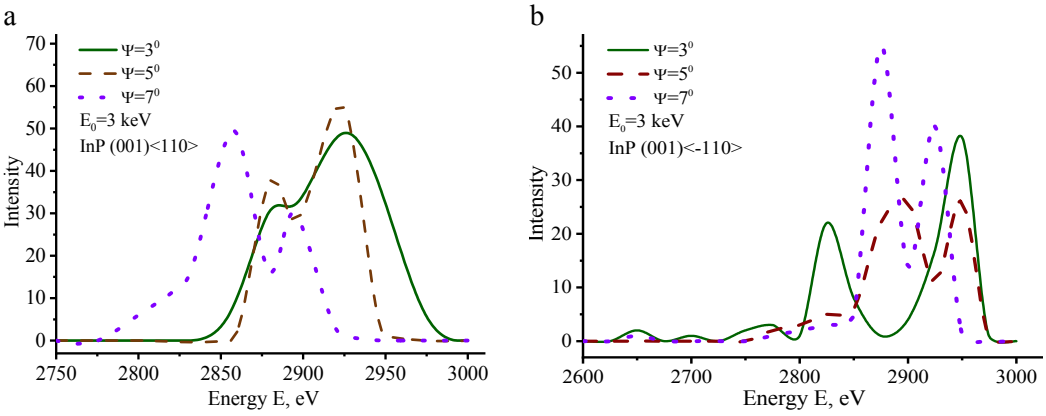



**Figure 3.** Energy distributions of Ar ions from the defect structure InP(001)<110> (a), InP(001)<ĭ10> (b) with the initial energy 3 keV and ψ = 3º, 5º, 7º .

We compare these energy distributions with the case of Xe ion scattering from the defect surfaces of InP(001)<110> and InP(001)<ĭ10>. At the scattering Xe ions from the direction InP(001)<110> we observed separate peaks of surface atomic row, defects and

semichannel. These peaks are similar ones in the case Ar ions. In the direction InP(001)<ĭ10> we can observe separate peaks of surface atomic rows, defects and semichannel more clearly.

For study of formation of peaks in the energy distribution we shall consider characteristic trajectories for above mentioned directions.

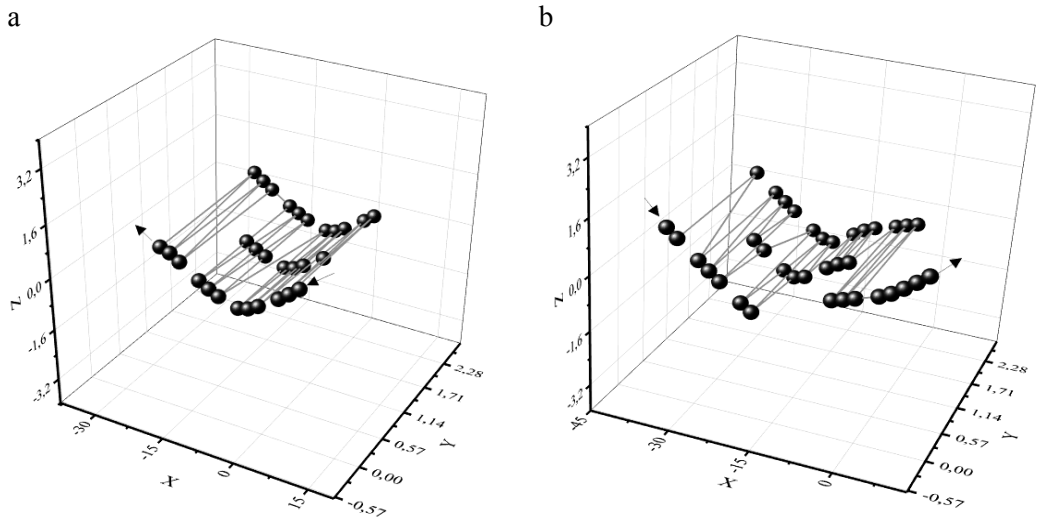



**Figure 4.** Characteristic trajectories of Xe ions (line) from the defect structure InP(001)<110> (a), InP(001)<ĭ10> (b) with the $E_0$ = 3 keV and ψ = 7º.

In Figure 4 presents the characteristic trajectories of Xe ions (lines) from the defect structure InP(001)<110>(a) and InP(001)<ĭ10> (b) with $E_0$ = 3 keV and ψ = 7º .

At firstly from these pictures we can see point defect structures for above mentioned direction and one of the simple trajectories scattering ion. It can be seen that in the absence of a surface atom, the incident ion collides with the next atom of the surface. Our calculations showed that the absence of an atom leads to a decrease in the number of collisions of incidence particles with atoms of the surface.

Study of characteristic trajectories scattering ions also will get more information about penetration of ions into the surface layers.

We calculated all physical parameters ion-atom collision. In the case Xe ion scattering from point defect of surface InP(001)<110> (Fig. 3a) the coefficient of collision is 29, inelastic energy loss is 61 eV. In the case InP(001)<ĭ10> (Fig. 3b) the coefficient of collision is 36, inelastic energy loss is 77 eV. These parameters and pictures show that by using LEIS method we can get information about point defect surfaces and we can determine displacement of point defects on the surface.

## III. CONCLUSION

The present study shows, for low energy ion scattering from point defect structures, the theoretical interest is in the calculation of the distributions of the defects, while for LEIS the dependence of the energy of the scattered projectile ions on scattering angle and the depth at which the scattering centre is located is the primary interest. Essentially the relevant theory is required to relate the yield of the detected scattered ions as a function of

energy at a reference scattering angle to the density and depth distribution of the different scattering atoms. It is necessary therefore, to consider the theory of elastic scattering processes in order to determine the energy loss per collision as a function of the scattering angle and the masses of the colliding particles. In principle this information enables the range of the projectile particle to be calculated and the distribution of displaced target atoms to be determined.

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