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INVESTIGATION OF TRAJECTRORY AND ANGULAR DISTRIBUTIONS SCATTERED Ar IONS FROM THE DEFECT InP(001) SURFACE

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Abstract. The Ar^+ ions scattering from the defect InP(001)<110>,<ī10>surfaces at the grazing incidence have been simulated by the computer simulation method. The trajectory and angular distributions of scattered argon ions on above mentioned surface semichannels have been calculated.

Keywords: computer simulation, ion scattering, semichannels, semiconductors.

Nuqsonli InP(001) sirtidan sochilgan Ar ionlarining trektoriyalari va burchak taqsimotlarini tadqiq qilish

Annotatsiya. InP(001)<110>,<ī10> sirtidan Ar^+ ionlarining kichik burchaklarga sochilish jarayoni kompyuterda modellashtirish usuli bilan o‘rganildi. Sochilgan argon ionlarning traektoriyalari va burchak taqsimotlari o‘rganildi.

Kalit so‘zlar: kompyuterda modellashtirish, ion sochilish jarayoni, yarim kanal, yarimo‘tkazgichlar.

Исследование траектории и угловые распределения при рассеяние ионов Ar с дефектной поверхностью InP(001)

Abstract.Малоугловое рассеяния ионов Ar^+ с поверхностью InP(001)<110>,<ī10> изучена с помощью метода компьютерного моделирования. Траектории и угловые распределения рассчитаны для ионов аргон, рассеянных вышеупомянутой поверхности.

Ключевые слова: компьютерное моделирование, рассеяния ионов, полуканалы, полупроводники.

1. Introduction.

In the last few decades, research on surfaces and interfaces bas grown to a mature branch of science. Subject of surface science is the study of processes on or properties of the interface between two media. The knowledge obtained can be fruitfully applied in various technological fields such as microelectronics, micro precision mechanics and heterogeneous catalysis. This works mainly concentrates on the surface analysis by means of ion scattering spectroscopy. The applications discussed will be on the solid-vacuum interface. The insight was grown, that for the understanding of many surface related problems, properties which are known from bulk physics cannot directly be extended to the surface[1]. It can easily be apprehended, that there will be a difference between bulk and surface atoms. In the bulk, without defects, an atom is fully surrounded by neighbor atoms and it is in equilibrium with its neighbors. If a surface is being made, for instance by cleavage of a crystal, bonds of the atoms in the cleavage plane with part of their neighboring atoms will be broken and the equilibrium will be disturbed. Breaking the bonds between atoms costs energy; the surface contains extra energy, the surface energy. Because of the disturbance of the equilibrium of the bulk atoms, it is not likely that the freshly cut surface is in the energetically most favorable state. The surf ace atoms will rearrange, so that the surface energy will be minimized. Three processes by which this minimization of the surface energy can take place will be mentioned [2-4].

Recently, Low Energy Ion Scattering (LEIS) has gained some momentum with the availability of high-end instrumentation for real-world surface analytical applications. These instruments make the unique capabilities of LEIS accessible by implementing a special analyzer design, allowing the quantitative analysis of the elemental composition of the outermost atomic layer of a material with high sensitivity and mass resolution. The technique [5] is based on the scattering of noble gas ions that are directed at the surface with a kinetic energy of 1 – 8 keV. In binary collision some of the ions are scattered back from the surface and can be detected by the energy analyzer. In the collision event, the ions exhibit a characteristic energy loss that is measured and used to determine the mass of the surface atom that was acting as the scattering partner. In contrast to non-dedicated

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instruments, the sensitivity of the analyzer is high enough to detect all required information of a given area before the surface is modified by the ion bombardment. The energy resolution and scattering geometry allow separating virtually any pair of elements, even with overlapping isotopes [6-7]. Applications of LEIS range from fundamental research to industrial materials, especially in the field of thin films and catalysis. The extreme surface sensitivity and the ability to analyze extremely rough and insulating samples make it the ideal technique for catalysis applications, where the functionality of the material is localized in the outer surface and simultaneously the concentrations of the analyte on the support may be very low. With detection limits in the range of a few atomic per cent for light elements up to the 10 ppm range for heavy elements – always as a fraction of the outermost atomic layer – modern LEIS does not have a need for model systems with higher concentrations of the active phase, but works on productions catalysts. On these samples, the technique can determine the amount of metal on the support that is really available to the catalysis, which is important for optimizing material usage. Amongst others, poisoning processes and formation of coke can be studied, including the localization of nucleation of coke. Recently [8] even the size of nanoparticles has been determined with a non-imaging methodology that does not suffer from statistical errors caused by the limited field of view of imaging techniques.

2. Computational method and results.

The present computer program for a calculation of the ion trajectories is based on the binary collision approximation. The binary collision approximation (BCA) has long been used in computer simulations of the interactions of energetic atoms with solid targets, as well as being the basis of most analytical theory in this area. While mainly a high-energy approximation, the BCA retains qualitative significance at low energies and, with proper formulation, gives useful quantitative information as well. 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.The foundations of the BCA in classical scattering are reviewed, including methods of evaluating the scattering integrals, interaction potentials, and electron excitation effects.For the description of the particle interactions the Biersack-Ziegler-Littmark (BZL) potential which gives quite good agreement with experiment over a wide range of interatomic spacing was used[9]. The inelastic energy losses were regarded as local depending on the impact parameter and included into the scattering kinematics. These losses have been calculated on the basis of Firsov model modified by Kishinevsky [10]. 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 sputtering and implantation results is insignificant.

The angle of incidence of primary ions ψ and the polar escape angle δ of scattered atoms were counted from a target surface and the azimuthal escape angle φ - from the incidence plane of the ions. The number of incident ions is 10^4. The incident ions and the recoil atoms were followed throughout their slowing-down process until their energy falls below a predetermined energy: 25 eV was used for the incident ions, and the surface binding energy was used for the knock-on atoms.

The possibilities of this code are following: 1) to carry out the calculations without inelastic energy losses or with their inclusions on one of three models: Kishinevsky, Firsov, Oen-Robinson (for light particles); 2) to vary the interaction potentials: Born-Mayer, Moliere, BZL; 3) to compute the time integral or to use the hard sphere model; 4) to calculate the parameters of the scattering ions for different values of mass ratio of colliding particles; These calculations do not require the change of code structure and may be performed by choice input parameters.

Using this methodology was simulated the behaviour of the scattering of 5 keV Ar^+ ions from defect InP(001)<110> and <$\bar{1}$10>surfaces have been investigated at the grazing incidence. It has been shown that the behaviour of the scattering depend to the orientation of single crystal. The structure of InP are very interesting. The atoms In and P located layer by layer in directions <110> and <$\bar{1}$10>.

In Fig.1 the simple trajectory at the angle incidences $\psi=5^0$ (a) and 13^0(b) with a initial energy 5 keV of Ar^+ ions bombarding of InP(001)<110> surface are shown.

It is seen the ion moved inside the semichannel in both angle of incidence. We can see from the structure some defects like absence of atom. In the case $\psi=5^0$ the coefficient of collision - 23, inelastic energy loss -121eV . But in the case $\psi=13^0$we can also observe quasi double scattering effect in semichannel. The quasi single scattering prevail in the case $\psi=11^0$. In the case of $\psi=13^0$the coefficient of collision - 7, inelastic energy loss -53 eV

a b

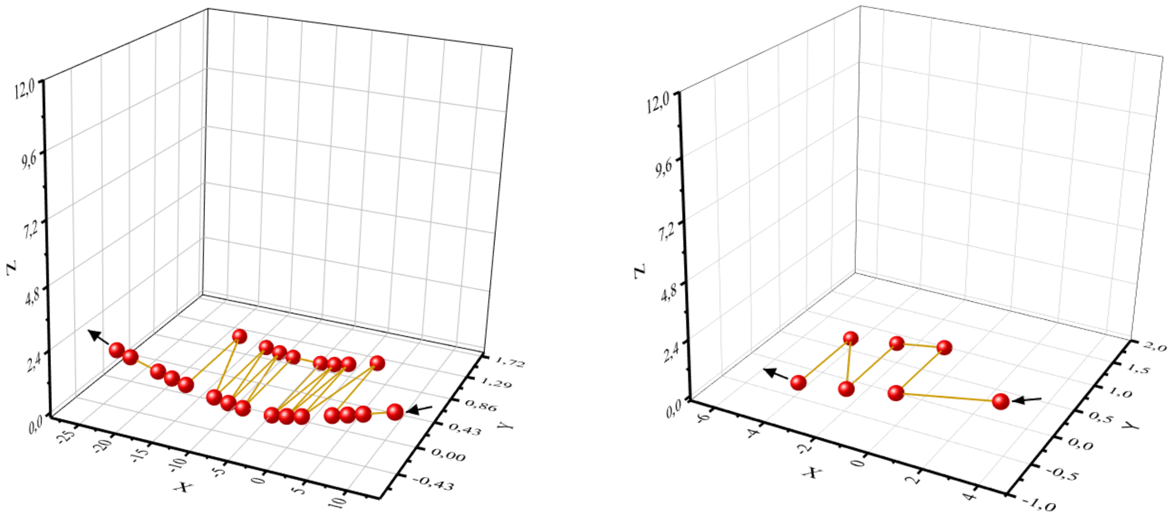

Fig.1. Simple trajectory on the angle of incidences $\psi=5^0$ (a) and 13^0(b) for 5 keV Ar^+ ions bombarding of InP(001)$\langle 110\rangle$ surface.

In Fig.2 presents the on of the characteristic trajectory on the angle o fincidences $\psi=5^0$ (a) and 13^0(b) for 5 keV Ar^+ ions bombarding of InP(001) $\langle\bar{1}10\rangle$surface. In this case the semichannel which formed on the surface. It is seen in the case $\psi=5^0$ (fig.2a) the ion at first scattered from four atoms which located on the surface. There are observed collision with atoms which located at the bottom of semichannel (five atoms). And then the ion turn to the up of semichannel and fully scattered from this semichannel. The coefficient of collision - 31, inelastic energy loss -108eV . In the case $\psi=13^0$ (fig.2b) the ion after capture by semichannel have almost same trajectory, but the number of collision with a semichannel atoms is difference. The coefficient of collision is 8 and inelastic energy loss is 44eV.

Also was received an angular distribution of Ar^+ ions, scattered from the defect InP(001)$\langle\bar{1}10\rangle\langle 110\rangle$with a initial energy 5 keV and on the angle of incidence $\psi=5^0,9^0,13^0$.

a b

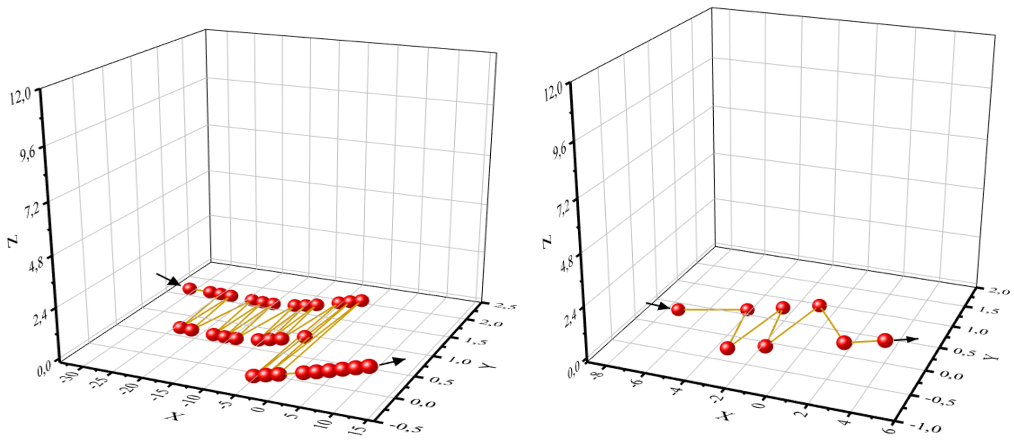

Fig.2. Characteristic trajectory on the angle of incidences $\psi=5^0$ (a) and 13^0(b) for 5 keV Ar^+ ions bombarding of InP(001) $\langle\bar{1}10\rangle$surface.

The analysis of angular distributions on the InP(001)$\langle 110\rangle$ and $\langle\bar{1}10\rangle$ directions we can see high intensity at the angle of incidence $\psi=5^0$(fig.3a). The high intensity peaks on the angular distribution are observed by the effect ion focusing. At the ion incidence $\psi=9^0$ also more intensity peak are observed since values of this angle very close to the ion focusing angle. At the ion bombarding InP(001)$\langle\bar{1}10\rangle$ direction dominated the effect mirror scattering of ions(fig.3b). The mirror effect, especially the mirror effect, has prevalence on $\psi=13^0$. The high intensity on angular distributions' will get more information about effects ion focusing.

a b

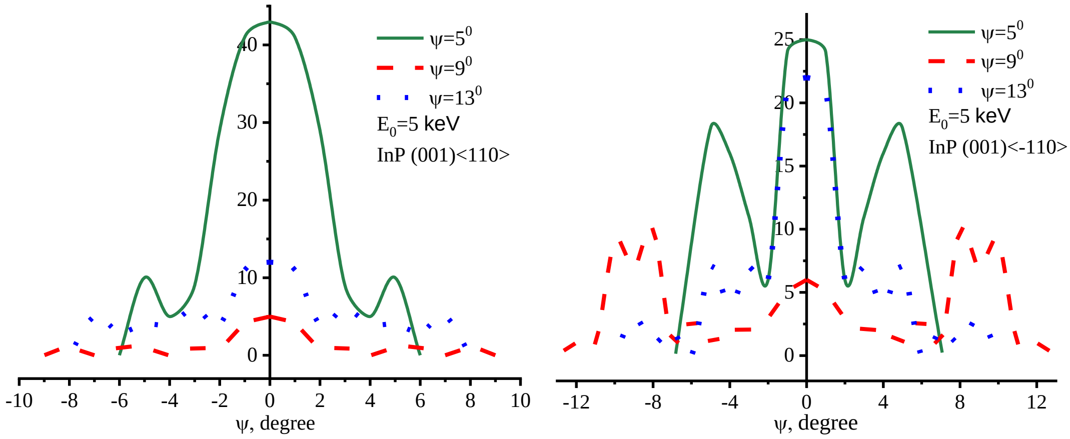

Fig.3. Angular distribution at the angle incidences $\psi=5^0,9^0,13^0$ for 5 keV Ar^+ ions bombarding of InP(001)<110>(a) and <ī10>(b) surfaces.

3. Conclusion.

It was shown that the scattered Ar ions from the defect InP(001) surface have special trajectories. The incidence ions had collision with surface atoms which located on atomic chains and semichannels. The fact that the inelastic losses exceed the elastic ones for small angle of incidence is due to an increase in the number of collisions and the particle trajectory length in the surface region, as well as to the absence of small impact parameters in the course of scattering. The predominance of the inelastic energy losses should reveal itself in the efficiency of the various inelastic processes accompanying the glancing ion scattering from a single crystal surface. The study of angular distributions of scattered ions from defect surfaces can give opportunity determinate the effect of ion focusing.

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