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INVESTIGATION OF THE ION SCATTERING PROCESS FROM THE A3B5 SEMICONDUCTORS BY THE COMPUTER SIMULATION METHOD

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Abstract: Scattering of Ar^+ ions from InP(001) at the grazing incidence was studied by the binary collision approximation method. The energy and angular distributions was obtained. At the energy distribution observed few peaks corresponding to the ions scattered from atomic chains and semichannels. Received results are interested at the study of semiconductor surfaces.

Keywords: computer simulation; ion scattering; semiconductors; binary collision approximation;

I. INTRODUCTION

In the last few decades intensive research has focused on $A^{III}B^{V}$ semiconductor surface structures [1]. On the one hand, the forces driving the surface structure formation are important for the understanding and control of material growth at a microscopic level. Usually, however, the surface structures formed in the technologically relevant gas phase epitaxial are not known in detail, but are simply assumed to be similar to those of the clean surface in ultrahigh vacuum [2]. On the other hand, semiconductor surfaces allow for the two-dimensional or even one-dimensional confinement of electrons, thus giving rise to peculiar many-body effects which are of fundamental interest. The electronic and structural properties of III-V compound (001) surface reconstructions, by contrast, are generally believed to be governed by a few simple principles [3]. One of the element from the group III-V compound semiconductors is a indium phosphide (InP) which used to produce efficient lasers, sensitive photo detectors and modulators in the wavelength window typically used for telecommunications, i.e., 1.55 micron wavelengths, as it is a direct band gap III-V compound semiconductor material. InP is the most important material for the generation of laser signals and the detection and conversion of those signals back to electronic form. Due to its high index of refraction, devices are very small, but the optical loss is also relatively high, so InP is not typically used for passive functions.

Therefore the surface of the group III-V compound semiconductors investigated by the many methods. And one of them is a ion scattering spectroscopy.

The ion scattering process has been the subject of both scientific investigations for a long time and recent rapid developing nanotechnologies and thin-film technologies. This process underlies such well-known methods of surface science as ion scattering spectroscopy. Physically, the energy range under consideration is characterized by the dominance of elastic over inelastic energy losses, and by the possibility of considering classical binary collisions using single-center potentials and disregarding the binding energy of the scattering ion in the crystal lattice. The first of these factors determines the upper, and the second, the lower boundary of the energy range.

In the present paper we will briefly review the theoretical findings on the structure of the (001) surface of InP. These findings are explained and put in perspective using surface phase diagrams derived from first-principles binary collision approximation collision calculations.

II. COMPUTATIONAL METHODS AND RESULTS

The theoretical investigation of atomic collision processes in crystals caused by ion irradiation is usually done using computer simulation, because real physical conditions (e.g., complicated interatomic interaction potential, surfaces, interfaces, and defects) can be taken into account much easier than it is possible by using analytical methods [4]. The simulation used in our calculations to construct the trajectories of the ions or projectile scattered by target atoms is based on the binary collision approximation [5] with two main assumptions: (1) only binary collisions of ions within target atoms or between two target atoms are considered, and (2) the path in which a projectile goes between collisions is represented by straight-line segments (Figure 1). In the binary collision model, particles move along straight-line segments, representing asymptotes to their trajectories in laboratory system, and one determines

not a particle trajectory but rather the difference between the angles characterizing the initial and final directions of motion.

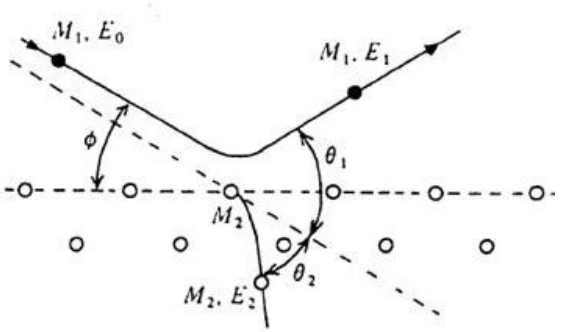


Figure.1. Scheme of binary collision approximation method

For the description of the particle interactions, the repulsive Biersack–Ziegler–Littmark (BZL) potential [6] 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 ε (E_0, p) were regarded as local depending on the impact parameter *p* and included into the scattering kinematics. These losses have been calculated on the basis of Firsov model modified by Kishinevsky [7] and contain direct dependence on the impact parameter:

$$\varepsilon(Eo,P)=\frac{0{,}310^{-7}vZ_1(Z_1^{1/2}+Z_2^{1/2})(Z_1^{1/6}+Z_2^{1/6})}{(1+\frac{0{,}67\sqrt{Z_1}r_0}{a_{tf}(Z_1^{1/6}+Z_2^{1/6})})}+(1-0{,}68\frac{V(r_c)}{Er})$$

where, *v* is the velocity of relative atomic motion, Z_1 is a greater, and Z_2 the smaller of the atomic numbers, and r_0 is in units of Å.

The expressions for the ion E_i energies after binary collision, taking into account inelastic losses, can be written as follows [8]:

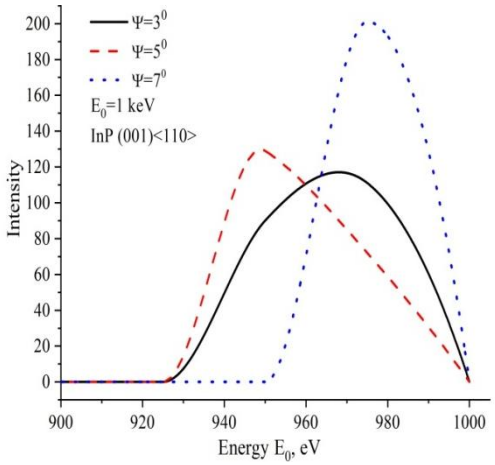
$$E_1=(1+\mu)^{-2}E_0(\cos\theta_1\pm\sqrt{(f\mu)^2-\sin^2\theta_1})^2$$

where f = [1 – (1 + μ)/με(E_0, p)/E_0]; θ_i and θ_r are the angles of ion and recoil scattering in the laboratory system of coordinate; E_0 is initial energy of impinging ion; p is impact parameter, and $\mu = m_2/m_1$. Estimating the accuracy of models for various values of the impact parameter in the low-energy range, it is necessary to notice that in a small impact parameter region (p < 0.5 Å), it is more preferable to use the Kishinevsky model; however, in the region of large impact parameters, all three models give approximately the same results, and they are useful even when the energy E_0 ~ 100 eV.

In Figure 2 presents the energy distributions of Ar^+ ions, experiencing specular scattering on chains of atoms on a clean InP(001)<100> surface with initial energies E_0=1 keV and 3 keV, angle of incidences $\psi=3^0,5^0, 7^0$. At the surface the atoms In and P located layer by layer. Therefore this surface mono crystals can be covered by only In or P atoms. In our simulations we considered surface semichannel formed by two surface P atom and one In atom from second layer. The acceptance of the analyzer collecting scattered particles, constituted by polar scattering angles is $\Delta\theta = \pm 0.5°$. In the case, when we use as the initial energy of bombardment ions was E_0=1 keV, in the energy distribution we can observe only one intensive peak. Our calculation shows that this peaks formed by the ions, which scattered from surface atomic chains. The bombardment ions can't get into inside the mono crystal surface. In the case E_0=3 keV, the energy distribution have two peaks. Ions scattered from surface atomic chains formed a peak at high energy part of distribution and second peak formed by the ions scattered from surface semichannnels. Comparing this two energy distributions shown that the increasing initial energy of incidence ions at the grazing incidence call to penetrate into mono crystal.

Figure 3 presents the angular distribution for above two cases. It is seen that in all case the angular distribution we can observe two-peak structure.

For a grazing incidence angle $\psi=3^0$ and scattering angle $\theta=6^0$ a distinct double-peak structure is observer in the primary ion energies (in our case 1 keV and 3 keV). The height of the high energy peak will be rather considerable, and under certain conditions it may be comparable with the height of the low-energy peak. From the angular distribution, in particular, for $\psi=7^0$ and $14=6^0$ and for primary ion energy 1 keV the height of the high- energy peak exceeds 75% of the height of the single peak.



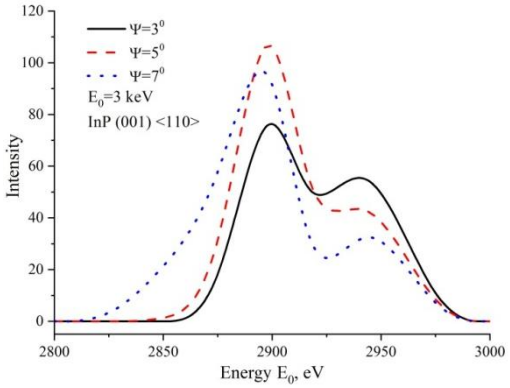


Figure.2. Energy distribution of scattered Ar^+ ions from InP(001)<110> at the ψ=3^0,5^0, 7^0 and E_0=1 and 3 keV.

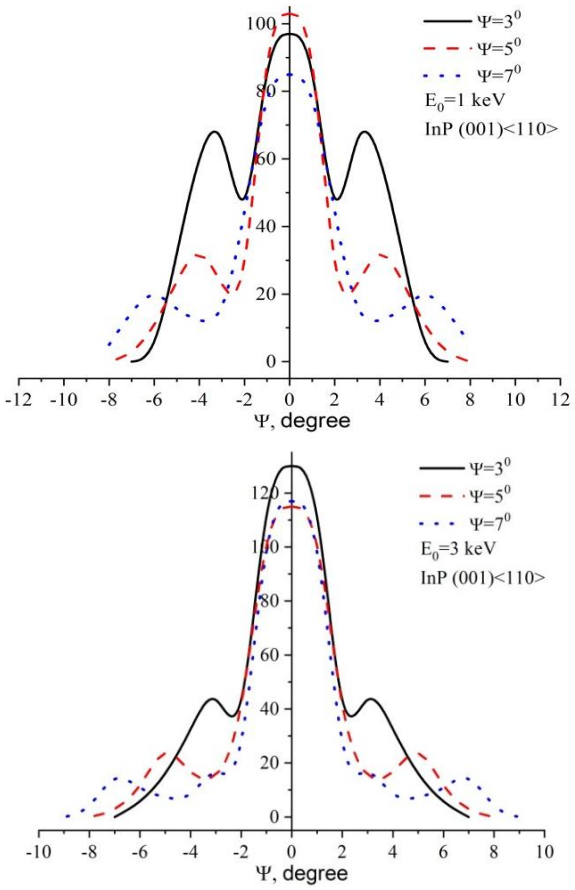


Figure.3. Energy distribution of scattered Ar^+ ions from InP(001)<110> at the ψ=3^0,5^0, 7^0 and E_0=1 and 3 keV

III. CONCLUSION

There is a clear and distinct peak in the energy spectrum shows that LEIS technique can be used effectively to identify the elements of the $A^{III}B^V$ semiconductor. On the other hand as azimuthally scan shows that there is symmetry of mirror scattered particles from $A^{III}B^V$ semiconductor. There are peaks in the scan that happens at mirror scattered, indicated in the $A^{III}B^V$ semiconductor symmetry is one-segment. This symmetry is forbidden in terms of crystallography.

V. REFERENCES

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