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АКТУАЛЬНЫЕ ВОПРОСЫ СОВРЕМЕННОЙ НАУКИ, ОБРАЗОВАНИЯ И ВОСПИТАНИЯ В РЕГИОНЕ

CONTENTS

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ANGULAR AND ENERGY DISTRIBUTIONS OF LOW-ENERGY ARGON IONS AT THE SCATTERING FROM $A^{III}B^{V}$ SEMICONDUCTOR SURFACE

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Abstract. The Ar^{+} ions scattering from the InP(001)$\langle 110\rangle$,$\langle\bar{1}10\rangle$ surfaces at the grazing incidence have been simulated by the computer simulation method. The trajectory, energy and angular distributions of scattered argon ions on above mentioned surface semichannels have been calculated.

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

Аннотация. С методом компьютерного моделирования смоделировано рассеяния ионов Ar^{+} с поверхностью InP(001)$\langle 110\rangle$,$\langle\bar{1}10\rangle$.

Рассчитаны траектории, энергетические и угловые распределения ионов аргон полуканалах вышеупомянутых поверхностей.

Ключевые слова. Компьютерное моделирование, ионное рассеяния, полуканал, полупроводники.

Annotatsiya. Argon ionlarining kichik burchaklarda InP(001)<110>**,**<$\bar{1}$10> sirtidan sochilishi kompyuterda modellashtirildi. Yuqorida keltirilgan yarim kanallardan sochilgan ionlarning traektoriyalari, energetik va burchak taqsimotlari o'rganildi.

Kalit so'zlar: kompyuterda modellashtirish, ion sochilish, yarim kanal, yarim o'tkazgichlar.

1. Introduction

During the exploration of the III–V compound semiconductors, the fundamental properties of indium phosphide (InP) were studied in detail. But for almost two decades since its first discovery as a useful semiconductor material [1-3], it has received little attention for device applications because its properties were similar to those of GaAs but it was less convenient to prepare. The superior performance of InP Gunn diodes compared to those made from GaAs motivated the device-oriented work on InP materials in the 1960s. This superior performance primarily came from its higher peak-to-valley ratio in velocity–field characteristics and from its larger thermal conductivity. Other InP device applications, which stimulated research from the early 1970s until today, were components for optical communication in the $1.3 \le \lambda \le 1.6\,\mu$m wavelength region where optical fibers have minimum dispersion and loss. These components include single-junction photo voltaic cells, various light sources and detectors.

Although indium phosphide and related materials applications started with long-wavelength light sources and detectors in optical fiber communication systems, it has expanded too many different device applications. Today InP has emerged as the third most important semiconductor in the world after Si and GaAs[4,5].

In the early to mid-1980s, there was an emphasis on research in InP materials for microwave and millimeter-wave power transistors. Recently output power density as high as 1.8 W/mm at 30 GHz, has been reported. These impressive results come about as a result of higher electron saturation velocity, peak-to-valley ratio of velocity-field characteristics, thermal conductivity, and breakdown field, along with a lower ionization coefficient and dielectric constant. Lower interface states compared to GaAs have also allowed more successful MIS structures to be fabricated in this material system.

Using InP at the construction many devices are bounded it surface structures. Therefore the surface consist almost all physical-chemical properties of the crystal. So, at the study of the surface structure InP are used many methods. One of them is an ion scattering spectroscopy [6].

Low energy ion scattering (LEIS) is a surface analysis method that can identify atoms in the topmost layer of a material. It consists of directing a beam of monoenergetic ions at a surface and measuring the kinetic energy of the scattered ions. If a beam of inert-gas ions with incident energy below a few keV is used, nearly all ions that survive scattering result from events involving surface atoms. The energy loss of an incident ion following a binary collision is kinematically related to the mass of its collision partner, so energy analysis of scattered ions provides mass analysis of the surface. Angle-resolved LEIS, in which the orientation of the sample surface is varied with respect to the incident ion beam, further provides real space structural information about surface atoms. The information gathered is obviously of particular importance when multicomponent metallic systems are investigated. In such systems preferential segregation or favored surface terminations may cause the topmost layer to differ significantly in composition from underlying layers. Ion scattering methods, covering a wide range of energies from ~1 keV to ~1 MeV, and mainly using low atomic number ions such as H^+, He^+ and Li^+, but also often including Ar^+ and Ne^+ at low energies, have been used in a range of surface structural studies [7,8]. The basic physical principle exploited is of elastic scattering shadow cones, such that atoms behind a scattering atom on the incident ion trajectory may be hidden from the incident beam within a certain range of relative lateral displacements but will scatter incident ions if this lateral displacement is exceeded. The visibility of scattering from these subsurface atoms as a function of incident direction thus provides information of the relative locations of the surface atoms and subsurface atoms. Similar effects occur for the outgoing scattered ions, with surface atoms 'blocking' the scattered ions from subsurface atoms and preventing them from reaching the detector in certain directions. The precision of these methods is generally highest for higher energy ions for which the shadow cones are narrowest, when values of ~0.02—0.03 Å may be achieved. While each ion which scatters from a surface atom causes significant local damage due to the recoil of the scattering atoms, the information on this scattering atom relates to its position before the scattering event. For sufficiently low incident flux density, therefore, these methods can provide information on surfaces essentially devoid of damage induced by the incident beams.

Low-energy ion scattering spectroscopy is an exciting technique that allows to study the structure and chemical composition of a materials surface. In this materials characterization method the sample is bombarded with a stream of ions and the positions, velocities and energies of the scattered ions are observed. The energy of scattered ions depends on the mass of the target, so there are distinct peaks in the energy spectrum of the scattered ions. These peaks give information about the samples elemental composition. The uniqueness of this technique lies in its sensitivity to the very first atomic layer on a sample and with forward scattering setup it is even capable of directly observing hydrogen atoms.

The aim of this paper is to make an assessment of the attainable level of quantification in low energy ion scattering spectroscopy depth profiling in terms of both the depth and concentration parameters. With regards to depth, straight forward analytical calculations on a model target system will be shown to lead to a direct relationship between depth of scattering and the energy difference between ions scattered at the surface and those at greater depth. The approach used, which is also valid for complex, multi-layered compound targets, offers a clear and readily understandable insight in what can be achieved. However, in more complex layered systems, spectra can only be effectively interpreted using computer simulations that are based on the same analytical approach, but the use of simulation makes the physical basis of the approach less transparent.

2. Computational method and results

In LEIS the ions is much smaller than the effective range of the scattering potential. Unless the scattering angle is extremely small, diffraction effects can be neglected and the interaction process can be described classically. The repulsive atomic potential of the surface atoms will only become comparable to the energy of the incident ions at very short distances (typically 0,5 A), As a consequence, the surface may be described by means of binary collisions between single ions and single surface atoms.

The surface atoms can be considered as free atoms since the interaction times during a collision (10^{-15}s) are considerably shorter than the times associated with lattice vibrations (typically 10^{-13}s). The vibrational energy of the surface atoms ($\approx$ 0.025 eV at room temperature) can also be neglected as compared with the energy of the incident ions. The act of collision ion and surface atoms was shown in fig.1.

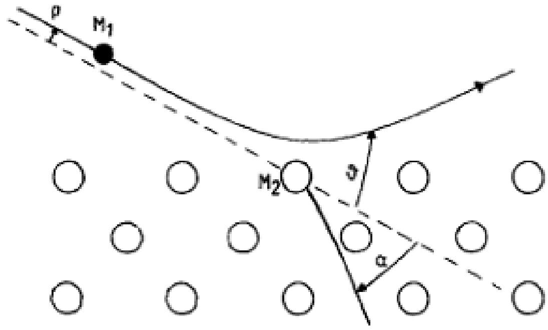

Fig.1. Schematic representation of the collision of an incident ion (mass M_1.) and a surface aton (mass M_2). The inpact parameter p determines the scattering angle Θ.

The present computer program for a calculation of the ion and recoil trajectories is based on the binary collision approximation. 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 Ne^+ and Ar^+ ions from InP(001)<110> and <$\bar{1}$10> surfaces have been investigated at grazing incidence. It has been shown that the behaviour of the scattering depend to the orientation of single crystal. The structure of InP are very interesting. The atoms In and P located layer by layer in directions <110> and <$\bar{1}$10>.

In Fig.2 the simple trajectory at the angle incidences $\psi=11^0$ (a) and 13^0(b) for 5 keV Ar^+ ions bombarding of InP(001)<110> surface are shown.

It is seen the ion moved inside the semichannel in both case. In the case $\psi=11^0$ the coefficient of collision - 21, inelastic energy loss -88 eV. But in the case $\psi=13^0$ we can observe quasi double scattering effect in semichannel. The quasi single scattering prevail in the case $\psi=11^0$. The coefficient of collision - 15, inelastic energy loss -62 eV.

In Fig.3 presents the simple trajectory at the angle incidences $\psi=11^0$ (a) and 13^0(b) for 5 keV Ar^+ ions bombarding of InP(001) <$\bar{1}$10> surface. In this case the semichannel which formed on the surface. It is seen in the case $\psi=11^0$ (fig.3a) the ion at first scattered from four atoms which located on the surface.

The are observer collision with atoms which located at the bottom of semichannel (five atoms). And then the ion turns to the up of semichannel and fully scattered from this semichannel. The coefficient of collision - 15, inelastic energy loss -83eV. In the case $\psi=13^0$ (fig.3b) the ion after capture by semichannel have almost same trajectory, but the num ber of collision with a semichannel atoms is difference. The coefficient of collision - 18, inelastic energy loss – 96eV.

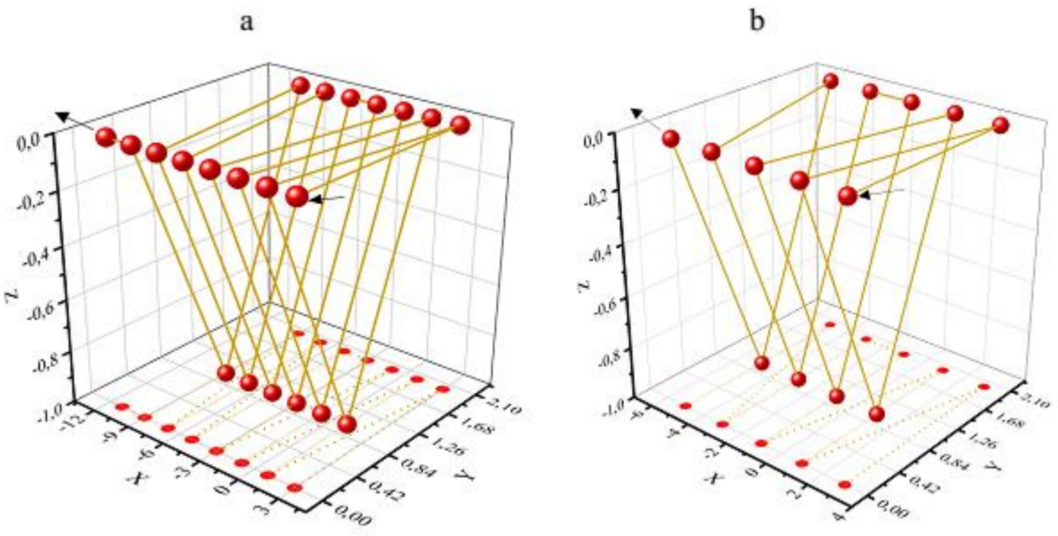

Fig.2. Simple trajectory at the angle incidences $\psi=11^0$ (a) and 13^0(b) for 5 keV Ar^+ ions bombarding of InP(001)<110> surface.

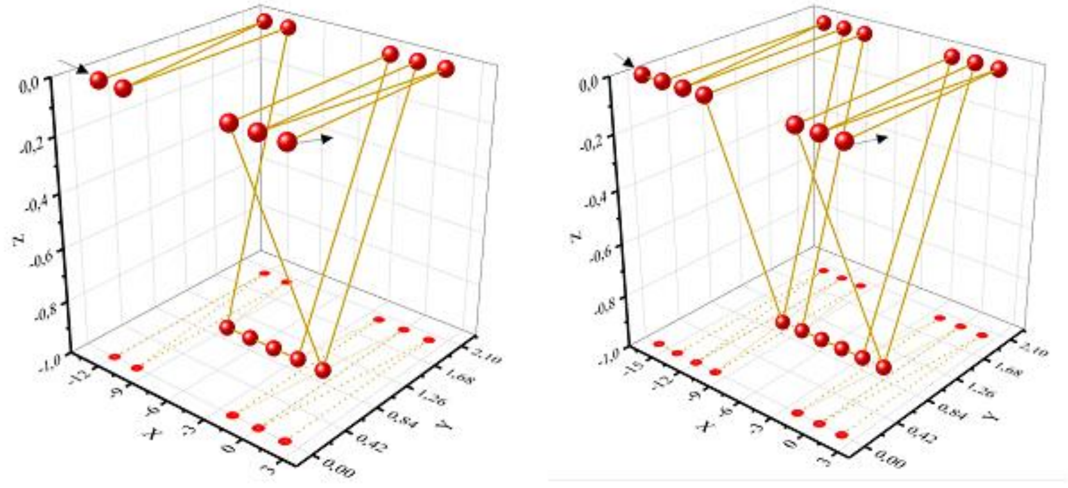

Fig.3. Simple trajectory at the angle incidences $\psi=11^0$ (a) and 13^0(b) for 5 keV Ar^+ ions bombarding of InP(001) <$\bar{1}$10> surface.

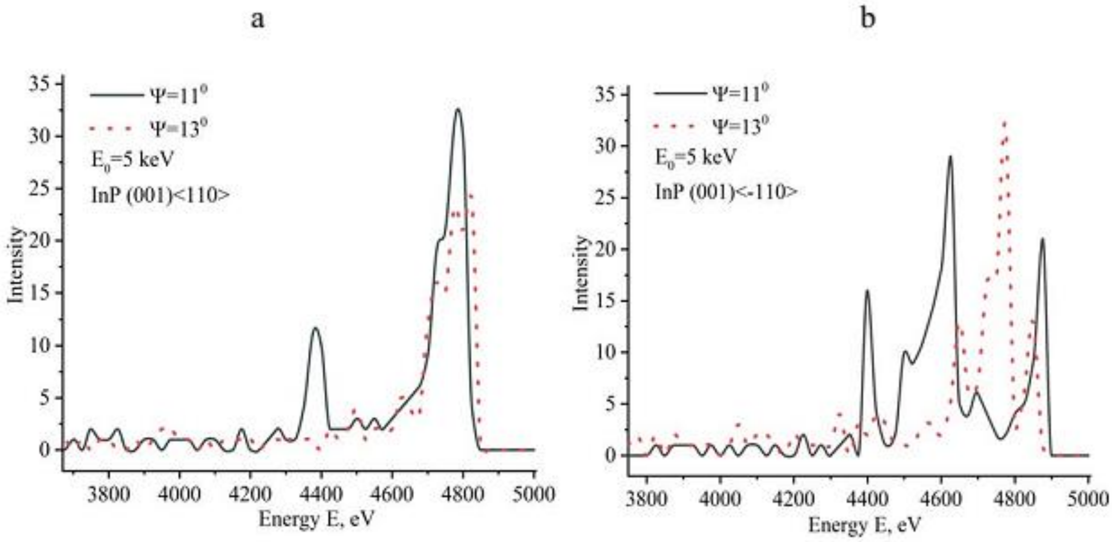

Fig.4. Energy distribution at the angle incidences ψ=11⁰ and 13⁰ for 5 keV Ar⁺ ions bombarding of InP(001)<110>(a) and <ī10>(b) surfaces.

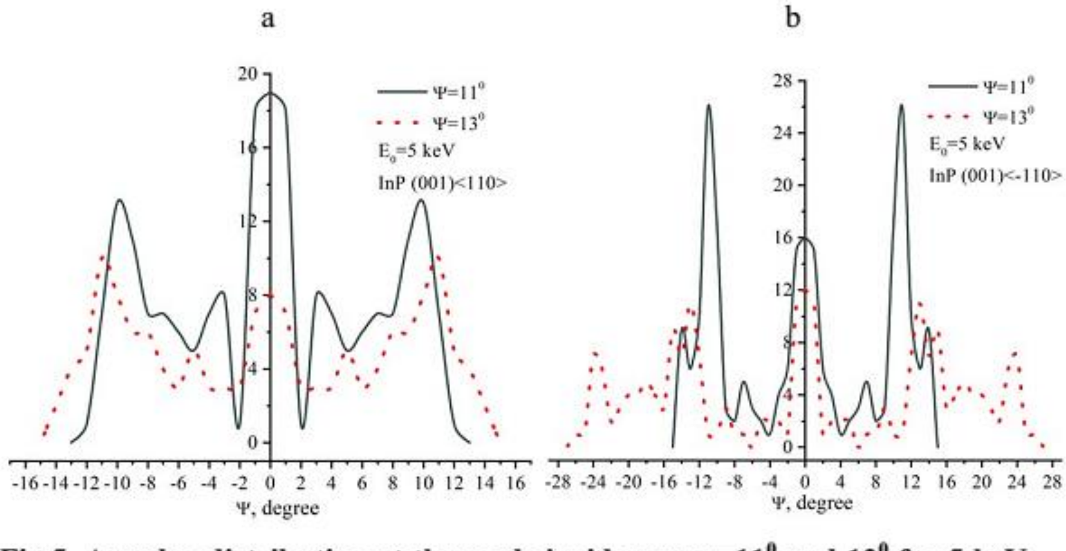

Fig.5. Angular distribution at the angle incidences ψ=11⁰ and 13⁰ for 5 keV Ar⁺ ions bombarding of InP(001)<110>(a) and <ī10>(b) surfaces.

On the Fig.5. presents the energy distribution at the angle incidences $\psi=11^0$ and 13^0 for 5 keV Ar^+ ions bombarding of InP(001)<110>(a) and <ī10>(b) surfaces.

On the energy distribution, we can observe doubly peaks spectrum. The peak, which formed on the higher energies, corresponded to the ions scattered from from surface atomic chains. Another peak, which formed low energies, corresponded to the ions scattered from surface semichannels.

The analysis of angular distributions on the InP(001)<110>(fig.5a) direction shown in both snapshots we can see high intensity at the angle of incidence $\psi=11^0$. This high intensity peak connected with a ion focusing effect. At the ion incidence $\psi=13^0$ also more intensity peak are observed since values of this angle very close to the ion focusing angle. At the ion bombarding InP(001)<$\bar{1}$10> direction dominated the effect mirror scattering of ions(fig.5b). The mirror effect has prevalence on $\psi=13^0$ in this case.

3.Conclusion

It was shown that the elastic energy losses are considerably smaller than the inelastic ones in a region of glancing scattering. 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.

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