Analysis of InGaP(001) surface by the low energy ion scattering spectroscopy

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Abstract. Ion scattering spectroscopy, which is a variation of low energy ion scattering (LEIS) that employs glancing scattering angles, is performed on InGaP(001) surfaces. LEIS energy distribution are simulated by computer simulation along the <110> and <ī10> direction, and the match of the positions of the flux peaks shows that the top three atomic layers are bulk-terminated. A newly observed feature are identified as a minimum in the multiple scattering when the ion beam incidence is along a low index direction. Calculated trajectories of scattered ions. This new method for analysis of large-angle LEIS data was shown to be useful for accurately investigating complex surface structures.

1. Introduction
Surfaces play an important role in a large number of industrial applications such as micro-electronics and chemistry. Due to the miniaturization of electronic devices, the surface-bulk ratio of these devices is increasing. Therefore, their properties are more and more determined by the surface. Nowadays, integrated circuits are often grown by depositing material on a semiconductor surface. Studying such a surface is more complicated than studying the bulk, both theoretically and experimentally. Theoretically, because the translational symmetry that simplifies the treatments of bulk properties, is not present perpendicular to the surface. Experimentally, because ultra-high vacuum conditions are needed in order to keep a freshly created or cleaned sample surface sufficiently long in its original state, since at ambient pressure a mono-layer may absorb in only $10^{-9}$ s. Especially the fact that equipment guaranteeing ultra-high vacuum conditions only became available commercially in the early 1960's, caused the late start of surface science. Despite this, its results are widely applied in technological fields such as micro-electronics and heterogeneous catalysis. The fact that the properties of a surface differ from those of the bulk can be illustrated in the following manner: consider an atom in the bulk. Such an atom is in equilibrium with all the atoms surrounding it. When a surface is made by cleaving a crystal, the bonds of the atoms at the cleavage plane are broken. Thus, the atoms at the freshly cut surface are no longer in equilibrium. By breaking the bonds the surface has also obtained extra energy, the surface energy. Therefore, in most cases the surface structure will change in order to minimize the surface energy. This can be achieved by chemical bond formation with adsorbing particles, by atomic displacement either parallel (reconstruction) or perpendicular (relaxation) to the surface, or by change of the chemical composition of the outermost atomic layers (segregation). There are many analytical techniques
available in surface science to obtain information about a sample surface. Each of these has its advantages and drawbacks, and provides only a specific kind of information. Therefore, in general a combination of different analysis techniques is used to characterize a surface [1-2].

Most surface analysis techniques use the interaction of a beam of particles with the sample surface to obtain the information. These particles can be either ions, electrons or photons. An important aspect of a surface analysis technique is the information depth, i.e. the depth in the sample from which the information is obtained. The information depth depends on the mean free path of the particles, and thus determines the surface sensitivity of an analysis technique. Because most of the surface effects take place in the outermost atomic layers, the information depth should preferably be limited to only a few atomic layers. Low-energy ion scattering (LEIS) is such a technique. In LEIS a primary beam of ions with an energy typically between 0.1 and 10 keV, is directed at a sample surface [3-4]. The ions interact with the atoms in the surface and due to this interaction they lose a certain amount of energy.

LEIS method also useful for the study structure of many component materials. Today, one of the many component materials is semiconductors, which have one or many elements [5-6].

One of them is a InGaP is an important semiconductor for the fabrication of optoelectronic and electronic semiconductor devices such as heterojunction bipolar transistors [7] and diode lasers[8]. Indium gallium phosphide is a wide band gap semiconductor, which is used, in high-power and high frequency electronics because of its superior electron velocity with respect to more common semiconductors silicon and gallium arsenide.

In this paper we presents investigation of InGaP(001) surface structure by the method of LEIS. At the calculations as a bombardment ion was used Ar ions.

2. Computational method and results
When an ion penetrates a solid, the ion will interact with the atoms in the solid. This interaction is a many particle problem and requires, at first instance, a quantum mechanical description. Since the quantum-mechanical model is too complicated to be of any practical use for computer simulation, a number of approximations is made in order to obtain a much simpler model: the binary-collision approximation (BCA) model. This model forms the basis of most computer codes for ion-scattering simulation. An important issue in ion-scattering simulation is the choice of the interaction potential, since it describes all quantum-mechanical details of the interaction between an ion and an atom. Within a solid, an ion interacts not only with the atomic nuclei but also with the electrons. This interaction causes two types of electronic processes to occur: inelastic energy loss and charge exchange. In our calculation, we used the potential of Biersack-Ziegler-Littmark (BZL) [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 angle of incidence of primary ions $\psi$ and the polar escape angle $\delta$ of scattered atoms were counted from a target surface and the azimuthal escape angle $\phi$ - from the incidence plane of the ions. In the figure 1 presents scheme of surface semichannel.

![Figure 1. The scheme of ion scattering by the surface semichannel.](image-url)
The incident ions were followed throughout their slowing-down process until their energy falls below a predetermined energy: 25 eV was used for the incident ions. The angle of incidence of the ion beam relative to the surface was changed in the range $\psi = 3^\circ$ and $7^0$, polar and azimuth scattering angles have been marked in $\delta$ and $\varphi$, respectively (figure1). The aiming points filled a rectangle whose sides were divided into 1000 and 1000 segments in the beam incidence plane (I coordinate) and in the perpendicular direction (J coordinate), respectively (figure1).

Using this methodology was simulated the scattering of 1 keV Ar$^+$ ions from InGaP(001)<110> and <ī10> surfaces at the grazing incidence. On the direction <110> formed surface semichannel, which consist In and Ga atoms. Atom Ga located on the surface layer and atom P on the second layer. And on the direction <ī10> formed surface semichannel by the atoms In which located surface layer, atoms Ga which located on second layer and atoms P which located on the third layer.

In figure 2 was shown $\delta$ (I) dependence at the angle of incidences $\psi=3^0$ and $7^0$ with initial energy 1 keV Ar$^+$ ions bombarding of InGaP(001)<110>(a) and <ī10> surfaces.

This dependence is very interesting for the separation of scattered ions from different parts of the semichannel. By studying this dependence, we can divide the scattered particles into three groups: the scattered ions from the atomic chain, the semichannel walls, and the bottom of the semichannel. Note that the scattered ions from the bottom of the semichannel and from the atomic chain mainly undergo mirror scattering. It can be seen that the scattered ions from the semichannel wall at small angle of incidence ($\psi=3^0$) have only positive values (mirror scattering), and with an increase in the angle of incidence ($\psi=7^0$) of the ions have both positive and negative values. Also, note that the geometric parameters of the semichannel also affect the dependence $\delta$ (I). Figure 2b shows that the dependence differs from the case <110>. Because in the case of <ī10>, the width and depth of the semichannel is greater than <110>.

![Figure 2](image_url)

**Figure 2.** The $\delta$ (I) dependence at the angle of incidences $\psi=3^0$ and $7^0$ with initial energy 1 keV Ar$^+$ ions bombarding of InGaP(001) <110>(a) and <ī10>(b) surfaces.

We also calculate trajectory of scattered ions. Couple of the simple trajectories scattered ions with the initial energy 1 keV presents on the figure 3. Using computational model we calculate couple of trajectories of scattered ions. On the figure 3a presents trajectory scattered ions at the angle of incidence $\psi=3^0$ on the point D from figure 2a. In this case the coefficient of collision- 39, energy of scattered ion -970 eV. On the figure 3b presents trajectory scattered ions at the angle of incidence $\psi=7^0$ on the point C from figure 2a. In this case the coefficient of collision- 68, energy of scattered ion -911 eV. This trajectories shows that by the increasing angle of incidence ions the depth of penetration of ions increases.
Figure 3. Trajectory scattered ions at the angle of incidence $\psi=3^0$ and $7^0$ on the points C(a) and D(b).

Figure 4. Energy distribution of scattered Ar$^+$ ions at the angle of incidences $\psi=3^0$ (dark yellow) and $7^0$ (red color) with the initial energy 1 keV bombarding of InGaP(001)<110>(a) and <110> surfaces.

On the figure 4 presents energy distribution of scattered Ar$^+$ ions at the angle of incidences $\psi=3^0$ (dark yellow) and $7^0$ (red color) with initial energy 1 keV bombarding of InGaP(001)<110> and <110> surfaces. At the angle of incidence $\psi=3^0$ on the both directions are observed only one peak (I) on the energy distribution. It means that the bombarded ions can’t penetrate to the semichannel and all incidence ions scattered from surface atomic chains. In the case <110> are observed intensive peak at large values of the energy of the scattered ions (I). This peak formed by ions scattered from the surface atomic chain. It should be noted, that the intensity of this peak increases with an increase in the angle of incidence of the ions. The second peak (II), which formed near the peak of the atomic chains, refers to the ions scattered from the semichannel. It can be seen that in the case of <110>, this peak has a large energy range and intensity than <110> case. This large energy range explained by a large geometric parameter of the semichannel.

3. Conclusion

LEIS simulations are performed for InGaP(001) <110>(a) and <110> surfaces. Calculated polar angle of scattering shows that we can separate group ions scattered from surface atomic chains and semichannel. And in all values of impact point we can plot trajectories of scattered ions. With the help of such simulations, the trajectories responsible for the features are much better understood. This includes common double peaks as well as a novel trajectory that involves interaction of the projectile with surface semichannels.

Our LEIS results have shown that the LEIS technique is quite suitable for surface investigations and diagnostic of many component materials.
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