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Investigation of Angular Spectrum of Scattered Inert Gas Ions from the InGaP (001) Surface

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In this work by computer simulation the low energy ion scattering by clean InGaP (001) <110> multicomponent single crystal under grazing ion bombardment conditions have been investigated, analyzed and the new data have been obtained. The effective original algorithms and computer codes of above mentioned ion-impact processes have been developed and created. The relationship between the spatial variables of the scattered beam (mainly azimuthal angular spectra) and the type of ions has been established. The correlation between focusing properties of surface semichannel with a type of bombardment ion at the different angle of incidence has been shown. It is shown that changes in the type of atoms of the semichannel lead to a change in the focusing properties of the surface semichannels.

Keywords: Ion scattering, Semichannel, Computer simulation, Angular distribution, Ion focusing.

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Introduction

InGaP has received increased attention recently because of the large direct bandgap attainable in this ternary. Initial experiments indicated that the maximum direct band gap is 2.2 eV, which makes Indium Gallium Phosphide (InGaP) a potentially efficient electroluminescent source of radiation up to the green portion of the visible spectrum. InGaP hetero bipolar transistors (HBT) epitaxial wafers will be used in high-frequency transmitter power amplifiers for the third-generation cellular phones. These HBTs will be small in size, and have high amplifying efficiency and good linear gain with low strain. Compared with field effect transistors, HBTs show lower power strain in broadband region and lower electricity consumption, and can be operated with a single power source. Compared with AlGaAs HBTs, InGaP HBTs have higher reliability and are advantageous in terms of manufacturing process [1, 2].

The InGaP HBT epitaxial wafer is drawing attention as a key material for devices in the third-generation cellular phones due to its advantages, including improved DC properties and high reliability. With the full-fledged start of the third-generation cellular phone services in the autumn of this year, demand for InGaP HBT epitaxial wafers is expected to increase sharply [3].

Therefore, investigation of surface structure InGaP thin film very interesting. To study the surface properties of this material, along with numerous methods, the method of low energy small angular scattering of ions is also used.

Low energy small angle ion scattering (LESAIS) mostly used for investigation of elemental structure and properties of the outermost atomic layer of the surface. This method is a one of the powerful tools for studying the relationships between surface phenomena such as cleaning, adhesion, thin film growth and so on. At present time, almost all of these results have been obtained on ions falling on the surface at large angles, and several models have been developed. Little has been done, however, with small sliding angles. However, very little experimental work has been done to study these processes in multicomponent substances, and no specific models have been developed to study these processes. The lack of experimental results in this direction hinders not only the solution of the fundamental problem, but also the solution of practical problems. In many cases, investigation of collision of fast particles with surface of solid body depends on azimuthal angle of scattering of particles from surface as a result of collision of fast particles with surface. Calculation of the azimuthal angle of ion scattering is very complicated and is determined by a large number of collisions. These difficulties interfere with analytical calculations, and the best method remains the computer simulation method. From this point of view, studies of the surface and near-surface structures of multicomponent semiconductor thin films using ion scattering spectroscopy and their re-surface use in modern micro- and nanoelectronics [4-8].

In this paper presents the investigation of InGaP(001) surface structure by the method of low energy small angular scattering of ions.

Computational method and results

When a low-energy (< 10 keV) ions hit a surface, several effects may occur. One of the possible effects is that the ion is scattered back from atoms in the outermost atomic layer of the surface. The energy and angular distribution of these ions provides information concerning the composition and structure of the surface. It will be shown that the scattering process between ions and surface atoms can be described classically which makes the interpretation relatively straightforward. Low energy small angle ion scattering (LESAIS) can be carried out with many types of ions. Usually noble gas ions (He , Ne , Ar) are used. The high neutralization probability of these ions prevents ions from leading the surface after a long interaction time with the solid. This makes LEIS suitable for the selective probing of the outermost layer of the surface. In this chapter some of the features of LESAIS are introduced [9, 10]. In LESAIS one very often uses a beam of noble gas ions. Due to their high neutralization probability, the fraction of particles, that return in a charged state after scattering from deeper layers, is very small. This and the fact, that only the ionized particles returning from the sample surface are analyzed, make LESAIS a technique that is well suited to studying the outermost layers of atoms. The interpretation of the spectra obtained with a LESAIS technique is in general a difficult task, because a large number of particles is involved in the scattering process. Besides this, the ions are influenced by electronic processes, such as inelastic energy loss and neutralization, during the scattering process. Therefore, computer simulations are often used as an aid in the interpretation. In this thesis we will discuss the aspects, both physical and algorithmic, of ion-scattering simulation in order to develop a computer code that is well suited to LEIS simulation. Two basic models for computer simulation have been worked out in the past: the classical dynamics (CD) model and the binary-collision approximation (BCA) model. The BCA can be used in computer simulations of the interactions of energetic ions with solid surface. Also can be the basis of most analytical theory in this area. In the low-energy region, the trajectories of colliding particles are determined in the first approximation by the elastic interaction forces of atoms. These are the Coulomb forces of interaction between the nuclei and electrons of atoms. They act at atomic distances between interacting particles. Consequently, to calculate the trajectory of an oncoming ion, it is necessary to consider its interaction with a set of atoms of the crystal lattice simultaneously. However, at the collision of very low energy ion with a crystal atom, we can limit ourselves to considering isolated paired particle collisions. The fact that lattice atoms are free in collisions, i.e. behave as atoms of dense gas, is confirmed by results of investigation of interaction time and energy of colliding particles.

For further development of mathematical modeling of the scattering process of ions of medium and low energies in a wide range of angles of incidence and scattering, we used the laws of two heavy particle collisions and considered the scattering of the ion beam from the surface of a monocrystalline sample based on the model of paired one-, two-, etc. multiple collisions. 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) [11]. 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 [12].

The angle of incidence of primary ions ψ were counted from a target surface and the azimuthal escape angle φ-from the incidence plane of the ions. In the Fig. 1 presents scheme of surface semichannel [13].

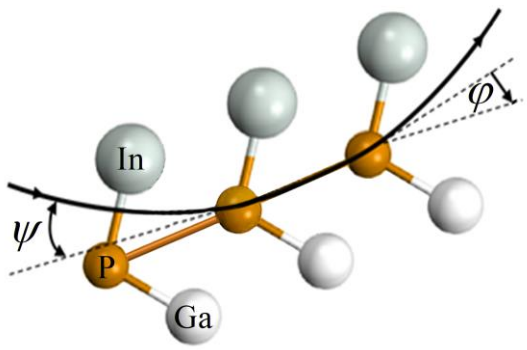

Fig. 1. The scheme of ion scattering by the surface semichannel.

This surface semichannel consist In and Ga atoms which located on the parallel surface atomic rows and atoms P which located on the second atomic layer. The walls of the semichannel formed by In-P and Ga P atoms. The bottm of the semichannel formed by only P atoms. The angle of incidence of the ion beam relative to the surface was changed in the range $\psi = 3$ - 11°, azimuth scattering angles have been marked in φ (Fig. 1).

Ion scattering is a relatively simplified problem compared with the diversity of geometrically complex trajectories encountered in ion implantation or with sputtering processes. The individual acts of scattering are relatively few and, if the surface is ordered (as in the crystalline targets), the collisions are well defined spatially, so that the modelling necessitates relatively few stochastic parameters. It thus becomes possible to obtain precise physical constants, parameters and dependencies that describe of bombarding ion-target atom interactions [14, 15].

Using this methodology was simulated the scattering of Ne^+, Ar^+ and Xe^+ ions from InGaP(001)<110> surface by the initial energy 5 keV at the grazing incidence (angle of incidence $\psi = 3°,5°,11°$). On the <110> direction formed surface semichannel, which consist In and Ga atoms on the surface layer and P atom which located on the second layer. The width of this surface semichannel is 4.01 Å.

In the Fig. 2 presents the azimuthal angular distribution of low energy scattered ions from the InGaP(001)<110> surface at angle the of incidence ψ=3°.

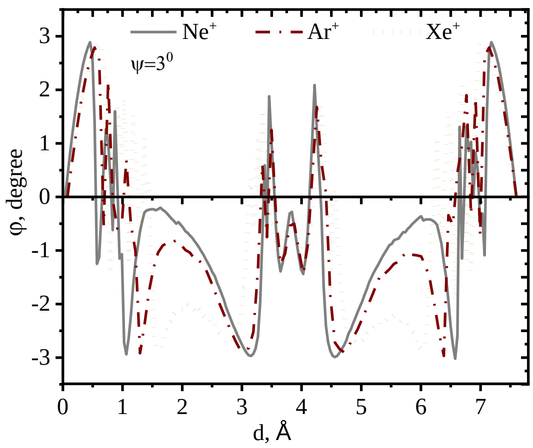

Fig. 2. The azimuthal angular distribution of low energy scattered ions from the InGaP(001)<110> surface at angle the of incidence ψ=3°.

The character of distribution for all types of ions looks same, at the angle of incidence at angle the of incidence ψ=3°.

Then the distribution going down and a zigzag dependence. It is a second part. The third part of the distributions is formed near the center of the semichannel and the values of the azimuthal angle are close to zero. The distance of third part determines the focal property of the semichannel. In this angle of incidence, with increasing masses of bombarding particles, a difference are observed at the onset of these groups. It should be noted that at this angle of incidence, ions couldn't penetrate inside the semichannel.

In the Fig. 3 presents the azimuthal angular distribution of low energy scattered ions from the InGaP(001)<110> surface at angle the of incidence $\psi = 7°$. The first part of distribution is a same for all types of ions. The second part looks very complicated since the azimuthal angle of scattering has both positive and negative values. This is because the ions after penetrate inside the semichannel scattered from different types of semichannel walls which formed by atoms In-P and Ga-P atomic pairs. In this case, the focusing properties of the semichannel are better in the case of the Xe ion.

In the Fig. 4 presents the azimuthal angular distribution of low energy scattered ions from the InGaP(001)<110> surface at angle the of incidence $\psi = 11°$. In this dependence, it is possible to observe a smoother dependence than in the above cases. The results obtained showed that the walls of the semichannel focus more ions than the bottom of the semichannel. This is due to the fact that an increase in the angle of incidence leads to an increase in the effect of the semichannel wall during focusing of ions. It can be seen from the dependence that the focusing effect clearly prevails in the case of scattering of Ne ions.

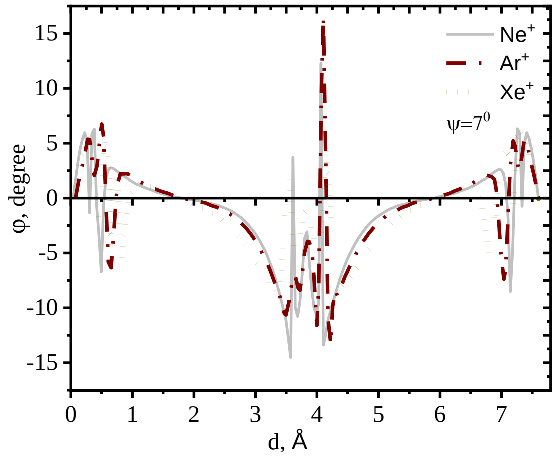

Fig. 3. The azimuthal angular distribution of low energy scattered ions from the InGaP(001)<110> surface at angle the of incidence $\psi = 7°$.

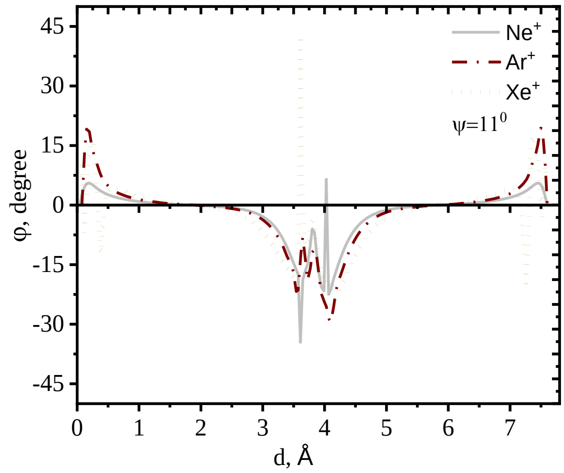

Fig. 4. The azimuthal angular distribution of low energy scattered ions from the InGaP(001)<110> surface at angle the of incidence $\psi = 11°$.

Conclusion

The azimuthal angle of distribution of Ne, Ar and Xe ions scattered from InGaP(001)<110> have been received by the method of computer simulation. The focusing properties of bombardment ions were discussed. In our calculations, the direct relations between the spatial variables of the scattered beam (mostly the azimuthal angular spectra) with the type of ions were identified.

Our calculation shows that the LESAIS can be used as a one of the method for a diagnostic and investigations of surface of many component thin films.

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М.К. Карімов, У.О. Кутлієв, С.Б. Боболжонова, К.У. Отабаєва

Дослідження кутового спектру розсіяних іонів інертного газу з поверхні InGaP (001)

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У роботі методом комп’ютерного моделювання проведено дослідження розсіювання низькоенергетичних іонів на очищеному багатокомпонентному монокристалі InGaP (001) <110> в умовах бомбардування іонами, здійснено аналіз та отримано нові дані. Розроблено та створено ефективні оригінальні алгоритми та комп'ютерні коди вищезгаданих процесів іонного впливу. Встановлено зв’язок між просторовими змінними розсіяного пучка (переважно азимутальними кутовими спектрами) і типом іонів. Показано кореляцію між фокусуючими властивостями поверхневого напівканалу з типом бомбардуючих іонів при різному куті падіння. Показано, що зміни типу атомів напівканалу призводять до зміни фокусувальних властивостей поверхневих напівканалів.

Ключові слова: розсіювання іонів, напівканали, комп’ютерне моделювання, кутовий розподіл, іонне фокусування.