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Scattering of low-energy Ne^+ ions from the stepped surface of InGaP(001)<110> at the small angles of incidence

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Scattering of Ne^+ ions at small angles of incidence from a stepped InGaP(001) <110> surface by the $E_0 = 5$ keV was simulated using computer simulation. The trajectories of dechanneled ions from defect surface, as well as their energies at the scattering and scattering angle, are studied. It is shown that before dechanneling, the frequency and amplitude of the trajectory of ions, which move the surface channel formed by the stepped atom, increase. The energy distributions of these ions are obtained and the part of the spectrum corresponding to these ions is determined. It has been established that the energetic dechanneled ions formed low intensity peaks on the low-energy part of the spectrum.

Keywords: Ion scattering, Semichannel, Defect, Computer simulation.

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Introduction

The study of the surface properties of solids is one of the main directions in the creation of microelectronic elements. When studying surfaces, many spectroscopy methods are used. Along with this, ion scattering spectroscopy is also used. This method considers the interaction of ions with surface atoms. At the beginning of research on the scattering of ions by the surfaces of solids, it was rather difficult to conclude that the interaction of a scattering ion with the atoms of a solid was a pairwise interaction. Experiments proceeding from a gas discharge, where the energies of the bombarding particles are low and the conditions on the surfaces of massive targets are almost always rather uncertain, contributed to the development of the concept of reflection as from a solid wall [1–7]. Very well-established systematic fundamental, experimental studies of the spatial and energy distributions of reflected particles from the surfaces of solid bodies with a disordered arrangement of atoms and ionized recoil atoms using equipment unique at that time made it possible to reliably establish that in the case of heavy ions, sharp peaks are observed in the energy distributions of reflected particles , whose position on the energy scale corresponds to a single quasi-elastic scattering of bombarding particles on individual target atoms. It was shown that in the case of reflection of light ions, single peaks are observed only at sufficiently low energies; as the ion energy increases, the distributions broaden and take on a domed shape. Currently, these obtained results have been used by the staff of scientific centers to create the basis for the theory of ion scattering and eventually the creation and development of the ion scattering spectroscopy method [8-12].

In this paper, we present studies of ion scattering from stepped InGaP(001)<110> surface. At the moment, there is a lot of experimental data on ion scattering spectroscopy from an ideal surface. There is a small amount of work studying the scattering of ions from a stepped surface. Therefore, we studied the scattering of Ne^+ ions from a stepped surface. Note that when studying the scattering process of ions, they are mainly chosen He^+, Ne^+, Ar^+ and Xe^+ ions.

I. Computational method and results

It is known that during the scattering of ions with low and medium energies, the forming trajectories of scattered particles are mainly determined, as is known, mainly by the elastic interaction of colliding particles [13]. Moreover, the forces which formed during such an interaction are Coulomb forces and from the action is preserved between the interacting particles. Due to this, it becomes difficult to calculate the trajectory of the scattered ion, since it undergoes interaction with all particles of the crystal. On the other hand, it takes a lot of machine time. In this case, it should be noted that at low energies, the act of interaction of an ion with surface atoms can be considered as a successive collision. Indeed, theoretically it is possible to imagine that the lattice atoms are free during collisions, i.e. they can behave like an atom of a dense gas.

We used in this study the method which based on the binary collision of two particles.so. the falling particles are the incident ion and the atom of the surface. Thus, in our calculations of particle scattering from the target surface, we considered them as pair interactions (binary collision approximation model).

At the moment, the MARLOWE and TRIM programs are the main modeling programs based on the method the approximation of paired collisions for the study of processes occurring during the bombardment of solids by charged particles. The basis of these two programs are almost the same. And the main difference is that MARLOWE is designed for the study of crystalline materials, and TRIM is for amorphous materials [14]. In the MARLOWE program [15], the scattering angle is determined by numerical calculation of the classical scattering integral or using previously calculated and tabulated values of these integrals for the Moliere potential [16].

We have simulated a semi-infinite monatomic step on the InGaP(001)<110> surface. This monoatomic step and some trajectories are shown in Fig.1. We examined the steps "up" on the surface. Surface atoms and steps consist of different kinds of atoms. that is. in our case, from Ga and P atoms, and on the adjacent atomic chain from In and P atoms. In this surface, the P atomic chains, which form surface steps, are located directly above the surface Ga and In atomic chains.

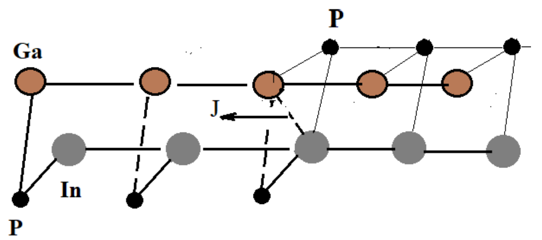


Fig. 1. Monoatomic step forming on the InGaP(001)<110> surface.

We studied trajectories for different values of the aiming point. Note that the aiming points in our case are the distances from the bombardment point to the step atom.

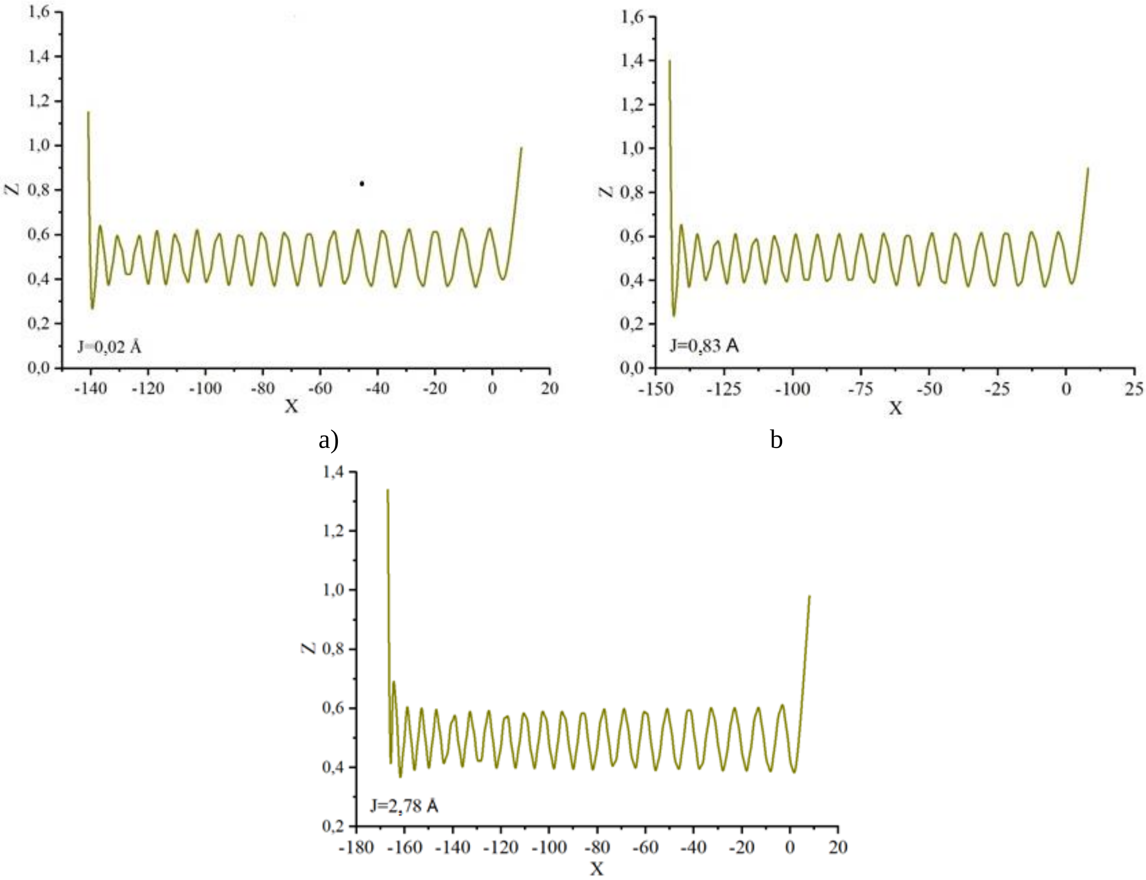
In Fig.2a. the projection of the ion trajectory on the InGaP(001)<110> surface is shown, captured into the channel at the value of the impact point of J = 0.4 Å at the angle of incidence $\psi = 5°$. It should be noted that the X-axis represents the ion path for each aiming point value. And the channel depth (Z) is located in the ordinate axis. In this value of the impact point, we can say that the ion falls near the surface Ga atomic row, and then is captured into the channel, formed by the atomic rows P and Ga. Our calculations showed that immediately after being captured into the channel, the ion moves under the influence of Ga and P atoms. Therefore, it has a higher frequency in the initial part of the trajectory. The ion has a fairly high mileage in this case. After that, you can see how the frequency of the ion trajectory narrows. This means that the ions are scattered from the wall of the channel, which consists of P atoms and Ga atoms. It can be seen from snapshot that the frequency of the ion trajectory inside the channel narrows, that is, it also begins to approach the upper atoms closer, and eventually an ion exit from this channel is observed (ion dechanalization). Due to the large trajectory, this ion left the channel with an energy of 1178 eV, while the inelastic energy loss was 2159 eV, the azimuthal scattering angle was -60°.

In Fig.2b. present next trajectory, i.e. in this case the aiming point value increased and it was 0.83 Å. The nature of the trajectory changed at X = 110. After this value, the amplitude began to fit in, and the ion approached closely to the walls of the channel, which consisted of surface atoms and atoms of the step. In this trajectory, the dechanneled ion had an energy of 1620 eV, an inelastic energy loss of 1952 eV, and an azimuth scattering angle of 61°.

In Fig. 2c. present trajectory incidence ion when J = 2.77 Å. The ion trajectory has a zigzag character. At first it had a large amplitude, and then the amplitude decreased and this led to dechanneling. Before leaving the channel, the ion collided hard with a Ga atom located in the lower part of the channel and escaped into vacuum. In this trajectory, the energy of the dechanneled ion is 1239 eV, the loss (inelastic energy) is 1930 eV, and the azimuth scattering angle is 61.72°.

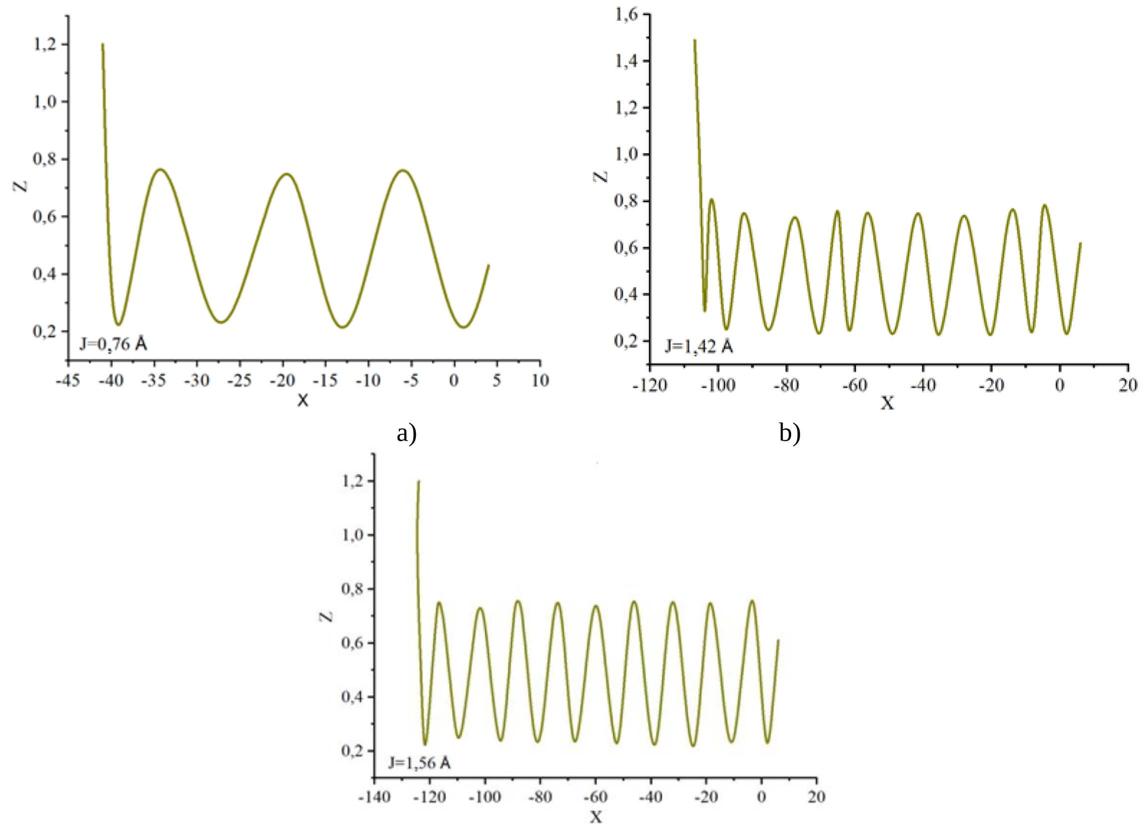
Now consider the trajectory of an ion trapped in a channel consisting of In and P atoms. This channel forms an adjacent atomic row, that is, parallel to the channel formed by Ga and P atoms. Figure 3a shows the trajectory of a dechanneled ion at J = 0.02 Å. From snapshot we can see that the ion trajectory has almost the same amplitude and frequency. And before existing from channel, the frequency of the trajectory decreased and the ion left the channel after scattering from the channel wall. The energy of the dechanneled ion is 3622 eV, the inelastic energy loss is 417 eV, the azimuth angle is 50.57°.

Fig.3b shows the trajectory of a dechanneled ion at J = 1.42Å. The amplitude and frequency of this ion trajectory begin to change almost near of the end the trajectory. We can observe that the frequency of trajectory changed after X= 100 and the process of ion dechanneling was observed. The last collision occurred with the channel wall. The energy of the dechanneled ion is 2482 eV, the inelastic energy loss is 963 eV, and the azimuth scattering angle is 19.77°.



c)

Fig. 2. Projection of the ion trajectory at the glancing angle $\psi = 5^0$ captured into the channel at different values of the aiming point: a – 0.4Å, b – 0.83Å, c – 2.77Å.



c)

Fig. 3. Projection of the ion trajectory at the glancing angle $\psi = 9^0$, captured into the channel at different values of the aiming point: a – 0.76Å, b – 1.42Å, c – 1.56Å.

In Fig. 3c presents the trajectory of dechanneled ion on the aiming point J = 1.55 Å. It can be seen that the ion trajectory has a rather long length, and before dechanneling, the frequency of the trajectories increased before the channel exit. Collisions occurred with the wall of the channel consisting of P-In atoms. The energy of the dechanneled ion is 733 eV, the inelastic energy loss is 1001 eV, the azimuthal scattering angle is 108.1°.

In Fig.4a present a projection of the trajectory of the ion that entered the channel. This happened at the value shown at the value of the impact point of 0.63 at the glancing angle of incidence $\psi = 9°$. In this value of the impact parameter, one can see that the influence of the Ga atomic rows is very large, since the ion is mainly scattered from this atomic row. The trajectory of the ion is not stable and therefore it quickly dechannels. Dechanneled ion energy 1437 eV, inelastic energy loss 349 eV, azimuth scattering angle 63°.

In Fig.4b present the projection of the trajectory of the ion trapped in the channel is shown at the aiming point of 1.20 Å. It can be seen from the trajectory that this ion is captured by the channel and then, after scattering by two atomic chains dechanneled. This trajectory also looks like trajectory of focused ions. Due to the existence of such a trajectory, one can argue about the focusing property of the channel, that is, some part of the ions can be focused. The energy of the dechanneled ion is 282 eV, the inelastic energy loss is 275 eV, the azimuthal scattering angle is 72.73°.

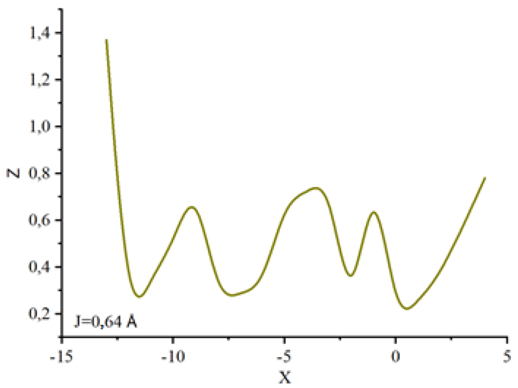
In Fig. 4c present the trajectory of scattered ion at J = 2.63 Å. In this case we can see that the channeled ion has a longer trajectory than the next trajectory. The trajectory of the ion is unstable and the ion leaves this channel after several collisions with the upper and lower atoms of the channel (P-Ga atoms). The energy of the dechanneled ion is 1487 eV, the inelastic energy loss is 531 eV, the azimuthal scattering angle is 99,34°.

Fig.5a shows the trajectory of a dechanneled ion at J = 2.14 Å. These impact point values are very close to the surface atomic rows of In. In this case, the ion directly penetrates the channel through the channel walls and, after collision with the upper and lower atoms (P-In), moves in the opposite direction. Then this channel will show. The ion trajectory looks like the trajectory of a focused ion. This ion has an energy of 2236 eV, inelastic energy loss 170 eV, azimuth scattering angle 82,41°.

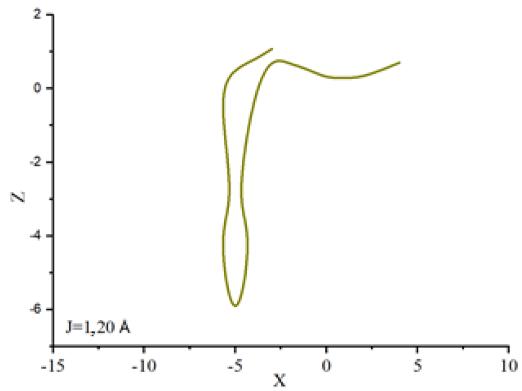
Fig. 5b shows the trajectory at J = 1.85 Å. At this value of the impact point, the ion entered the channel and, after three collisions, left this channel. Note that the last ion collision was the lower atoms of the channel, consisting of In atoms. This ion has an energy of 1405 eV, inelastic energy loss 316 eV, azimuth scattering angle 91,50°.

Fig. 5c shows the trajectory at J = 0.64 Å. We see that the trajectory of this ion is not quite long, but before dechanneling, it scattered with the lower atoms of the channel (In). This ion has an energy of 1444 eV and an inelastic energy loss of 386 eV, and an azimuth scattering angle of 35.88°.

Fig.6 shows the energy distribution of scattered Ne^+ ions at the bombardment of stepped InGaP(001) <110> surface with E_0= 5 keV, at angles of incidences $\psi = 5°$ and 9°. At the $\psi = 5°$ (fig.6a), the several intense peaks observed in the energy spectrum. On the energy



b)



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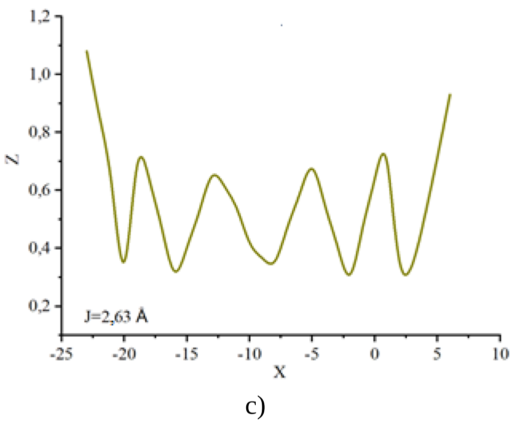
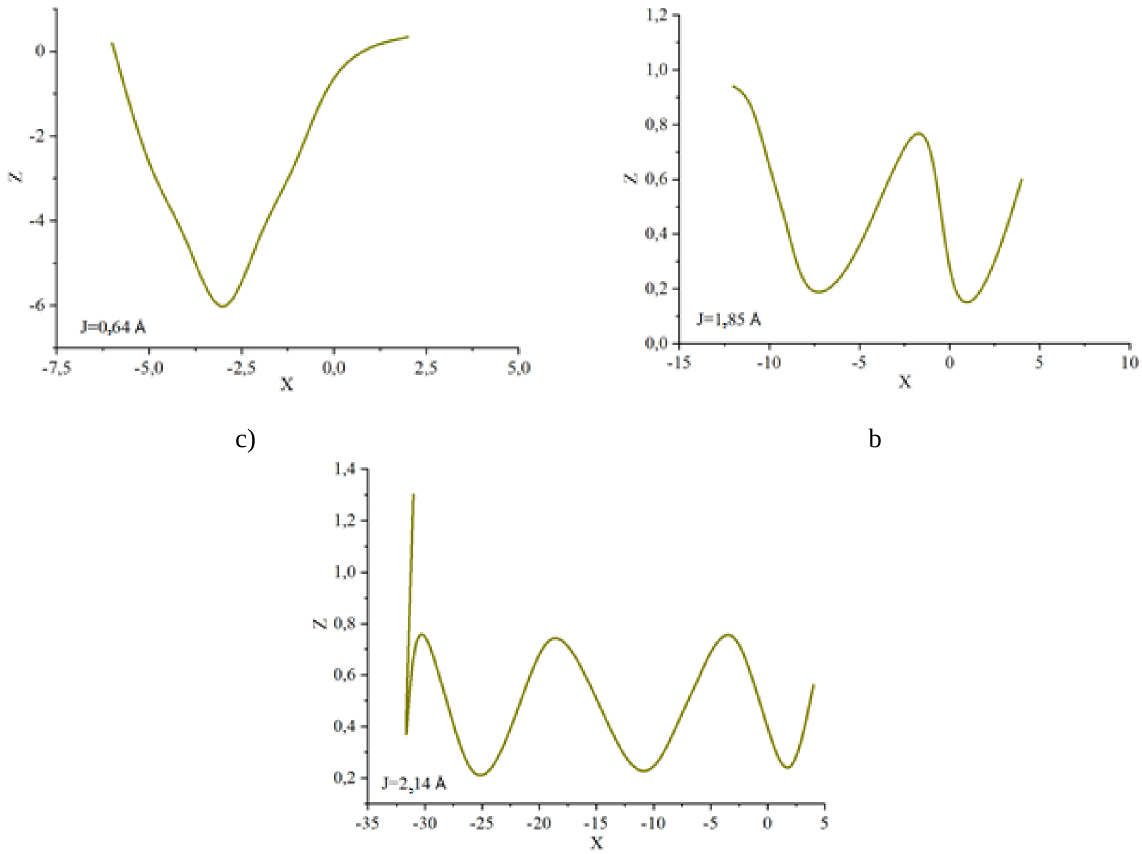


c)

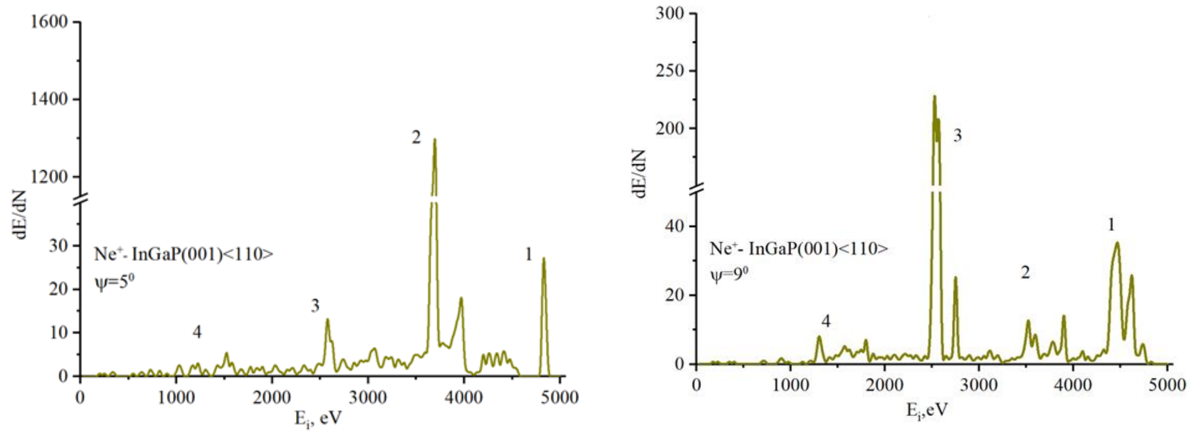
Fig. 4. The projection of the trajectory of the ion at the glancing angle 9^0 captured into the channel at different values of the aiming point: a – 0.64Å, b – 1.20Å, c – 2.83Å.



c) b

c)

Fig. 5. Projection of the ion trajectory at an angle of incidence 9^0, captured into the channel at different values of the aiming point: a – 0.63Å, b – 1.85Å, c – 2.14Å.



a) b

Fig. 6. Energy distributions of scattering Ne^+ ions from InGaP(001)<110> surface at the ψ=5° (a) and 9° (b) by E_0 = 5 keV.

distribution, we observe the most intense peak 2, which formed by ions whose scattered to the angle 90^0. Our studies show that the trajectory of these ions consists of two parts - scattered from the ideal part and from the first step atom. The next intensively peak 1 formed by the ions scattered from surface atomic chains. Low intensively peaks (3-4) formed by ions which captured to surface channel formed by P atoms (step atoms). Analyzing the trajectories of these ions, we can say that the ions first scatter from the ideal part of the surface InGaP (001) <110>, and then, before leaving surface channel, they scatter from the stepped surface. Moreover, peak 3 refers to ions scattered angle of 10^0-150^0, and the peak 4 remaining low-intensity peaks refer to ions scattered angle of more than 150^0 and less than 180^0.

Fig. 6b. shows the energy distribution of scattered Ne^+ ions at the bombardment of the stepped InGaP (001) <110> surface with E_0 = 5 keV at ψ = 9°. We observe that the intensity of the scattered ion peak 2 decreased and peak 1 increases. The peak 3 increases and this indicates the capture of ions into the surface channel formed by step atoms has increased. This shows the dechanneling of ions in large quantities between two atoms of the surface atomic series.

Conclusion

We have considered the trajectories and energy distributions of scattered Ne^+ ions at small angles of incidence on a stepped InGaP(001)<110> surface with $E_0 = 5$ keV. The trajectories of dechanneled ions are analyzed and the dechanneling conditions are discussed. The resulting energy distributions prove the existence of dechanneled ions. The spectra of dechanneled ions are formed in the low-energy part of the spectrum.

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Розсіювання низькоенергетичних іонів Ne^+ зі ступінчастої поверхні InGaP(001)<110> при малих кутах падіння

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Методами комп'ютерного моделювання розглянуто розсіювання іонів Ne+ під малими кутами падіння від ступінчастої поверхні InGaP(001) <110> на E_0 = 5 кеВ. Досліджено траєкторії деканалованих іонів з поверхні дефекту, а також їх енергію при розсіянні та від кута розсіяння. Показано, що перед деканалуванням зростає частота й амплітуда траєкторії іонів, які переміщують поверхневий канал, утворений східчастим атомом. Отримано енергетичні розподіли цих іонів і визначено частину спектра, що відповідає цим іонам. Встановлено, що енергетичні деканаловані іони формують піки низької інтенсивності в низькоенергетичній частині спектра.

Ключові слова: іонне розсіювання, півканали, дефекти, комп'ютерна симуляція.