

# Energy And Angular Distributions Scattered $\text{Ne}^+$ Ions From The GaP(100) Surface

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**Abstract**—The peculiarities of the low energy  $\text{Ar}^+$  and  $\text{Ne}^+$  ions scattering from the GaP(100)  $\langle\bar{1}10\rangle$  and  $\langle 110\rangle$  surface at grazing incidence has been investigated by the computer simulation. In our calculations was used the binary collision approximation. The energy and angular distributions of the particles reflected from the GaP(100)  $\langle\bar{1}10\rangle$  and  $\langle 110\rangle$  surface have been calculated. On the energy spectrum the characteristic peaks corresponding to scattering of ions by the surface atomic chains and semichannels are observed. The situation and intensity of these peaks depend on the geometrical form of the surface semichannels.

**Keywords**—ion scattering; computer simulation; energy and angular distribution

## I. Introduction

Currently, there are many experimental data on ion scattering from the single-component surfaces, and developed a number of methods for the understanding the processes of ion scattering from single crystals. The situation is different in the case of ion scattering from the multi-component crystals, in particular two-component crystals, which play an important role in modern microelectronics and nanoelectronics. There are many of unresolved problems, including the mechanisms of ion scattering and the laws small angle ion scattering from these surfaces[1].

The low-studied processes included the processes of interaction of fasted ions with solid surfaces and their scattering. In this paper we present energy and angular distributions scattered  $\text{Ne}^+$  ions from the surface of GaP(100)  $\langle\bar{1}10\rangle$ ,  $\langle 110\rangle$  by method of computer simulation.

## II.COMPUTER SIMULATION AND RESULTS

The simulation program used in the present work based on the binary collision approximation with two

main assumptions: (i) only binary collisions of ions with target atoms or between two targets atoms are considered; and (ii) the path which a projectile goes between collisions is represented by straight-line segments [2-3]. 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. While this approach permits one to cut the required computer time (compared with direct integration of the equations of motion), it also entails a systematic error due to the fact over short segments of path, the real ion trajectory differs from the asymptotes used to replace the former. This error was estimated in [4] for the Cu-Cu pair, a number of potentials and three values of energy. It was established that the deviation of an asymptote from the real trajectory is essential only for head-on collision and high energies.

For the particles interaction description the Biersack-Ziegler-Littmark (BZL) potential [5] 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 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 [6-8].

On Fig.1. shows the energy distribution of the ions  $\text{Ne}^+$  scattered from the surface of the GaP (100)  $\langle\bar{1}10\rangle$  with initial energy  $E_0 = 5$  keV and at different values of grazing angles  $\psi=3^0, 5^0, 7^0$ .

It is seen that in all cases the energy spectrum comprises two peaks, one of which is formed at low energies and refers to ions scattered from semichannel and next peak formed at high energies, relates to the ions scattered from the atomic chain.

When the slip angle is  $\psi=3^{\circ}$ , the peak of the scattered ions semichannel formed at the energy  $E = 4700\text{eV}$ , and the peak of the scattered ions semichannel ridge, formed by  $E = 4900\text{eV}$ . This shows that the share of energy loss of ions scattered from the semichannel, more than the ions scattered from the surface of the atomic chain. It should be noted that the peak of the scattered ions from semichannel has a greater intensity. This proves that at a value close to the above, i.e. when  $\psi=3^{\circ}$ , there is the effect of refocusing.

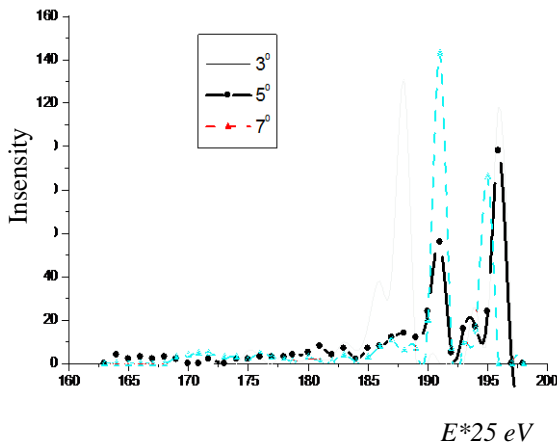


Figure.1. The energy distribution of the ions  $\text{Ne}^+$  scattered from the surface of the  $\text{GaP}(100)\langle 110 \rangle$  with initial energy  $E_0 = 5 \text{ keV}$  and at different values of grazing incidence  $\psi=3^{\circ}, 5^{\circ}, 7^{\circ}$ .

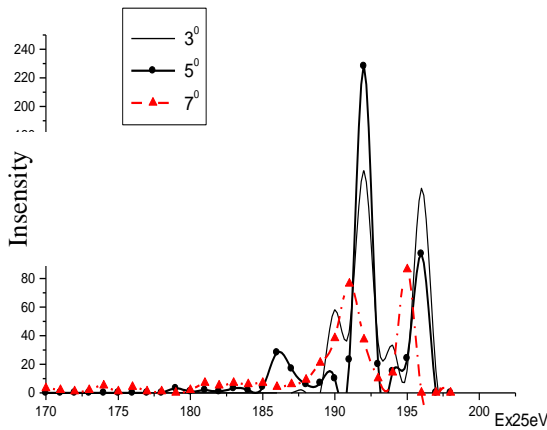


Figure.2. The energy distribution of  $\text{Ne}^+$  ions scattered from the  $\text{GaP}(100)\langle 110 \rangle$  surface at the initial energy  $E_0=5\text{keV}$  and angle of incidence  $\psi=3^{\circ}, 5^{\circ}, 7^{\circ}$

In the case where the slip angle is  $\psi=5^{\circ}$  also seen the emergence of two intense peaks in the energy spectrum. It should be noted that in this case, the peak of the scattered ions from semichannel, shifted toward higher energies ( $E = 4775\text{eV}$ ) and has a small intensity.

The next peak, i.e the peak scattered ions from the crest semichannel remains unchanged ( $E=4900 \text{ eV}$ ), but is characterized by low intensity.

If the value of slip angle  $\psi=7^{\circ}$  ion energy distribution is completely transformed, i.e the peak of ions scattered from the atoms located on the crest of semichannel, shifted towards lower values of the energy ( $E = 4825 \text{ eV}$ ). Note that when the incidence angles is  $\psi=3^{\circ}$  and  $5^{\circ}$  then the values of energy ions scattered from the crest semichannel remained unchanged. If the value of the incidence angle is a  $\psi=7^{\circ}$ , then the peak observing by scattered ions from the semichannel has greater intensity, with the value of the energy of these ions remains unchanged, as is the case when  $\psi=5^{\circ}$ .

It should be noted that the high intensity of the scattered particles from the semichannel, due to the effect of ion focusing.

On the Fig.2. presents the energy distribution of  $\text{Ne}^+$  ions scattered from the  $\text{GaP}(100)\langle 110 \rangle$  surface at the initial energy  $E_0=5\text{keV}$  and at the angles of incidence  $\psi=3^{\circ}, 5^{\circ}, 7^{\circ}$ .

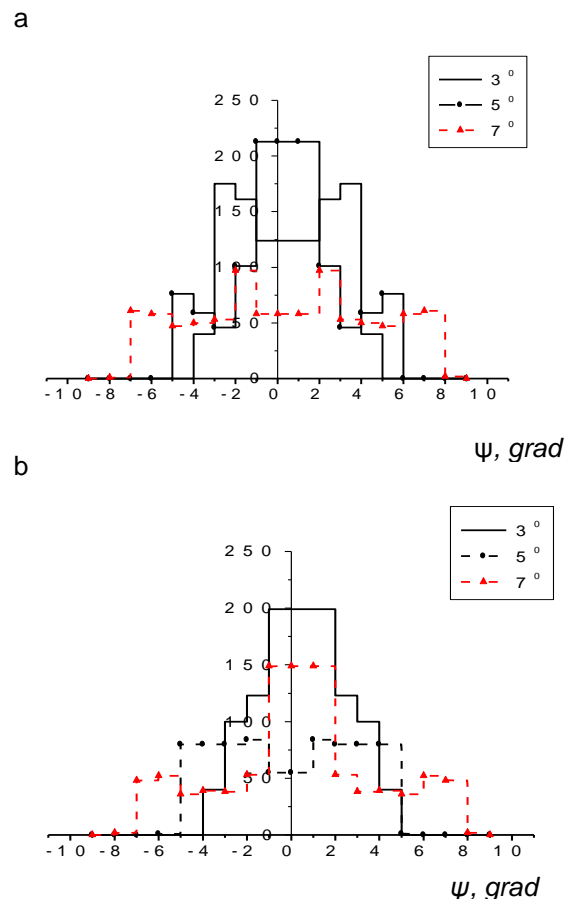


Figure 3. The spatial angular distribution of scattered ions  $\text{Ne}^+$  semichannels formed on the surface of  $\text{GaP}(100)$  in the direction of  $\langle 110 \rangle$ (a) and  $\langle 1\bar{1}0 \rangle$ (b) at grazing angles  $\psi=3^{\circ}, 5^{\circ}, 7^{\circ}$ , with initial energy  $E_0 = 5 \text{ keV}$ .

The energy distribution consists two peaks, corresponding to scattering ions from the atomic

chains ( at the greater value of the energy) and semichannels, consequently.

Analysis present energy distribution has shown that we can observe more big intensity of scattered ions from the semichannel, exists at values of the grazing angles  $\psi=3^{\circ}, 5^{\circ}$ . This is depended with that exactly under these values of the grazing angles, amount ion diffused from the semichannel, in contrast with amount ion well over, scattered from atomic chain.

It should be noted that the values of the incidence angle, close to the  $\psi=3^{\circ}, 5^{\circ}$  observed effects of refocusing and multiple focus.

If the value of incidence angle  $\psi=7^{\circ}$  the intensity of the reflected ions from the crests semichannel greater than the intensity of particles reflected from semichannel. Comparisons of these relationships have shown that the peak of the scattered particles from the semichannel, biased towards high values of energy at grazing angles  $\psi=3^{\circ}, 5^{\circ}$ .

On the Fig.3. shows the spatial angular distribution of scattered ions  $Ne^{+}$  semichannels formed on the surface of GaP (100) in the direction of  $\langle 110 \rangle$  (a) and  $\langle 110 \rangle$  (b) at grazing angles  $\psi=3^{\circ}, 5^{\circ}, 7^{\circ}$ , with initial energy  $E_0 = 5$  keV. When the value of slip angle  $\psi=7^{\circ}$  there is a wide, but not intensive distribution. This is because at this value grazing angle is not observed effect of ionic and respectively focus the reflected number of particles in this case is very small.

Analysis of these distributions shows that in both cases there is an intense reflection at grazing angle  $\psi=3^{\circ}$ . This because at grazing angles which are close to the  $\psi=3^{\circ}$  is dominated by the effect of ion focusing. For the remaining grazing angles observed greater spatial angular distribution of scattered  $Ne^{+}$  ions from the surface semichannel.

It should be noted that the intensity of the reflected particles at  $\psi=5^{\circ}$  and  $7^{\circ}$  mainly depends on the mass of the bombarding particles. Comparison of these distributions indicate that in the case of  $Ne^{+}$  ion bombardment of reflected intensity values of the above particles at glancing angles less than in the case of  $Ar^{+}$  ion bombardment.

### III. Conclusion

We have a detailed analysis of the calculated energy and angular distribution of the small-angle scattering of  $Ne^{+}$  ions block atoms single crystals GaP (100)  $\langle 110 \rangle$ ,  $\langle 110 \rangle$  with  $E_0 = 5$  keV. It is shown that the energy distribution can be clearly divided contribution ion scattering surface region (over 10 layers) that form a plurality of discrete peaks in the low energy part of the spectrum.

Thus, a study using computer simulations of energy and angular distributions of scattered ions from the surface of the two component mono-crystals, which leads to the development of a method

for quantitative analysis of composition and surface structure.

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