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ENERGY AND ANGULAR DISTRIBUTIONS OF SCATTERED Ar^+ IONS WITH A BLUE PHOSPHORUS SURFACE AT SLIDING ANGLES

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This article presents the theoretical results of energy and angular distributions of Ar^+ ions from the surface of blue phosphorus at a small value of the angle of incidence and initial energy receiving by computer simulation method. It is shown that at a small value of the initial energy of ions from the trajectory of scattered ions it is possible to obtain the general shape of the surface semichannel. Moreover, increasing the value of the initial energy makes it possible to obtain the full shape of the semichannel, as well as the shadow behind the semichannel, which provides information on the location of the atom of the second layer. It is established that in the energy distribution due to an increase in the value of the initial energy a multi-peak structure is formed. This makes it possible to determine the surface structure. The obtained angular distribution shows that there is a specular and multiple scattering of ions from the target.
Keywords: *Ion scattering; Semichannel; Computer simulation; Ion bombardment; Energy and angular distributions*
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INTRODUCTIONS

Low-energy small-angle ion scattering (Low Energy Ion Scattering (LEIS) is one of the most sensitive and accurate methods of material surface analysis [1-5]. This method allows obtaining information about the composition, structure and properties of the upper atomic layer of a solid. LEIS is based on the detection of ions scattered from the sample surface at small angles. The ions used typically have energies of several hundred to several thousand electron volts. Due to the small penetration depth of the ions (less than one nanometer), the method provides exceptionally high sensitivity to atoms located on the surface itself [6-8]. One of the main advantages of LEIS is its ability to selectively analyze only the upper atomic layer, unlike other spectroscopic methods that penetrate deeper into the material. This makes it an indispensable tool for studying surface modification processes, adsorption, catalysts, and for monitoring surface cleanliness.

Blue phosphorus is an allotropic form of phosphorus with unique electronic and structural properties, making it a promising material for micro- and nanoelectronics. Unlike black phosphorus, blue phosphorus has a stable two-dimensional hexagonal lattice similar to graphene, but with semiconductor properties. One of the key parameters determining the suitability of a material for microelectronics is the band gap. For blue phosphorus, it is in the range from ~1.9 to 2.0 eV (depending on the number of layers and the substrate), making it suitable for creating field-effect transistors, photodetectors and other components of nanoscale electronics [9-13]. Therefore, due to the great interest in the structure of blue phosphorus, we studied the energy and angular distributions of scattered Ar^+ ions from the surface of blue phosphorus at low values of the initial energy and incidence angle.

METHOD OF RESEARCH AND DISCUSSION OF RESULTS

Binary Collision Approximation Method (BCA) is widely used to model the interaction of ions with a solid surface, especially in problems related to ion scattering, ion implantation and surface structure analysis [14]. The BCA method is based on the assumption that the motion of ions during interaction with target atoms can be described as a sequence of independent two-particle collisions – between the probe ion and an individual atom of the material. In this case, many-body interactions and collective effects are ignored, which significantly simplifies the calculations. There are many advantages of this method [15]. BCA allows modeling the processes of ion interaction with a surface without significant resource costs, especially in comparison with more complex methods such as molecular dynamics. Despite its approximate nature, the method gives good quantitative estimates for a wide range of energies (from tens of eV to several MeV) [16]. It is especially effective in modeling processes in low-energy ion scattering methods, where interactions are limited to the upper layers.

In our calculations, we considered a semichannel formed on the surface of blue phosphorus (Fig. 1). It has a zigzag form. And this semichannel was divided into two parts from the middle. And the first part of the semichannel was divided

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into 1000 aiming points (in the direction of I). Ar^+ ions with small values of initial energy at sliding angles were directed to each aiming point.

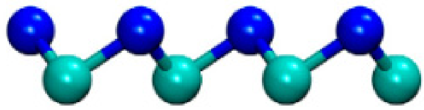

Figure 1. The semichannel, formed on the surface of blue phosphorus

One of the main objectives of this work was to study the trajectory of scattered ions, since the trajectory of scattered ions mainly determines the formation of peaks in energy and angular distributions. We analyzed the trajectories of scattered Ar^+ ions with an initial energy of E_0 = 1 and 3 keV and at angles of incidence ψ= 9-15^0. The choice of such a value of the incidence angle is due to the fact that the width of the semichannel formed on the surface of blue phosphorus is quite wide and is 4.2 Å. To study the trajectory of scattered ions from this semichannel, it was sufficient to study the trajectory of ions scattered from half of the semichannel, since the remaining ion trajectories are symmetrical.

RESEARCH METHOD AND RESULTS

Fig. 2 shows the trajectories of scattered Ar^+ ions with an initial energy of E_0 = 1 keV and at angles of incidence ψ = 9, 11, 13 and 15^0. At ψ= 9^0 (Fig. 2.1 a), the incident ions began to penetrate into the surface semichannel. And it is noticeably visible that the set of trajectories of scattered ions began to form the shape of a semichannel, as well as the location of the atom located at the bottom of the semichannel. It can also be seen that a small part of the ions penetrated into the crystal (were implanted). The number of trajectories of refocused ions is also large. And Fig. 2.1b shows the trajectories of scattered ions at ψ = 11^0. It is seen that the shape of the semi-channel was completely formed. And the ions were focused more clearly. The number of trajectories of overfocused ions decreased. Fig. 2.1c shows the trajectories of scattered ions at ψ=13^0. In this case, the location of the atom, which is at the bottom of the semi-channel and it focuses many ions, is clearly visible. The number of trajectories of overfocused ions also became even smaller. Most of the ions were implanted inside the crystal. At ψ=15^0 (Fig.2.1d), the number of implanted and focused ions increased significantly.

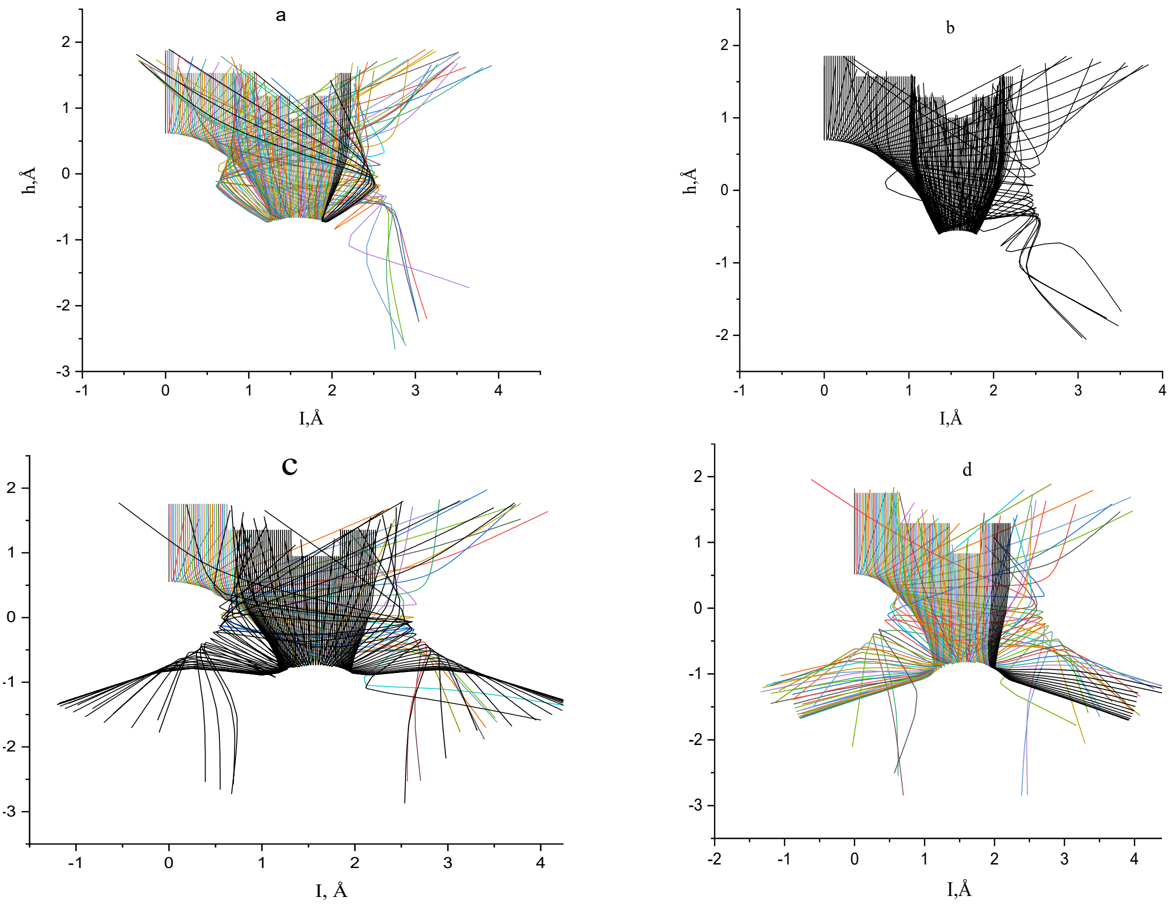

Figure 2. Trajectories of scattered Ar^+ ions from a surface semichannel that formed on the surface of blue phosphorus with an initial energy of E_0 = 1 keV and at angles of incidence ψ = 9, 11, 13 and 15^0

Fig. 3 shows the energy and angular distributions of scattered Ar^+ ions from the surface semichannel, which was formed on the surface of blue phosphorus with the initial energy $E_0 = 1$ keV and at angles of incidence $\psi = 9$, 11, 13 and 15^0. From the energy distribution (Fig.3a) it is evident that at the incidence angle values ($\psi = 9$, 11 and 13^0) the spectrum contains a single peak shape. This is due to the fact that the energy values of scattered ions from the bottom and the surface atomic row are close to each other.

And at $\psi = 15^0$ penetration of ions inside increased, which formed a complex trajectory and therefore an energy spectrum is observed, which has a two-peak shape. In the angular spectrum of scattered ions, two peaks are observed (Fig. 3b). The first peak refers to ions scattered from the plane of incidence and the second peak refers to mirror scattered ions.

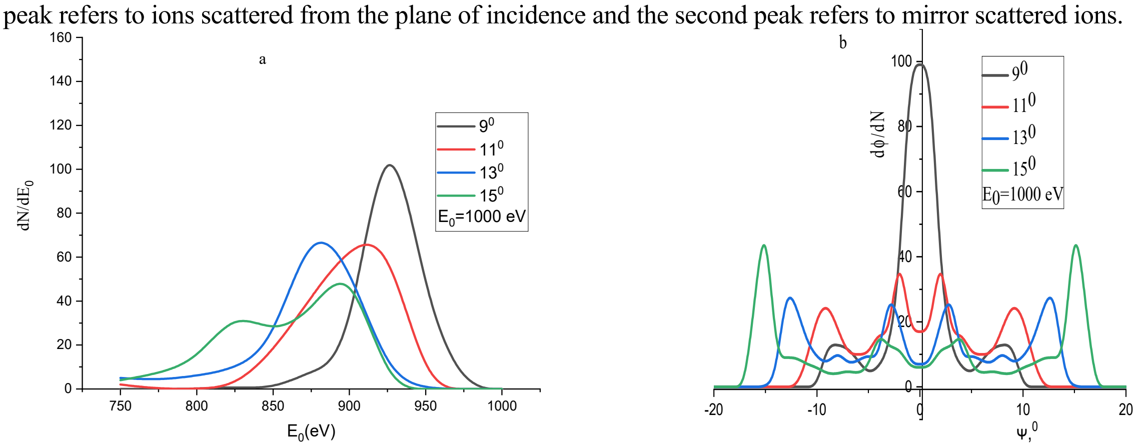

Figure 3. Energy (a) and angular (b) distributions of scattered ions Ar^+ from a semichannel formed on the surface of blue phosphorus with an initial energy of $E_0 = 1$ keV and at angles of incidence $\psi = 9$, 11, 13 and 15^0

Fig. 4 shows the characteristic trajectories of scattered Ar^+ ions from the semichannel formed on the surface of blue phosphorus with the initial energy $E_0 = 3$ keV at incidence angles ψ of = 9, 11, 13 and 15^0. At the $\psi = 9^0$ the Ar^+ ions penetrated the surface semichannel, and implantation of ions in small quantities is also observed (Fig. 4a). The ion trajectories consist of specularly scattered, focused and overfocused ion trajectories. In general, the shape of the surface semichannel can be determined. Fig. 4b shows the trajectory at $\psi = 11^0$. At this value of the ion incidence angle, the full shape of the semichannel can be seen. It can also be seen that the number of implanted ions has increased than at $\psi = 9^0$.

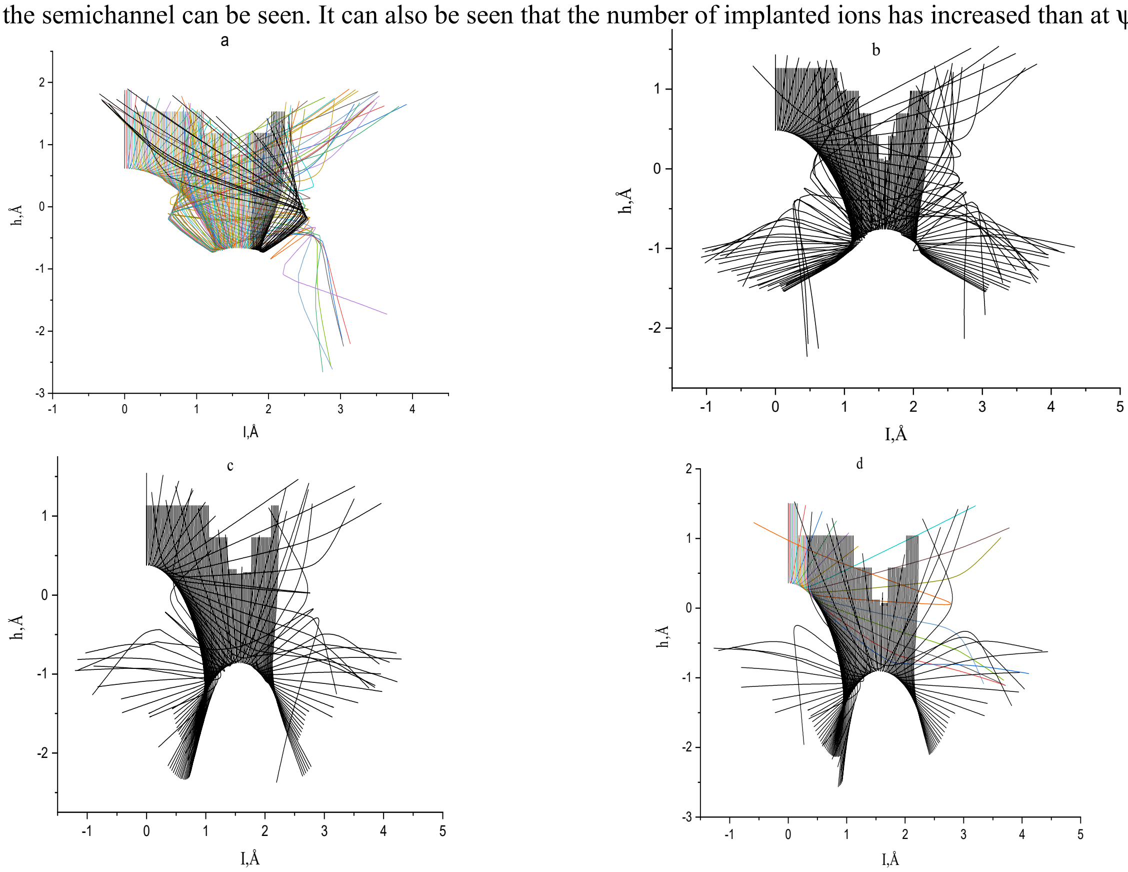

Figure 4. Energy (a) and angular (b) distributions of scattered ions Ar^+ from a semichannel formed on the surface of blue phosphorus with an initial energy of $E_0 = 3$ keV and at angles of incidence $\psi = 9$, 11, 13 and 15^0

It should be noted that from the trajectory of scattered ions, the location of the atom of the semichannel, located at the bottom of the semichannel, could also be more clearly seen. This can be observed by the formation of a shadow on the back side of the atom. Fig. 4c shows the ion trajectory at $\psi=13^0$. From the figure one can see that the implantation of ions into the crystal occurs around the atom located at the bottom of the semi-channel. It should be noted that at this value of the angle of incidence of ions, trajectories are observed, scattered from the surface atomic row, from the semi-channel and implanted ions (crossing the walls of the semi-channel). And at $\psi= 15^0$ the shadow formed behind the atom of the semichannel, located at the bottom of the semi-channel, narrowed even more compared to $\psi=13^0$ due to the increase in the angle of incidence. It should be noted that at this value of the angle of incidence the number of ions that crossed the walls of the semichannel decreased.

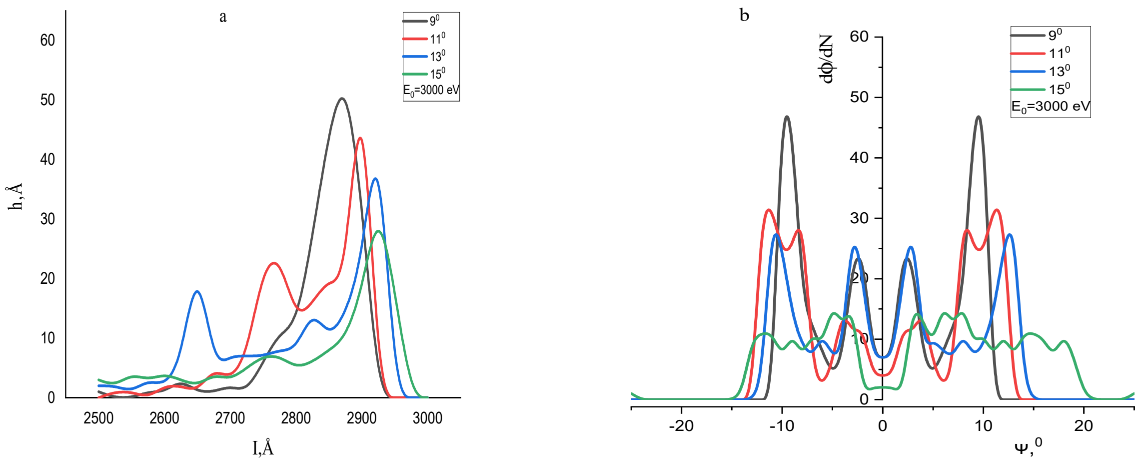

Figure 5. Energy and angular distributions of scattered Ar^+ ions from a surface semichannel that formed on the surface of blue phosphorus with an initial energy of $E_0 = 3$ keV and at angles of incidence $\psi = 9$, 11, 13 and 15^0

Fig.5 shows the energy and angular distributions of scattered Ar^+ ions from the surface semichannel, which was formed on the surface of blue phosphorus with an initial energy of $E_0 = 3$ keV at the angles of incidence $\psi = 9$, 11, 13 and 15^0.

The energy distribution (Fig. 5a) contains two peaks in all values of the incidence angle. The peak formed by the high-energy part of the distribution refers to ions scattered from the surface atomic row, and the peak located in the low-energy part of the distribution refers to ions scattered from the bottom of the semichannel. A low-intensity peaks formed by the low-energy part of the distribution refers to ions multiple scattered from the wall of the semichannel. Fig. 5b shows the angular distribution of scattered Ar^+ ions from the surface semichannel, which was formed on the surface of blue phosphorus with an initial energy of $E_0 = 3$ keV at the angles of incidence $\psi= 9$, 11, 13 and 15^0 . It is seen that the angular distribution also contains two peaks. The first peak refers to specularly scattered ions, and the second peak is formed at $\psi/ 2$ and it refers to ions multiple scattered ions inside the semichannel.

CONCLUSIONS

We have studied the energy and angular distributions of scattered Ar^+ ions from the surface semichannel, which was formed on the surface of blue phosphorus with the initial energy $E_0 = 1$ and 3 keV at the angles of incidence $\psi=9$, 11, 13 and 15^0 . It is shown that an increase in the initial energy leads to a splitting of the peak into at least two parts, which corresponds to ions scattered from the surface atomic row, from the semichannel. Low-intensity peaks of ions, repeatedly scattered from the wall of the semichannel are also observed. Thus, the trajectories of scattered ions are analyzed and it is shown that due to an increase in the initial energy, cones (shadow) are formed on the back side of the atom of the semichannel, located on the bottom of the semichannel.

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ЕНЕРГЕТИЧНИЙ ТА КУТОВИЙ РОЗПОДІЛ РОЗСІЯНИХ ІОНІВ Ar+ З ПОВЕРХНІ БЛАКИТНОГО ФОСФОРУ ПІД КОВЗАЮЧИМИ КУТАМИ

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У цій статті представлені теоретичні результати розподілу енергії та кутових розподілів іонів Ar+ з поверхні блакитного фосфору при малому значенні кута падіння та початкового отримання енергії методом комп'ютерного моделювання. Показано, що при малому значенні початкової енергії іонів з траєкторії розсіяних іонів можна отримати загальну форму поверхневого півканалу. Більше того, збільшення значення початкової енергії дозволяє отримати повну форму півканалу, а також тінь за півканалом, що надає інформацію про розташування атома другого шару. Встановлено, що в розподілі енергії внаслідок збільшення значення початкової енергії формується структура з багатьма піками. Це дає змогу визначити структуру поверхні. Отриманий кутовий розподіл показує, що існує дзеркальне та багаторазове розсіювання іонів від мішені.

Ключові слова: *розсіювання іонів; півканал; комп'ютерне моделювання; бомбардування іонами; енергетичний та кутовий розподіл*