

Ar + Ion Scattering Simulations with a Blue Phosphorus Surface at Small Incidence Angles

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Abstract: In this paper, characteristic trajectories and energy distributions of scattered Ar + ions from the surface of blue phosphorus with the initial energy $E_0 = 1$ keV and grazing angles $\alpha = 30^\circ, 50^\circ$ and 70° are discussed. It is shown that at small values of the incidence angle of bombarding ions, the shape of the surface semichannel (armchair shape) can be determined. The scattering coefficient and energy of scattered ions are calculated for the scattered ions. The calculated energy distributions of the scattered ions are analyzed. It is found that the peak of scattered ions from the surface atomic row and the bottom of the semichannel merge and the peak of scattered ions from the bottom of the semichannel is located in the low energy part of the peak.

Keywords: Ion scattering, semichannel, computer simulation, energy distributions.

INTRODUCTION

The methods of ion spectroscopy of surfaces (low-energy ion scattering spectroscopy (LEIS)) are based on processes occurring during the interaction of accelerated atoms and ions with the surface and near-surface layers of a solid. These processes are so diverse and complex that it is unlikely that a theory can be created that would describe them all from a unified standpoint. A number of theories have been developed to date, each of which describes a separate process or a limited group of processes to one degree or another. This module examines the main provisions and conclusions of some generally accepted theories, without which ion spectroscopy methods could not have arisen at all [1-5].

Blue phosphorus is a long-predicted and recently obtained allotropic modification of this element. Its properties were studied by chemists from Germany, who achieved the formation of a two-dimensional structure similar to graphene. With its single-layer honeycomb structure, it resembles probably the best-known 2D material, graphene. In analogy with its famous predecessor, it was then still called blue phosphorine. This new semiconductor material has since been investigated as an extremely promising candidate for optoelectronic devices[6].

In this work, we studied the trajectories and energy distributions of scattered ions at small angles of incidence and at low values of the initial energy of bombarding particles from the surface of blue phosphorus.

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METHOD

In this work we used the method of approximation of pair collisions [7-8]. In the region of low energies the trajectories of colliding particles are determined in the first approximation by the forces of elastic interaction of atoms. These forces arise from the Coulomb forces of interaction of nuclei and electron atoms and, therefore, act at any distance between the interacting particles. Consequently, to calculate the trajectory of the incident ion it is necessary to consider its interaction in the crystal lattice with all atoms simultaneously, which is very difficult. But at not very low energies ion-atom collisions can be considered as isolated pair collisions of particles. The fact that the atoms of the lattice are free during collisions, i.e. behave like atoms of a dense gas, are confirmed by the results of the study of the interaction time and energy of the colliding particles [9-10].

For further development of mathematical modeling of the process of scattering of ions of medium and low energies in a wide range of angles of incidence and scattering we used the laws of collision of two heavy particles. Thus, we will consider scattering of a beam of ions from the surface of a single-crystal sample based on the model of paired single-, double-, etc. multiple collisions. To describe the ion-atom interaction, the universal potential of Ziegler - Biersack - Littmark was used [11].

Fig. 1 shows a surface semichannel in the form of a "zigzag" that is formed on the surface of blue phosphorus. This semichannel was chosen as the main cell and this surface is divided into aiming points. And these aiming points were the bombardment points of the incident ion [12].

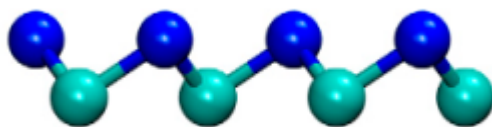


Fig. 1. Semichannel formed on the surface of blue phosphorus

We have investigated the trajectories of scattered Ar^+ ions from the surface of blue phosphorus at grazing angles of $\psi=3^0$, 5^0 , and 7^0 with the initial energy of $E_0=1$ keV. Figure 2a shows the projection of the trajectory of scattered Ar^+ ions from the surface atomic row to the middle of the semichannel of $\psi=3^0$. It is evident from the figure that the part related to ions scattered from the surface atomic row is much wider. This indicates the presence of two atomic rows. Figure 2b shows several trajectories scattered from the surface atomic row. It is evident that the trajectories are parallel to each other from two closely located atomic rows. The collision coefficient in this case is equal to 26, the energy of scattered ions is -983 eV. Figure 2c shows the trajectories of scattered ions from the bottom of the semichannel. It is evident that the ion scattered from the semichannel moves along the surface of the semichannel and does not penetrate into it. The collision coefficient in this case is 20-22, the energy of scattered ions is 961-971 eV.

Fig. 3a shows the projection of the trajectory of scattered Ar^+ ions from the surface atomic row to the middle of the semichannel $\psi=5^0$. The nature of these trajectories also shows that there are two P atoms on the surface. The lower line of the trajectory shows the shape of the surface semichannel and this shape is slightly narrowed compared to $\psi=3^0$. Fig. 3b shows the trajectory of ions scattered from the surface atomic row and the parallelism of the trajectory is preserved in it. The collision coefficient in this case is 20, the energy of the scattered ions is -979 eV. Fig. 3c shows the trajectory of scattered ions from the bottom of the semichannel. In this case, the ions penetrated into the semichannel. The collision coefficient in this case is 23, the energy of the scattered ions is -983 eV.

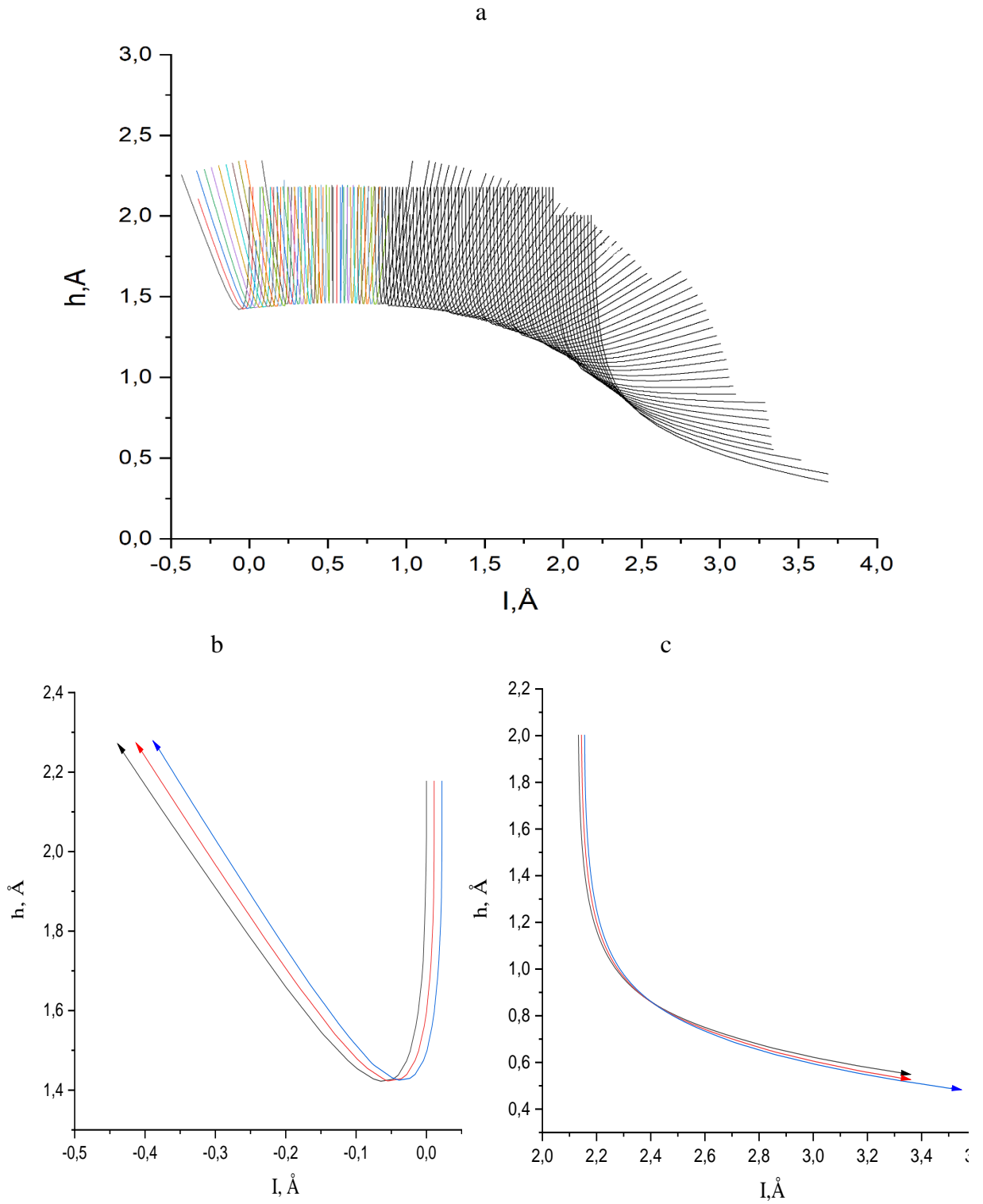


Fig. 2. Trajectories of scattered Ar^+ ions from the surface of blue phosphorus at $\psi=3^\circ$ and with an initial energy $E_0=1$ keV.

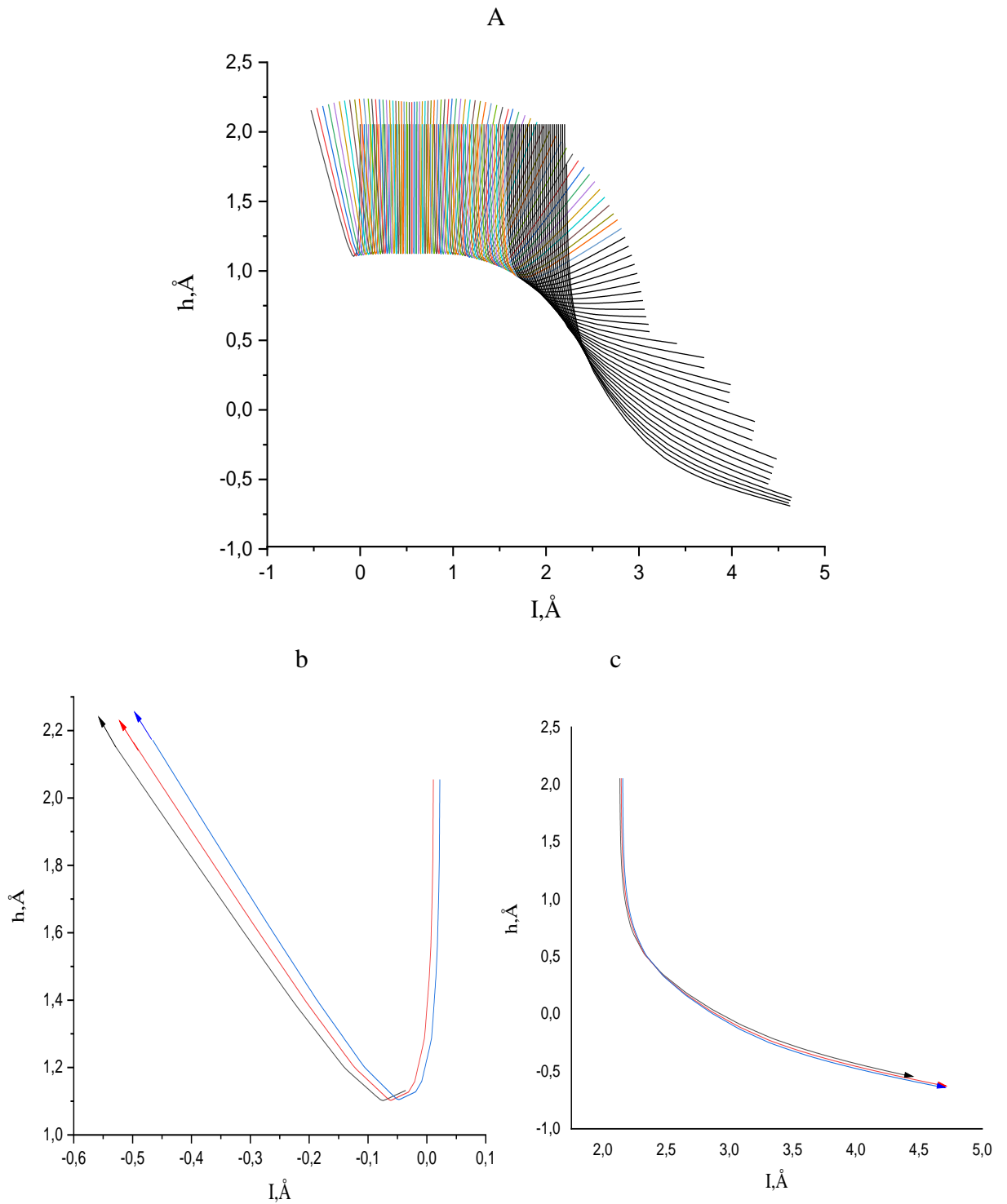


Fig. 3. Trajectories of scattered Ar^+ ions from the surface of blue phosphorus at $\psi=5^\circ$ and with an initial energy $E_0 = 1 \text{ keV}$.

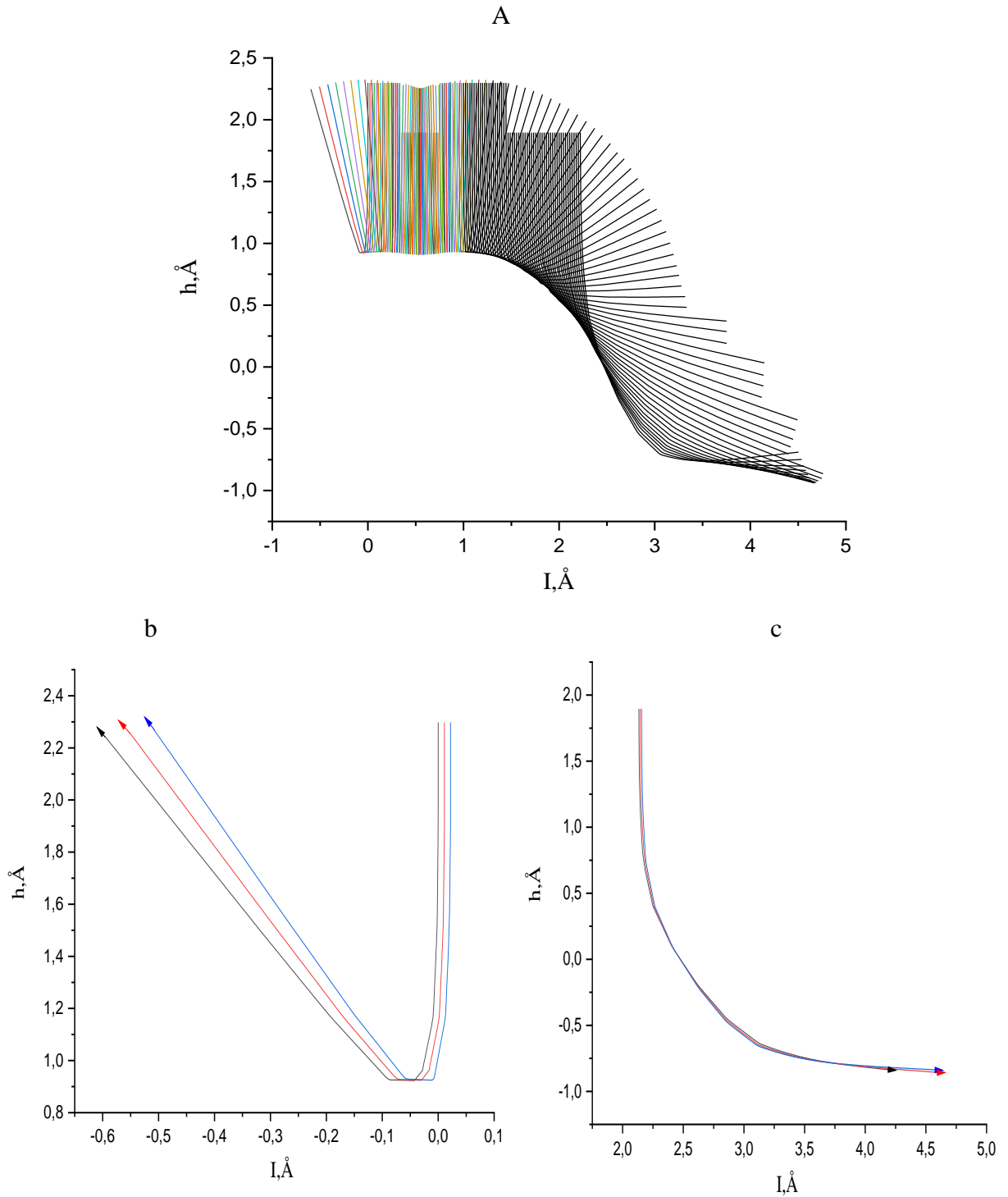


Fig. 4. Trajectories of scattered Ar^+ ions from the surface of blue phosphorus at $\psi=7^\circ$ and with an initial energy $E_0=1$ keV.

Fig. 4a shows the trajectory of scattered Ar^+ ions from the surface of blue phosphorus at $\psi=7^\circ$ and with an initial energy of $E_0=1$ keV. It is evident that at this value of the angle of incidence of the ions they penetrated even deeper into the semichannel, although there is almost no change in the trajectories of scattered ions from the surface atomic row. Fig. 4b shows the trajectory of scattered ions from the surface atomic rows. In this case, the collision coefficient in this case is 17, the energy of scattered ions is -969 eV. In Fig. 4c shows the trajectory of scattered ions from the bottom of the semi-channel. In this case, the parallelism of the trajectory is maintained and the collision coefficient in this case is 20, the energy of the scattered ions is 978 eV.

Figure 5 shows the energy distributions of scattered Ar⁺ ions from the surface of blue phosphorus at $\psi=3^\circ$, 5° and 7° with an initial energy of $E_0=1$ keV. It can be seen from the distribution that the intensity at $\psi=3^\circ$ is very high.

This is due to the fact that the ions are mainly scattered from the surface atomic row. And at $\psi=5^\circ$ and 7° the ions begin to penetrate into the surface semi-channel and energy losses are observed, which leads to a shift in the low-energy part of the spectrum of the peak of the surface atom. In all these values of the angle of incidence of ions, the peak of the surface semi-channel and the surface atom merge.

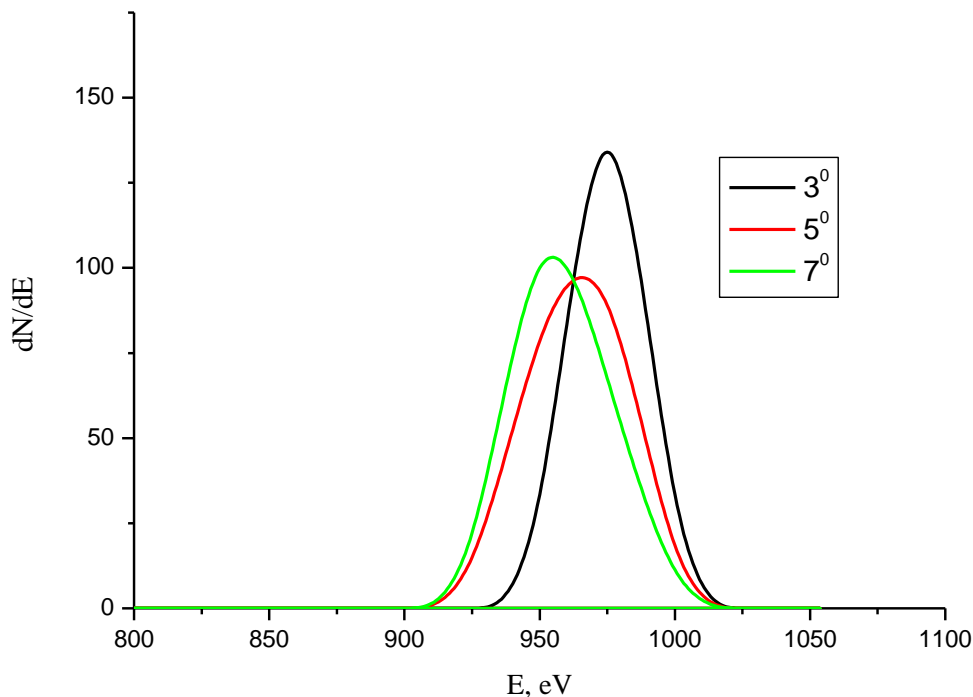


Fig. 5. Energy distributions of scattered Ar⁺ ions from the surface of blue phosphorus at $\psi=3^\circ$, 5° and 7° with an initial energy $E_0=1$ keV.

RESULTS

The study of Ar⁺ ion scattering patterns from blue phosphorus required analysis at graze angles of 30° , 50° and 70° with an initial ion energy of 1 keV. Scattered ion bombardment at a 30° incident angle exposed surface atomic rows to produce a broad range of trajectory paths. The experimental setup showed a scattering coefficient value of 26 while measuring an energy reading of 983 eV. At 50° and 70° incidence angles the ions reached deeper into the surface semichannel while their scattering trajectories became more focused. At 50° the scattering coefficient reached 20 while scattered ion energies maintained 979 eV, while at 70° the coefficient declared 17 with corresponding energies at 969 eV. Under 30° incident angle the energy distribution displayed peak intensity attributed to direct scattering from the surface atomic row. The ions penetrated into the semichannel when incidence angles reached 50° and 70° which led to both energy losses and spectral shift across the low-energy region. The combination of surface atomic row peaks and semichannel peaks occurred because these two regions maintained similar energy values.

DISCUSSION

The simulation data from blue phosphorus surface detects interaction patterns between incident ions as they scatter at different grazing angles (30° , 50° , 70°). Ar⁺ ions predominantly bombard surface atomic rows when incidence hits at 30° producing trajectories that widen accordingly because this angle matches blue phosphorus surface atomic structure. When incidence angles rise to 50 and 70 degrees measured from surface normal the ion trajectories become narrower and the

ions enter the surface semichannel to cause alterations in their scattering properties. Increased incident angles drive ion-surface interactions deeper into the material while simultaneously reducing scattering rates and shifting energy distributions toward less energetic outcomes. The energy peaks merge at higher grazing angles because ion scattering occurs from atomic rows on the surface combined with ion scattering from channel bottom features. The experimental results conform to predictions about ion focusing and channeling phenomena that intensify with increased angle of incidence.

The research shows that blue phosphorus surface semichannel structure shapes ion scattering dynamics significantly when using higher grazing angles. The merged energy peaks from surface atomic rows with semichannel signals indicate strong relationships between both surface and subsurface scattering mechanisms while additional study is necessary to define specific surface-subsurface interaction mechanisms. These research outcomes will provide a deeper knowledge about ion scattering behavior on blue phosphorus and other one-dimensional nanostructures which will benefit future surface analysis and material characterizers' work.

CONCLUSIONS

We have investigated the scattering of Ar^+ ions from the surface of blue phosphorus at grazing angles $\psi = 3^\circ$, 5° , and 7° with the initial energy $E_0 = 1 \text{ keV}$. The ion trajectories were studied, which showed the shape of the surface semichannel. It was shown that with an increase in the incidence angle of the bombarding ions, the shape of the trajectory narrows and the ions begin to penetrate into the surface semichannel. The energy spectrum obtained at these incidence angles of the bombarding ions also shows that with an increase in the incidence angle of the ions, the spectrum shifts toward low energy.

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