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Scattering Studies of Ar + Ions with a Black Phosphorus Surface at Small Incidence Angles

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Abstract: This article presents the results of studying the trajectory and energy distributions of scattered Ar+ ions from the surface of black phosphorus at grazing angles of □=30 and 70 with the initial energy of E0 =1 keV. It is shown that at large incidence angles (□>7 0) it is possible to analyze the appearance of the ion focusing effect by studying the nature and shape of the trajectory of scattered particles. The scattering coefficient and energy of scattered ions reflected from the bottom of the semi-channel and the surface atomic row are calculated. The energy distributions of scattered ions are calculated and it is shown that the peak of the surface atomic row and the bottom of the semichannel merge into one peak, due to the small difference in the energy of these ions, which is explained by the small value of the initial energy of the incident ions.

Keywords: Semichannel, ion scattering, computer simulation, ion focusing, energy distributions.

INTRODUCTION

It is known that such developments in modern advanced areas of production as microelectronics, metallurgy, thermonuclear technology and others face the problem of creating multicomponent materials with the required properties. In the process of analyzing such materials and monitoring their multicomponent structure, along with other methods, the method of ion scattering spectroscopy is widely used. Ion scattering spectroscopy allows you to quickly monitor and obtain information about the concentration of analyzed elements in the surface layers without destroying its structure [1-4]. In materials science, ion scattering spectroscopy is widely used in the process of analyzing the composition of diffusion layers, determining the dose and depth of embedded atoms, the thickness of the dielectric layer, and also to determine the degree of contamination of thin layers. In metallurgy, ion scattering spectroscopy is used to study corrosion, surface contamination and other processes. Many practical achievements in this area are associated with the obtained theoretical knowledge on ion scattering spectroscopy and sputtering of the irradiated surface [5-6].

Black phosphorus is the most stable thermodynamically and the least chemically active form of elemental phosphorus. Black phosphorus is a black substance with a metallic luster, greasy to the touch and very similar to graphite, and with a complete lack of solubility in water or organic solvents. One-, two-, three- and four-layer black phosphorus, both with and without an insulator. Some properties, such as the frequency at which active absorption of radiation begins, remained virtually unchanged. But others, such as the width of the forbidden zone (one of the main parameters of semiconductors) and the shape of the absorption spectrum, changed quite significantly. It turns out that by selecting the appropriate shell, it is possible to control the parameters of black phosphorus in a wide range, which opens up new prospects for the practical application of the material [7].

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 black phosphorus.

METHOD

In studying ion scattering we used the binary collision approximation method[8]. Two basic programs are based on the pair collision approximation, which are used to simulate a wide range of processes caused by the bombardment of solids by accelerated particles. It is assumed that the particles move between collisions along straight lines, which are the asymptotes of the particle paths in the laboratory coordinate system. Inelastic losses are assumed to be equal to the sum of local and nonlocal losses. Local losses are determined by the Oen-Robinson formula. Nonlocal energy losses are associated with continuous energy losses of a moving particle and are assumed to be proportional to the particle velocity. This method also allows one to simulate the interaction of ions with different types of crystalline solids. This is done using special procedures for rotating a single-crystal block, the parameters of which are the input data of the program. Thus, in order to simulate reflection from a target with a chaotic arrangement of atoms, the crystalline target is rotated randomly relative to the crystal lattice after each collision with the bombarding particle[9-10]. The Ziegler - Biersack - Littmark universal potential is used to describe ion-atom interactions [11].

Fig. 1 shows a semichannel formed on the surface of black phosphorus[] . It is evident that it has the shape of an " armchair". We have considered 1000 trajectories of incident Ar^+ ions on the surface of half of this semichannel[12].

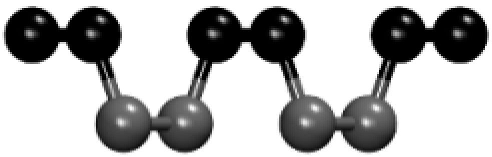

Fig. 1. Semichannel formed on the surface of blue phosphorus

We have investigated the trajectories of scattered Ar^+ ions from the surface of black phosphorus at grazing angles of $\psi=3^0$ and 7^0 with the initial energy of E_0 =1 keV. The choice of the initial energy values is due to the fact that many effects can be observed at these energy values and the mechanisms of these processes can be explained. Fig. 2a shows the general trajectory of scattered Ar^+ ions at $\psi=3^0$. It should be noted that these trajectories were obtained for half of the semichannel. It is evident from the figure that at this value of the incidence angle the ion will not be able to penetrate into the semichannel. And near the center of the semichannel, trajectories with two and one-third foci were observed. Next, we will look at individual trajectories of scattered ions from the surface atomic row and from the bottom of the semichannel.

Fig. 2b shows the projections of the trajectory of scattered ions from the surface atomic row. It is evident from the figure that the incident ions are mainly scattered from the atomic row without and with a small deviation from the initial direction. Our calculations showed that the scattering coefficient is 21 and the energy of the scattered ion is 985 eV. Fig. 2c shows the trajectories of scattered ions from the bottom of the semi-channel. It is evident that the trajectories have an oval shape. This is due to the fact that the ions are scattered only from the surface atomic row. Due to the oval nature of the trajectory, the scattering coefficient lies in the range of 59-63, and the energy is 961-971 eV.

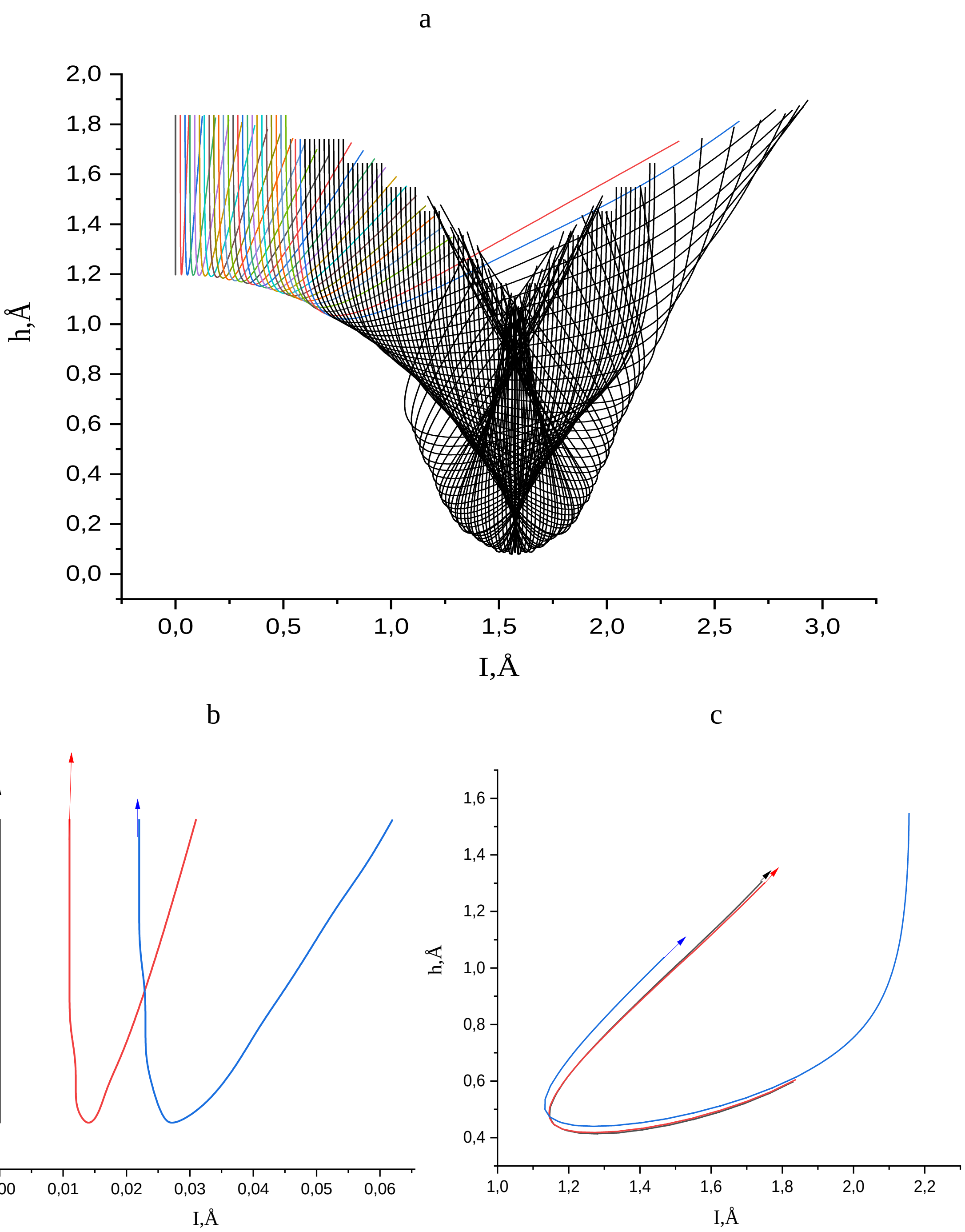

Fig. 2. Trajectories of scattered Ar^{+} ions with the surface of black phosphorus at $\psi=3^{0}$

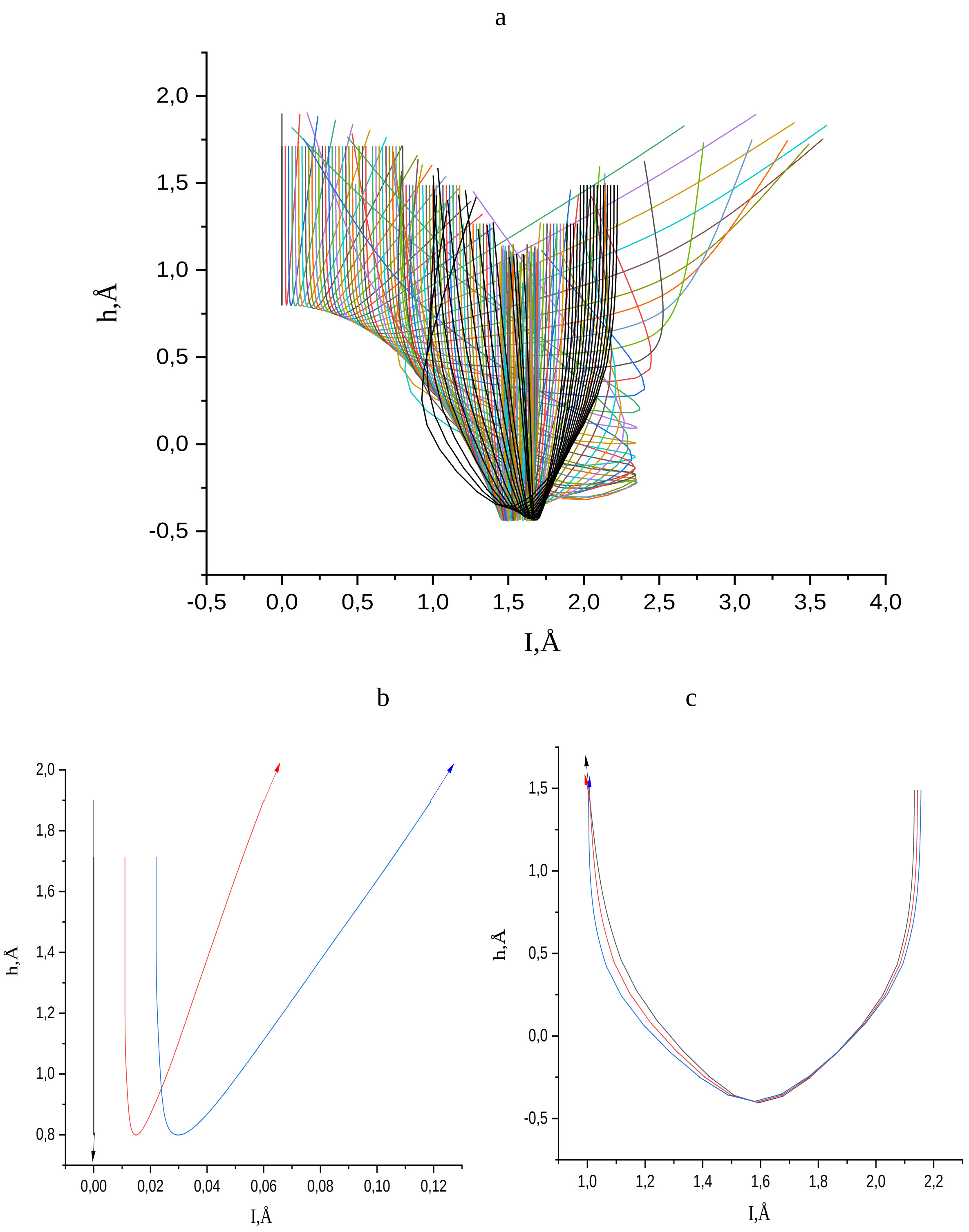

Fig. 3. Trajectories of scattered Ar^+ ions with the surface of black phosphorus at $\psi=7^0$

Fig. 3a shows the projections of the trajectory of scattered Ar^+ ions with the surface of black phosphorus at grazing angles $\psi=7^0$ with the initial energy E_0=1 keV. Comparison of this case with the case $\psi=3^0$ shows that the trajectories in this case are narrowed. Fig. 3b shows the trajectory of scattered ions from the surface half-channel. The nature of these trajectories is very similar to the case $\psi=3^0$ and is slightly narrowed. Our calculations showed that the scattering coefficient is 13 and the energy of the scattered ion is 972 eV.

Fig. 3c shows the trajectory of scattered ions from the bottom of the semi-channel. It is evident that the ion penetrating into the semichannel is scattered from the bottom of the semi-channel, and then from the surface atom and leaves the semichannel. It should be noted that by analyzing the nature and shape of the trajectory, one can explain the effect of ion focusing. In this case, the scattering coefficient of the trajectory lies in the range of 42-44, and the energy is 955-956 eV.

Fig. 4 shows the energy spectra of scattered Ar^+ ions with a black phosphorus surface at grazing angles of $\psi = 3^0$, 5^0, and 7^0 with an initial energy of E_0 =1 keV. It can be seen from the figure that the energy spectrum contains one peak. Our calculations showed that in the energy spectrum the peak of scattered ions from the atomic row and from the bottom of the semi-channel merge into one peak, since their energy values differ little.

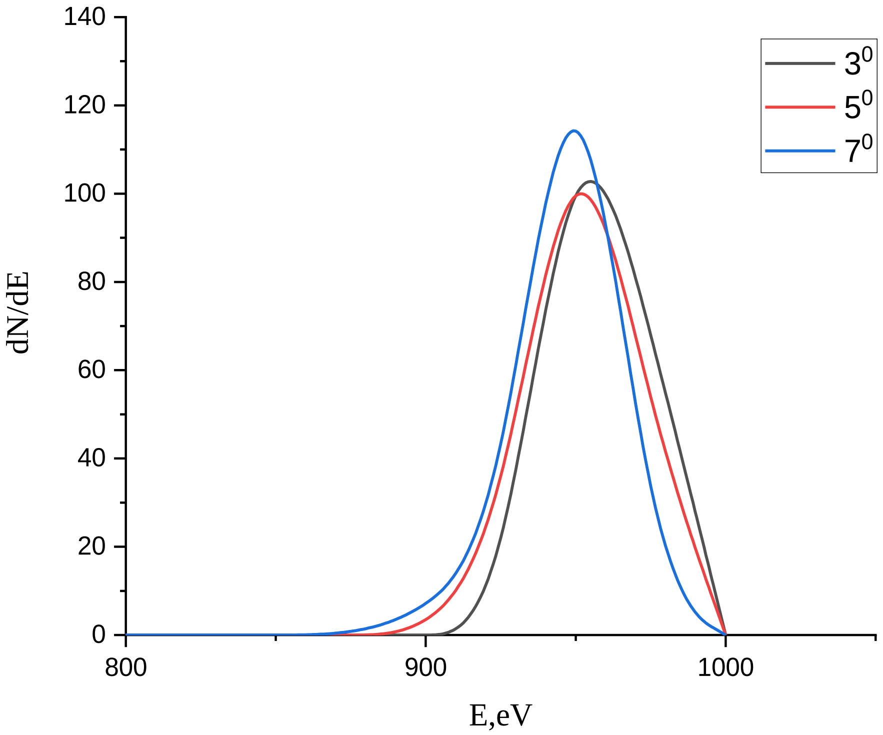

Fig. 4. Energy spectra of scattered Ar $^{+}$ ions from the surface of black phosphorus at grazing angles of $\psi = 3^0$, 5^0, and 7^0 with an initial energy of E_0 =1 keV.

RESULTS

Experimental results of Ar+ ion scattering with 1 keV energy examined black phosphorus at two incidence angles which produced different scattering patterns. When scattering occurred at a 30° angle the ions primarily hit the surface atomic row which produced little redirection from their original path. The research established that this scattering condition resulted in a 21 coefficient while recording scattered ion energy at 985 eV. Ion trajectories reflected from the bottom of the semi-channel exhibited an oval shape at a scattering coefficient spanning 59 to 63 and an energy range from 961 to 971 eV. Application of a 70° scattered angle narrowed down ion trajectories indicating stronger ion focusing properties. Analysis revealed surface atomic row ion scattering produced a scattering coefficient of 13 when the scattered ions measured 972 eV in energy. The bottom scattering produced results in which the scattering coefficient reached between 42 and 44 with energy readings between 955 and 956 eV.

During energy spectrum analysis the scattering peaks from ions that originated at the surface atomic row merged with those from the bottom of the semi-channel because the scattering sites remained nearly identical in energy. The analysis demonstrated consistent merger of peaks across 30°, 50° and 70° grazing angles that highlighted minimal energy variations in scattered ions originating from different surface elements.

DISCUSSION

The results of the scattering studies of Ar+ ions on the black phosphorus surface reveal significant insights into the dynamics of ion interactions at small incidence angles. When Ar+ ions hit the black phosphorus surface at 30° and 70° angles the trajectories and energy profiles produce separate configurations while the scattering properties and kinetic data differ between surface atomic row and semi-channel bottom. The surface atomic row interacts prominently with the registering ions when incident at 30° resulting in minimal trajectory deviations. The ion trajectories narrow when incidence reaches 70° while an increased immediate appraisability makes ions scatter between semi-channel bottom and surface atomic row. The measurement indicates that material-ions interactions show strong dependence on angular incidence because ion focusing reaches maximum strength at steep angles.

Multiple energy peaks merge due to the small difference in scattering site energies between surface atomic rows and semi-channels because incident ions start at low energy. These experimental results both enhance comprehension of ion surface interactions with black phosphorus structures and demonstrate how scattering response is influenced by controlled incidence conditions. Additional research should investigate incident ion energy levels to enhance knowledge about ion focusing mechanisms together with mechanisms of scattering from unique surface features. Exploring surface defects alongside impurities would enhance our understanding of both scattering dynamics and potential material assessment and surface management applications.

Conclusions

We have studied the scattering process of Ar^{+} ions from the surface of black phosphorus at grazing angles of $\psi=3^0$ and 7^0 with the initial energy of E_0 =1 keV. Characteristic trajectories of scattered ions at small incidence angles have been obtained. It has been shown that the trajectories of scattered ions from the surface atomic row and from the bottom of the semi-channel differ both in the value of the scattering coefficient and in the value of the energy of the scattered ions.

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