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Studying the Trajectory of Small-Angle Scattered Ar^+ Ions from CdTe(001) <110> Surface Semichannel

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Abstract: Based on cadmium tellurium (CdTe), photovoltaic cells are designed to absorb and convert sunlight into electricity. In this paper, we tried to describe the underlying mechanisms of scattering ions from surface semichannel formed on the CdTe(001)<110>. When analyzing the calculated trajectories near the center of the semichannel, a special trajectory was discovered, which consists of two focuses - the first refers to ion focusing and is located near the bottom of the semichannel, the second refers to overfocused ions and is located near the surface. The effect of ion focusing is observed at small angles of incidence and the number of trajectories at this value of the angle of incidence is quite large. It is shown that with an increasing angle of ion bombardment, the number of trajectories that have two focus decreases and then disappears. The collision coefficient and energy of scattered ions are calculated. It was found that the collision coefficients and energies are very close to refocused ions.

Keywords: ion scattering, computer simulation, refocusing, semichannel.

1. Introduction

The use of thin films in solar energy production is of great interest. Currently, many elements are used as thin films such as photovoltaic cells. Structure and surface energy are also interesting and these properties are studied by many methods [1-5]. Photovoltaic cells have also been created based on cadmium tellurium, which is the only thin-film technology with a lower cost compared to conventional solar cells made from other materials. Therefore, studying the composition and structure of cadmium tellurium is of great interest. Many methods are used for this. Along with these, low-energy ion scattering spectroscopy can also be used.

The advantage of the ion scattering method is that it does not form defects on the surface of the crystal when bombarded with ions. And now this method is successfully used in many branches of science and technology. CdTe(211)/Ge (211) has been studied using the medium energy ion scattering method to study stress relaxation. This structure was previously studied using 10 X-ray diffraction samples at different thicknesses. MEIS in channeling mode is a good alternative for high-depth-resolution defect profiling [6]. Te was also studied. This surface was obtained after etching a CdTe single crystal with bromine and methanol using two methods: X-ray photoelectron spectroscopy and dynamic low-energy ion scattering (LEIS).

Data from these methods were compared. The data obtained showed that the Te/Cd ratio had an exponential drop at a depth of 6 nm. At a depth of more than 6 nm, the substrate becomes stoichiometric. The information obtained about the composition at depth using LEIS turned out to be more detailed in comparison with ARXPS [7]. Therefore, this article presents the results of calculating the trajectory of scattered ions near a surface semichannel CdTe(001) <110> at small angles of incidence of Ar^+ ions.

2. Method and results

This work uses the binary method collision approximation, which is described in [8]. This method was founded in the middle of the last century and is still one of the successful methods for modeling the process of ion scattering. At this point, there are many potentials of ion-atom collisions, which have a good correlation with experimental data [9-12]. This work uses one of these interaction potentials, which is called Ziegler-Biersack-Littmark and it correlates very well with experimental results [13].

Figure 1 shows a semichannel formed on the surface of CdTe(001)<110>. When studying the trajectory of ions, we chose an aiming platform, which is described in detail in [14-15]. In this case, we moved from the surface atom to the middle of the semichannel by 1000 points in direction I (Fig. 1.).

An ion was directed to each point and thus we can consider 1000 trajectories. We considered only those aiming points that are close to the center of the semichannel. And in this way, we can study the characteristic ion trajectories of mainly scattered ions from the bottom of the semichannel.

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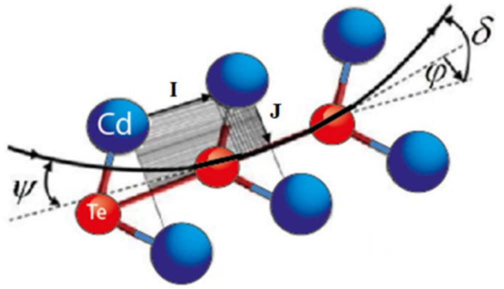

Fig. 1: Scheme of semichannel and ion trajectory

In Fig.2. The projection of the trajectory near the bottom of the semichannel formed on the surface of a CdTe (001)<110> single crystal is presented. Angle of incidence for Ar^+ ions $\psi=1.0^0$ (a), 1.3^0 (b) , 2.0^0 (c) and initial energy E_0 =500 eV. Our calculations showed that at this value of the angle of incidence there are very interesting trajectories near the center of the semichannel. It turns out that trajectories with two foci are observed a lot. It can be seen that the falling parts of all ion trajectories are parallel to each other. They first scatter from the half-cane wall and focus near the surface (intersecting each other). And then they rigidly collide with an atom that is located at the bottom of the semichannel and are scattered towards the wall of the semichannel. i.e. focus.

Further study of the trajectory showed that both are scattered from the wall of the semichannel (second focus) at large angles and intersect the falling part of the trajectory. Thus, focusing and refocusing of ions during scattering from the surface semichannel is observed. The energy of scattered ions for these trajectories (E_i) is 488-490 eV, the collision coefficient (Ks) is 32-33 , and for the longest trajectory Ks = 39 . These two focuses are very well depicted in Fig. 2b. These trajectories were obtained at a sliding angle $\psi=1.3^0$ and E_0=500 eV. It can be seen that the trajectories of several ions are almost parallel. Both focus lies inside the surface semichannel. Thus, there are two focuses.

The first focus, which lies near the bottom of the semichannel, is called ion focusing, and the second focus is called refocusing. In this case, E_i = 486-488 eV, Ks = 36 - 38. It should be noted that the effect of ion refocusing is observed at this value of the angle of incidence, since distinct two foci are observed. At sliding angle $\psi=2.0^0$ the projection of the incident part of the trajectory of scattered ions will change (Fig.2c) compared to Fig. 2b. The ion focusing effect begins to deviate, although it is still very small. Because the reflected parts undergo a change (narrows). These trajectories lost their parallelism. It can be seen that, reflecting from the bottom of the semichannel, the ions are scattered over a large angle with a noticeable difference. And this difference increased even more after scattering from the wall of the semichannel. In this case, the parameters E_i = 483-488 eV, Ks = 30-42.

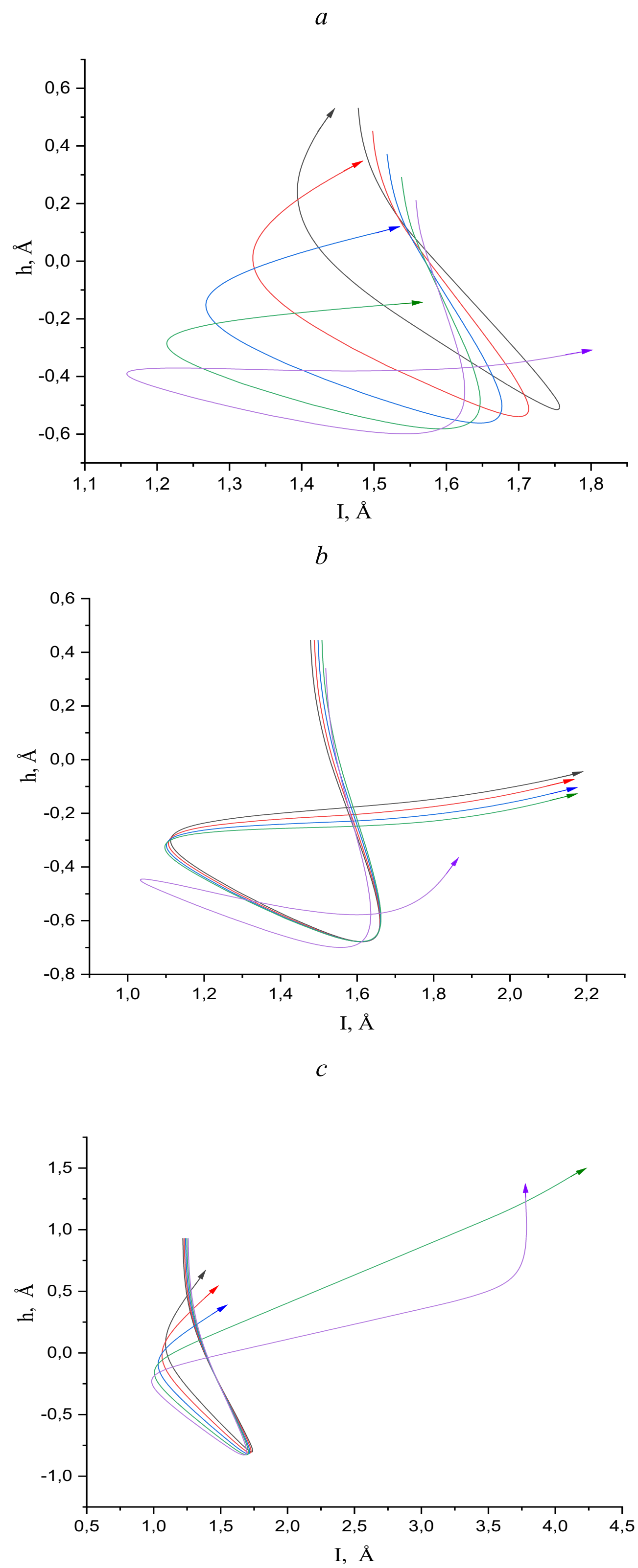

Fig. 2: Trajectories of scattered Ar^+ ions near the center of a semichannel formed on the surface of a CdTe single crystal (001) < 110> at an angle of incidence ψ= 1.0 ^{0} (a), 1.3 ^{0} (b), 2.0 ^{0} (c) and E_0 = 500 eV

We have obtained trajectories of scattered Ar^+ ions near the center of a semichannel formed on the surface of a CdTe(001)<110> single crystal at an angle of incidence $\psi=3^0$ and E_0 =500 eV (Fig. 3.). Analysis of the resulting trajectories showed that they have two types. The first type of trajectory refers to ions that fall near the center of the semichannel. It is clear from the trajectory of these ions that they are first scattered from the atom, located at the bottom of the semichannel. Then they are scattered from the wall of the semichannel towards the bottom of the semichannel. After scattering from the atom located at the bottom of the semichannel, they are directed into the interior of the single crystal. those. hyperchanneling is observed. These ions mostly remain in the single crystal.

The second type of trajectory is formed due to the process of ion refocusing. Those trajectories that are directed towards the surface of the CdTe(001)<110> single crystal refer to refocused ions. It can be seen that the trajectory of these ions first scatters from the bottom of the semichannel, and then from the wall of the semichannel and is directed towards the side of the surface. And then it leaves the surface because its energy is greater than the surface energy of the atoms. For this angle of incidence of ions E_i = 485-490 eV, Ks = 17-24

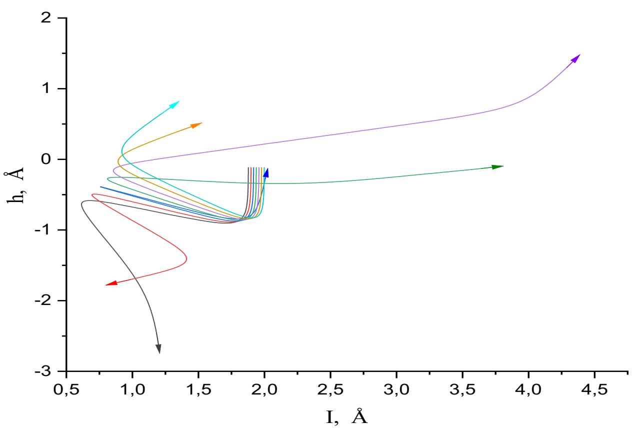

Fig. 3: Trajectory of scattered Ar^+ ions near the center of a semichannel formed on the surface of a CdTe(001) <110> monocrystal at an angle of incidence $\psi=3^0$ and E_0=500 eV

Ar^+ ions near the center of the semichannel formed on the surface of a CdTe(001)<110> single crystal at an angle of incidence $\psi=4^0$ and E_0 =500 eV to look at what changes the trajectories of scattered ions undergo with increasing angle of incidence (Fig.4.). It is clear from the figure that those ions that fell near the bottom of the semichannel after reflection from these atoms are directed towards the wall of the semichannel and penetrated into the adjacent semichannel (hyperchanneling process). In this case, the first trajectory has the shortest mileage and, accordingly, the smallest collision coefficient. At the following aiming point values, ions began to penetrate into the interior of the single crystal. And when an ion falls on the center of the semichannel, it scatters from the bottom, and then from the walls of the semichannel and leaves the semichannel. those. this ion is refocused. In this case, some of the ions leave the surface, and some of them remain in the crystal. The values of the main parameters in this case E_i= 481 -492 eV, Ks =13-22

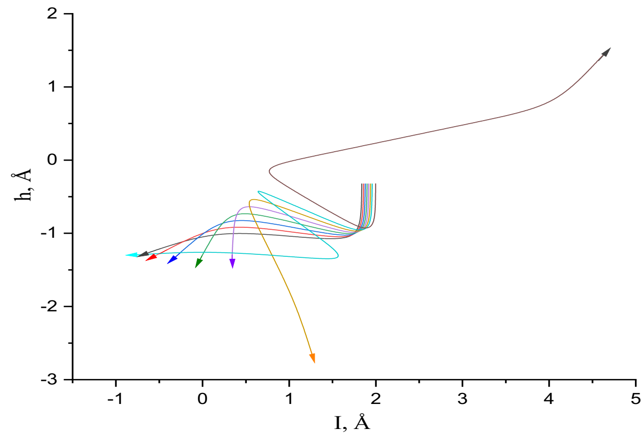

Fig. 4: Trajectories of scattered Ar^+ ions near the center of a semichannel formed on the surface of a CdTe(001) < 110> monocrystal at an angle of incidence $\psi=1.4^0$ and E_0=500 eV

At an angle of incidence $\psi=5^0$ on the above surface, trajectories similar to those at an angle of incidence $\psi=4^0$ are observed (Fig. 5). It can be seen that those values of the aiming point close to the bottom of the semichannel increase the range of scattered ions, which subsequently penetrated into adjacent semichannels (hyperchanneling). It should be noted that the first trajectory that is chosen in this case shows that the ion is reflected from the bottom of the semichannel, then from the surface atom and is directed into the semichannel. The ion is then reflected from the semichannel and directed into an adjacent surface atomic chain. The scattering angle from the surface atom is large and the ion is placed inside the single crystal since its energy is small to overcome the surface energy. By analyzing these trajectories, it is possible to determine the value of the surface energy of atoms. The values of the main parameters in this case E_i = 470-493eV, Ks =9-33

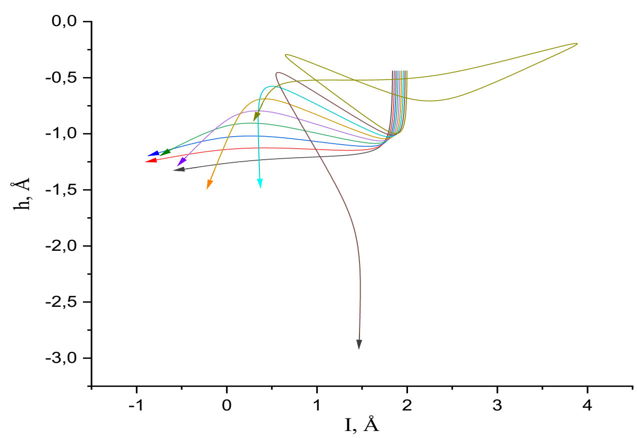

Fig. 5: Trajectories of scattered Ar^+ ions near the center of a semichannel formed on the surface of CdTe(001)<110> monocrystal at an angle of incidence $\psi=5^0$ and E_0=500 eV

3. Conclusions

We have studied the trajectories of Ar^+ ions near the bottom of the semichannel formed on the surface of CdTe(001)<110> monocrystal at angles of incidence ψ=1-5^0, with an initial energy E_0=500 eV. It is shown that ion scattering from the bottom and wall of the semichannel is observed at all values of the angle of incidence. The angle of incidence is determined and the effect of ion perfocusing, which has trajectories with double focus, is observed. For this case, the refocusing effect occurs at ψ=1.3^0. The results obtained showed that with increasing angle of incidence of bombarding ions, the effect of ion focusing is not observed. The results obtained are of interest when studying processes such as ion refocusing, implantation and hyperchanneling, which make it possible to understand these processes using the trajectory of scattered ions. Calculation of the ion trajectory makes it possible to determine the surface energy. If the ion energy is greater than the surface energy of the atoms, then the ion leaves the semichannel. But if it's the other way around, then the ion remains inside the surface layer.

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