EAST EUROPEAN JOURNAL OF PHYSICS. 2. 320-323 (2025)
DOI:10.26565/2312-4334-2025-2-39 ISSN 2312-4334

STUDIES OF IMPLANTATION OF O^+ IONS INTO SiO_2(001) FILMS AT THE SMALL-ANGLE ION BOMBARDMENT

U.O. Kutliev[a], A.S. Ashirov[a]*, G.X. Allayarova[b], A. Saidova[a]
[a]*Urgench State University, Urgench, Uzbekistan*
[b]*Karshi State University, Ko'chabog st,. Karshi, Uzbekistan*
**Corresponding Author e-mail: atabeks.ashirov@gmail.com*
Received January 22, 2025; revised April 2, 2025; accepted April 30, 2025

We have studied the process of ion implantation at small-angle ion bombardment of SiO_2 (001) film at low values of initial energy (up to 5 keV). Along with scattered O^+ ions· ion implantation is observed. It has shown that the geometric parameters of the surface semichannel affect the bombardment angle, which initiates the implantation process. It was found that in the case of a shallow semichannel, the implantation process is observed more than a deep semichannel at one value of the angle of incidence of ions. The dependence of implanted ions on the angle of their bombardment is obtained. It is found that few bombarding ions were implanted into the deep surface semichannel. This is explained by the influence of the second atomic row of the semichannel. The results obtained are of great interest in studying the ion implantation process.
Keywords: *Implantation; Ion bombardment; Computer modeling; Ion scattering; Focusing*
PACS: 34.50.-s

INTRODUCTION

During ion bombardment of a solid surface, many processes are observed that can be described both experimentally and theoretically [1-5]. Along with these processes, there is also the process of ion scattering and their implantation on surface areas. It is known that ion scattering spectroscopy (ISS) is an analytical method based on the study of the interaction of ions with the surface of materials. The main focus is on the analysis of the surface composition, structure and properties of thin layers and nanomaterials [6-8]. This method allows one to study the atomic composition, chemical state and surface topography with high sensitivity to the outer atomic layers. This method is successfully used along with many other methods for studying processes occurring on and near the surface. With this method, one can also study the ion implantation process and the characteristic trajectories of implanted ions [9-11].

Silicon dioxide (SiO_2), also known as silica, is widely used in various industries due to its unique properties, such as high chemical inertness, hardness and heat resistance. It is used to create insulating layers in microcircuits and other electronic devices, and is also used to obtain high-purity silicon required for solar panels. Therefore, the study of its structure and composition is of great interest. Artificial oxidation (implantation) of silicon is usually carried out in oxidizing furnaces similar to those used for diffusion in a carrier gas flow at high temperature (1000-1200°C). The basis of such furnaces, as in diffusion, is a quartz tube with silicon plates, heated either by high-frequency currents or in some other way [12-13]. In this work, the implantation of oxygen ions under small-angle bombardment with small values of initial energy was calculated using computer modeling. Trajectories were plotted and the number of implanted oxygen ions was calculated.

METHOD AND DISCUSSION OF RESULTS

In this work, the binary collision approximation method was used to describe the ion-atom interaction. For further development of mathematical modeling of the scattering process of medium and low energy ions in a wide range of incidence and scattering angles, we used the collision patterns of two heavy particles. Thus, we will consider the scattering of an ion beam from the surface of a monocrystal sample based on the model of paired single, double, etc. multiple collisions [14-15].

The pair collision approximation is the basis of two basic programs, with the help of which a wide range of processes caused by the bombardment of solids by accelerated particles are modeled: the program MARLOWE and the program TRIM [16, 17]. Both programs are based on practically the same formalism. The difference between these programs is that the first initially operates with crystalline targets, while the second with amorphous ones. To estimate the inelastic energy loss in an elementary collision act, we used the modified Kishinevski potential [18]:

$$\varepsilon(Eo,P)=\frac{0,310^{-7}\nu Z_1(Z_1^{1/2}+Z_2^{1/2})(Z_1^{1/6}+Z_2^{1/6})}{(1+\dfrac{0,67\sqrt{Z_1}r_0}{a_{tf}(Z_1^{1/6}+Z_2^{1/6})})}+(1-0,68\frac{V(r_c)}{Er})$$

where, a_{tf} = 0.468Å, ν and E_r -are the relative velocity and energy of the atom, Z_1 and Z_2 are the charge of the colliding ions and atoms, v -cm/s, E_r -eV, r_{min} in angstroms.

Cite as: U.O. Kutliev, A.S. Ashirov, G.X. Allayarova, A. Saidova, East Eur. J. Phys. 2, 320 (2025), https://doi.org/10.26565/2312-4334-2025-2-39

In our calculations, we considered 200 trajectories of bombarding oxygen ions separately for the <110> and <ī10> directions of the SiO_2 (001) film surface. The structure of the surface semichannels formed by SiO_2(001)<110> and SiO_2 (001)<ī10> is shown in Fig. 1a and Fig. 1b, respectively. The width of the semichannel formed in the <110> direction is 5.063 Å and the depth is 1.64 Å. And the width and depth of the semichannel formed in the <ī10> direction are 5.063 Å and 2.46 Å , respectively.

It is known that some of the ions are reflected from the film, and some of them remain inside the film (implanted). To study this issue, we obtained the dependence of the reflected particles on the angle of incidence of the bombarding O^+ ions to find out what part of the ions remains inside the SiO_2(001) film at low values of the initial energy (up to 5 keV). This dependence makes it possible to determine the percentage of implanted ions in the film. We calculated the scattering and implanted ions with low-angle ion bombardment. This work presents calculations exclusively of implanted ions. It should be noted that the width of the semichannel in SiO_2 (001)<110> is 5.063 Å, and the depth is 1.64 Å. In the direction of SiO_2(001)<ī10>, the width of the semichannel is also 5.063 Å, and the depth is 2.46 Å.

a b

Figure 1. Structure of the surface semichannel of the SiO_2(001) film in the directions <110> (a) and <ī10> (b)

Figure 2 shows the dependence of the number of implanted O^+ ions in SiO_2 (001) <110> films on the angle of incidence. We selected the values of the angle of incidence in the range of 1-30^0. This is due to the fact that small-angle implantation of ions on thin films. From the dependence it is evident that ions with an initial energy of E_0=1 keV to the value of the angle of incidence at $\psi \geq 9^0$ begin to penetrate into the film (black line). In this case, a small number of O^+ ions penetrate into the film and a large number of ions reflecting from the film was observed. At the initial energy value E_0 = 2 keV, the ions penetrate into the film in $\psi \geq 6^0$ (red line). Our calculations showed that at E_0 = 3 keV, ions penetrate into the film at $\psi \geq 5^0$ (pink line). And E_0 =4 keV, ions penetrate into the film at $\psi \geq 4^0$ (blue line). At values of E_0 = 5 keV, ions penetrate into the film at $\psi \geq 4^0$ (violet line).

At the next increase in the value of the angle of incidence of ions in all values of the initial energy, the number of implanted ions begin to increase. After the growth of the number of implanted particles, a small decline in the dependence is observed, which is located in the range ψ=12^0-17^0. Analysis of the particle trajectory showed that the decrease in the number of implanted ions is explained by the fact that in this value of the initial energy and angle of incidence of particles, the effect of ion focusing is observed. That is, what part of the ions are focused in the surface semichannels. After this decline, an increase in the number of implanted particles is observed and again the number of these particles decreases, which is explained by a decrease in the collision of ions with the surface atomic row and the wall of the semichannel.

Fig.3. shows the dependence of the number of implanted O^+ ions in SiO_2(001)<ī10> films on the angle of incidence. It is evident from the dependence that the process of implantation of ions with an initial energy of E_0 =1 keV begins to penetrate into the film $\psi \geq 2^0$ (black line). Moreover, at other values of the initial energy, the ions penetrate with $\psi \geq 1^0$. This is because the geometric parameters semichannels are large. For this semichannel, a two-peak structure is also observed. And a decrease in the number of implanted ions is observed with the ion focusing effect. Comparison of these two dependencies presented in Fig.2 and Fig.3. shows that with an increase in the number of atomic rows of the surface semichannel, the number of implanted ions increases. Our calculations showed that there is a decrease in the number of implanted ions when bombarded at the ψ =12^0-15^0 in the direction of SiO_2(001)<ī10>. The process of ion focusing explains this decrease in the number of implanted ions.

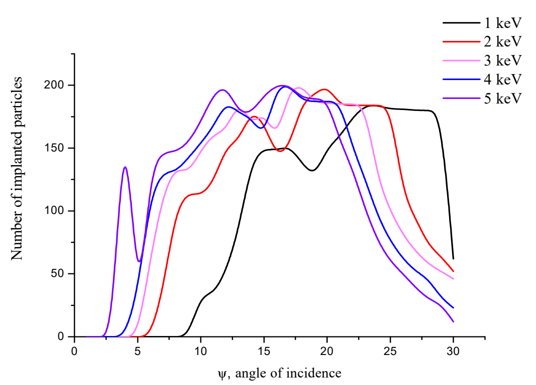

Figure 2. Dependence of the number of implanted O^+ ions in SiO_2(001)<110> films on the angle of incidence

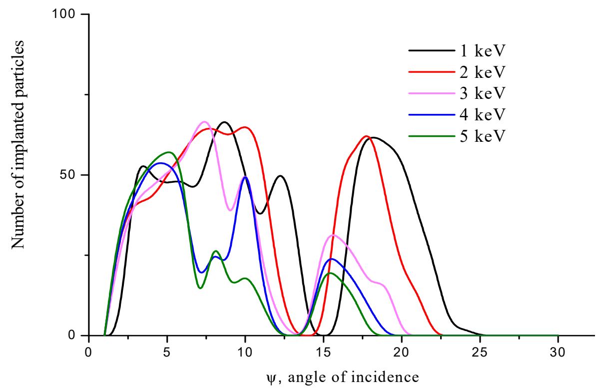

Figure 3. Dependence of the number of implanted O^+ ions in SiO_2(001)<ī10> films on the angle of incidence

For the study, we will consider two trajectories obtained for the SiO_2(001) film in the <110> and <1̄10> directions. Fig. 4 and Fig. 5 show several trajectories of implanted ions for the <110> and <1̄10> directions, respectively, at an incidence angle $\psi = 10^0$ and with an initial energy of $E_0 = 1$keV. It is evident from the trajectory shown in Fig. 4 that two trajectories (1 and 2) penetrated into adjacent semichannels and remain in the film as an implanted particle. And trajectory 3 shows that this ion is scattered from the surface semichannel. When bombarded in the <1̄10> direction by O^+ ions, straight and zigzag trajectories are also observed before implantation of ions (Fig. 5).

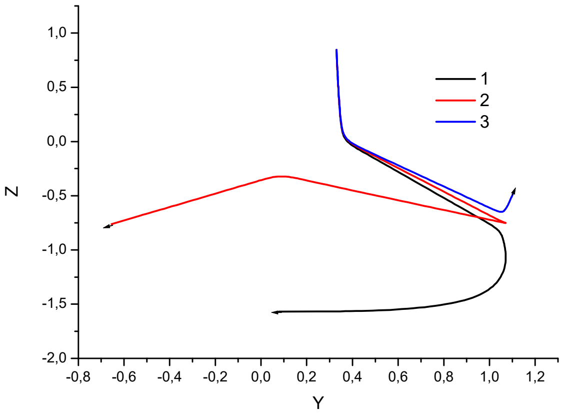

Figure 4. Characteristic trajectories of implanted O^+ ions in the SiO_2(001)<110> film at E_0=3 keV and $\psi = 10^0$

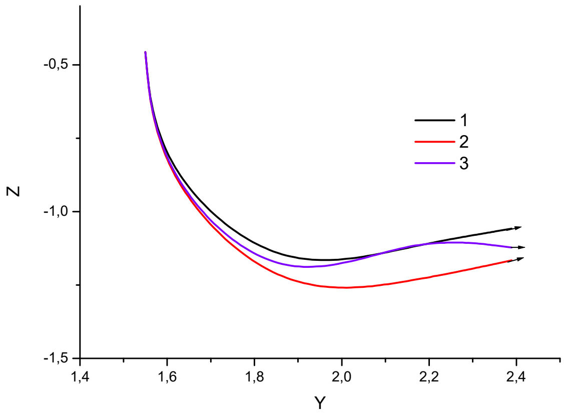

Figure 5. Characteristic trajectories of implanted O^+ ions in the SiO_2(001)<1̄10> film at E_0=3 keV and $\psi = 10^0$

Our calculations showed that the trajectories of the ions that remained (were implanted) in the films have different types. These trajectories were formed due to multiple scattering from the atomic chains under the surface layers, and they have a zigzag and linear shape in general.

CONCLUSION

We have studied the process of implantation of O^+ ions into SiO_2(001) films using computer modeling. The dependence of the number of implanted O^+ ions into SiO_2(001) films on the incidence angle has been obtained. It has been shown that the geometric parameters of the surface semichannels affect the process of ion implantation. The characteristic trajectories of the implanted ions on the films have been studied and the parameters of the implanted particles have been calculated. The obtained results make it possible to apply the ion implantation process to obtain materials with new parameters.

ORCID
Uchkun O. Kutliev, https://orcid.org/0000-0003-2241-2025; **Atabek S. Ashirov**, https://orcid.org/0000-0002-8731-7531

REFERENCES

[1] J.M. Haile, *Molecular Dynamics Simulation -Elementary Methods*, (Wiley-Interscience, New York, 1992).
[2] D.P. Woodruff, D. Brown, P.D. Quinn, T.C.Q. Noakes, and P. Bailey, "Structure determination of surface adsorption and surface alloy phases using medium energy ion scattering," Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, **183**(1-2), 128-139 (2001). https://doi.org/10.1016/S0168-583X(01)00472-4
[3] D.M. Muradkabilov, D.A. Tashmukhamedova, and B.E. Umirzakov, "Applying low-energy ion implantation in the creation of nanocontacts on the surface of ultrathin semiconductor films," Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques, **7**(5), 967–971 (2013). https://doi.org/10.1134/S1027451013050376
[4] Y.S. Ergashov, and B.E. Umirzakov, "Structure and Properties of a Bilayer Nanodimensional $CoSi_2$/Si/$CoSi_2$/Si System Obtained by Ion Implantation," Technical Physics, **63**(12), 1820–1823 (2018). https://doi.org/10.1134/S1063784218120058
[5] Z. Xie, and X. Luo, "Energy losses of highly charged Ar^{q+} ions during grazing incidence on tungsten surfaces," Frontiers in Physics, **12**, 2024. https://doi.org/10.3389/fphy.2024.1362594
[6] S.B. Utamuradova, S.K. Daliev, A.K. Khaitbaev, J.J. Khamdamov, K.J. Matchonov, and X.Y. Utemuratova, "Research of the Impact of Silicon Doping with Holmium on its Structure and Properties Using Raman Scattering Spectroscopy Methods," East Eur. J. Phys. (2), 274-278 (2024). https://doi.org/10.26565/2312-4334-2024-2-28
[7] S. Zainabidinov, S.I. Rembeza, E.S. Rembeza, *et al*., "Prospects for the use of metal-oxide semiconductors in energy converters," Appl. Sol. Energy, **55**, 5–7 (2019). https://doi.org/10.3103/S0003701X19010146
[8] N.Y. Yunusaliyev, "The Gas-Sensitive Properties of Tin Dioxide Films," East Eur. J. Phys. (4), 439-442 (2024). https://doi.org/10.26565/2312-4334-2024-4-52
[9] U.O. Kutliev, M.U. Otabaev, M.K. Karimov, F.K. Masharipov, and I. Woiciechowski, "Scattering of low-energy Ne^+ ions from the stepped surface of InGaP(001)<110> at the small angles of incidence," Physics and Chemistry of Solid State, **24**(3), 542-548 (2023). https://doi.org/10.15330/pcss.24.3.542-548
[10] U.O. Kutliev, M.U. Otabaev, and M.K. Karimov, "Investigation Ne ions scattering from the stepped InP(001)<1̄10> surface," Journal of Physics: Conference Series, **2388**(1), 012092 (2022). https://doi.org/10.1088/1742-6596/2388/1/012092
[11] M.K. Karimov, F.O. Kuryozov, S.R. Sadullaev, M.U. Otabaev, and S.B. Bobojonova, "Investigation of Defect InP(001) Surface by Low Energy Ion Scattering Spectroscopy," Materials Science Forum, **1049**, 192–197 (2022). https://doi.org/10.4028/www.scientific.net/MSF.1049.192

[12] H.H. Brongersma, T. Grehl, E.R. Schofield, R.A. Smith, and H.R. ter Veen, "Analysis of the outer surface of platinum-gold catalysts by low-energy ion scattering," Platinum Metals Review, **54**(2), 81-85 (2010). https://doi.org/10.1595/147106710X494358

[13] A. Rafati, Rik ter Veen, and D.G. Castner, "Low energy ion scattering: determining overlayer thickness for functionalized gold nanoparticles," Surf. Interface Anal. **45**(11-12), 2013-2016 (2013). https://doi.org/10.1002/sia.5315

[14] A.S. Ashirov, U.O. Kutliev, S. Xakimov, and S.K. Ismailov, "Low Energy Ar $^+$ Ions Scattering from SiO_2(001)<$\bar{1}$10> Surface under Grazing Incidencem," Materials Science Forum, **1049**, 152-157 (2022). https://doi.org/10.4028/www.scientific.net/MSF.1049.152

[15] U. Kutliev, M. Karimov, B. Sadullaeva, and M. Otaboev, "Investigation of the ion scattering process from the A3B5 semiconductors by the computer simulation method," COMPUSOFT: An International Journal of Advanced Computer Technology, **7**(4), 2749–2751 (2018). https://ijact.in/index.php/j/article/view/431/412

[16] M.T. Robinson, *MARLOWE Binary Collision Cascade Simulation Program, Version 15b, A Guide for Users*, (London, 2002).

[17] M.T. Robinson, "Computer Simulation Studies of High-Energy Collision Cascades," Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, **67**(1-4), 396-400 (1992). https://doi.org/10.1016/0168-583X(92)95839-J

[18] L.M. Kishinevsky, "Cross- sections of inelastic atomic collisions," Izvestiya Phys. Ser. **26**, 1410-1414 (1962). (in Russian)

ДОСЛІДЖЕННЯ ІМПЛАНТАЦІЇ ІОНІВ O+ У ПЛІВКИ SiO2(001) ПРИ МАЛОКУТОВОМУ ІОННОМУ БОМБАРДУВАННІ

У.О. Кутлієв[a], А.С. Аширов[a], Г.Х. Аллаярова[b], А. Саїдова[a]
[a]*Ургенчський державний університет, Ургенч, Узбекистан*
[b]*Каршинський державний університет, м. Карші, вул. Узбекистан*

Досліджено процес іонної імплантації при малокутовому іонному бомбардуванні плівки SiO_2 (001) при малих значеннях початкової енергії (до 5 кеВ). Поряд з розсіяними іонами O+ спостерігається імплантація іонів. Показано, що геометричні параметри поверхневого півканалу впливають на кут бомбардування, який ініціює процес імплантації. Встановлено, що у випадку неглибокого напівканалу процес імплантації спостерігається більше, ніж глибокого напівканалу при одному значенні кута падіння іонів. Отримано залежність імплантованих іонів від кута їх бомбардування. Виявлено, що кілька бомбардуючих іонів були імплантовані в глибокий поверхневий півканал. Це пояснюється впливом другого атомного ряду півканалу. Отримані результати представляють великий інтерес для вивчення процесу іонної імплантації.

Ключові слова: *імплантація; іонне бомбардування; комп'ютерне моделювання; розсіювання іонів; фокусування*