

The effect of temperature factor during heavy ion irradiation on structural disordering of SiC ceramics

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ABSTRACT

The paper presents the results of the influence of heavy ion irradiation on the formation of anisotropic distortions of the crystal structure and electron density distribution in SiC ceramics. The assessment of the change in the properties of the damaged layer was carried out using Raman spectroscopy methods, and using data on structural changes obtained using the X-ray diffraction method. The observed alterations in the spectral modes $E_1(\text{TO})$, $E_2(\text{TO})$ and $A_1(\text{LO})$ depending on the irradiation temperature indicate an anisotropic distortion of the structure, which has a clearly expressed dependence on the irradiation temperature, as well as the type of ions used for irradiation. The assessment results of changes in the electron density distribution contingent upon the irradiation temperature for both types of ion irradiation showed a direct correlation between the irradiation temperature growth and the electron density anisotropic distortion caused by the deformation of chemical bonds. In turn, the combination of the effects of thermal heating and ionization processes causes deformation distortion of chemical bonds, which is most pronounced at high irradiation temperatures, for which thermal expansion of the crystal lattice and accelerated diffusion of vacancy defects play a key role in disordering.

1. Introduction

The study of the kinetics of structural damage accumulation in ceramic materials using optical research methods is one of the most developing promising areas of research today due to the possibility of determination of the concentration dependences of defects associated with exposure to ionizing radiation, and determination of the connection between structural changes and effects associated with the softening of damaged layers [1–4]. In addition to study of the kinetics of structural damage caused by heavy ions, which allows simulation of the radiation damage processes caused by fission fragments or neutron exposure, much attention has recently been paid to research aimed at identification of the influence of temperature factors on radiation damage processes [5–7], since the potential of most ceramic materials consists in their use in extreme conditions, including those associated with exposure to high temperatures [8–12]. In this case, the evolution of structural damage resulting from the interaction of incident ions with the crystal structure, as a result of additional thermal effects, can be more pronounced, as has been shown in several studies [13–15], the

main results of which make it possible to postulate an adverse impact of high temperatures on the structural disorder degree. Thermal impact on the crystalline structure of structural materials is usually expressed in the volumetric broadening of the crystal lattice, caused by a change in the amplitude of atomic oscillations, alongside an elevation in the migration processes of vacancies and point defects in the structure [16, 17]. In combination with the ionization effect, thermal heating can lead to a more pronounced destabilization of the damaged layer, which in turn will lead to more intense disordering and amorphization of the damaged layer, which will negatively affect the properties of ceramics, as well as their service life.

The main idea of this article is to determine the influence of irradiation temperature in the case of high-dose irradiation, characteristic of the formation in the structure of the effect of deep overlapping of structurally deformed inclusions arising along the trajectory of ion movement, on the change in structural features and associated changes in electron density in SiC ceramics. In this case, the selection of irradiation temperature regimes was chosen based on data on the possible operating modes of this type of ceramics when considering them as

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structural materials for new generation reactors, including high-temperature reactors [18,19]. Much attention in the work is paid to determination of the irradiation temperature effect on alterations in structural features and anisotropic distortions of the distribution of electron density and chemical bonds caused by irradiation with heavy ions in the near-surface layer.

The use of Raman spectroscopy methods to study structural damage associated with heavy ion irradiation is one of the most promising methods of non-destructive testing of radiation damage in the near-surface layer, determining not only the quantitative concentration of defects, but also establishing qualitative changes associated with the crystal structure distortion, and changes in the chemical bonds Si – C, Si – Si, C–C. Thus, using the Raman spectroscopy method, structural changes in 4H–SiC and 6H–SiC ceramics [20] subjected to heavy ion irradiation were established, which made it possible to establish the amorphization kinetics, alongside the relationship between structural distortions and irradiation type. The relationship between the total disorder and the contribution from chemical disorder in the crystal structure caused by heavy ion irradiation in SiC ceramics, determined using the Raman spectroscopy method, was studied in Ref. [21]. Interest in SiC ceramics is not only due to their use as structural materials, but also to various other applications, including those related to optical materials and cathodoluminescence [22–24].

2. Experimental part

Polycrystalline SiC ceramics with a hexagonal type of crystal lattice were chosen as objects of study; the structural ordering degree is 98.0%. Commercial ceramics purchased from Dongguan Mingrui Ceramic Tech. Co. Ltd. were used as test samples. The degree of structural ordering was assessed using the X-ray diffraction analysis method, the results of which coincided with the passport data of the supplier company.

Irradiation of SiC ceramic samples for the purpose of simulation of radiation damage processes characteristic of modeling the effect of overlapping defective inclusions in a damaged layer was performed at the heavy ion accelerator DC-60, located at the Institute of Nuclear Physics of the Ministry of Energy of the Republic of Kazakhstan (Astana, Kazakhstan). Irradiation was conducted with heavy Ar⁺ (70 MeV) and Xe⁺ (230 MeV) ions, the irradiation fluence was $5 \times 10^{13} \text{ cm}^{-2}$. The choice of Ar⁺ and Xe⁺ ions for irradiation of the samples is based on the possibilities of simulation of radiation damage comparable to fission fragments of nuclear fuel when using this class of materials in the structural materials of the active zone. The variation of the irradiation

temperature was from 25 °C to 700 °C, the choice of which was based on the possibilities of simulation of the processes of radiation damage comparable to the impact of fission fragments that occur during the operation of materials in various extreme conditions. The irradiation temperature was controlled using a special controller, as well as a set of thermocouples recording the temperature of the sample on both sides, as well as the temperature of the heater. The maximum ion path length was determined according to calculation data using the SRIM Pro 2013 software code; a model taking into account the effect of cascade displacement formation was used for the determination.

Fig. 1 reveals the results of simulation of the ionization losses of heavy Ar⁺ and Xe⁺ ions along the ion trajectory in the damaged layer, performed in the SRIM Pro 2013 software code. The general appearance of the presented dependencies in Fig. 1a indicates that when the type of ions during irradiation changes from Ar⁺ to Xe⁺, the thickness of the damaged layer grows from 12 to 14 μm , while the values of ionization losses dE/dx_{electron} are about 6–7 keV/nm and 22–23 keV/nm for Ar⁺ and Xe⁺ ions, respectively, which indicates that the nature of the structural changes associated with ionization processes will be more pronounced when irradiated with Xe⁺ ions. Moreover, in this case, according to the data on the assessment of the values of energy losses during interaction with nuclei dE/dx_{nuclear} , the contribution from the interaction of Xe⁺ ions will be more pronounced than when irradiated with Ar⁺ ions.

As is known, the dominant mechanisms of radiation damage in materials during interaction with heavy ions are inelastic collisions associated with the ionization effect and the emergence of electron-phonon bonds that arise as a result of the transformation of the kinetic energy of incident ions during interaction with electron shells. In the case of inelastic interactions, the main effects arising as a result of the interaction of incident ions with the crystal structure, along the trajectory of the ions in the material, localized electronic excitations arise, the formation of which leads to local heating of the crystal lattice, as well as ionization processes, the occurrence of which leads to a change in the electron density.

In turn, elastic collisions that lead to the formation of interstitial atoms and vacancies in the structure of the damaged layer are caused by the interaction of incident ions with nuclei, are quite complex due to the structural features of the materials under study, which in turn requires detailed and comprehensive study. During elastic interaction of incident ions with atomic nuclei, their displacement occurs if the kinetic energy of the incident ions is sufficient to break the bond energy. At the same time, in the case of thermal heating of samples during irradiation, the

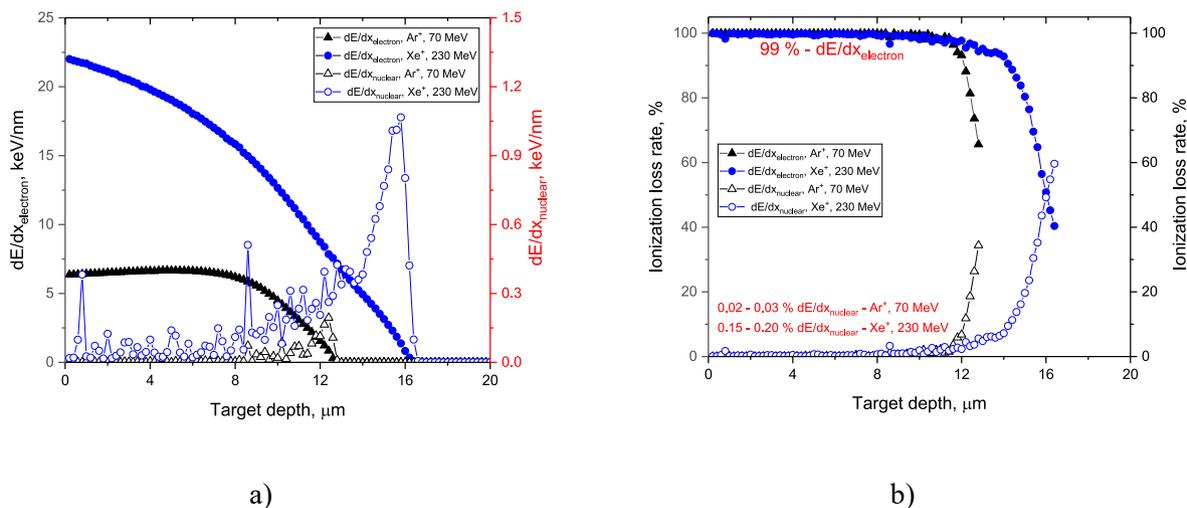


Fig. 1. Results of ionization loss modeling performed in the SRIM Pro 2013 software code: a) Dependence of the change in the value of ionization losses of ions along the trajectory of movement in the near-surface layer with a thickness of about 20 μm ; b) Assessment results of the distribution of contributions of ionization losses to the processes of deformation distortion of the crystal structure of SiC ceramics when irradiated with heavy ions Ar⁺ and Xe⁺.

effect of thermal expansion occurs, as well as changes in the amplitude of oscillations of atoms in the lattice nodes, which, with elastic collision of incident ions, can lead to more pronounced structural changes, since the crystalline structure in the case of temperature heating is in a metastable state. In this case, a change in the temperature of the thermal effect on the irradiated samples can initiate a greater number of structural changes, especially when in the system the contribution of ionization nuclear energy losses of incident ions during interaction with the crystal structure becomes greater due to a decrease in the ion velocity during multiple collisions. Fig. 1b demonstrates the assessment results of the influence of the contributions of energy losses of incident ions along the trajectory of their motion in the damaged layer, according to which it can be concluded that over most of the trajectory, the main contribution is made by the interactions of ions with electron shells, which are accompanied by ionization processes and changes in the electron density distribution, which are practically irreversible for dielectric materials [25,26]. At the same time, at a depth of about 12–15 μm , elastic collisions make their contribution, the role of which increases when ions are slowed down in the damaged layer.

The irradiation temperature was controlled by placing thermocouples on the sample and heating element to record the sample temperature during the entire irradiation process, as well as during heating and subsequent cooling. In order to avoid oxidation effects with a sharp temperature drop, the samples were cooled in a vacuum for 5–10 h until room temperature was reached, after which they were removed from the irradiation chamber. According to the estimated ion penetration depth in ceramics, in the case of irradiation with Ar^+ ions, the maximum penetration depth is about 12–12.5 μm , and in the case of irradiation with Xe^+ ions, the maximum penetration depth is more than 16 μm .

The study of structural changes associated with deformation distortion of chemical bonds in the damaged layer was carried out by means of a comprehensive analysis of the Raman spectra of the studied samples obtained using an EnSpectr M532 Raman spectrometer (Spectr-M LLC, Chernogolovka, Russia). The changes in the electron density distribution in the crystal lattice of the samples in the initial and irradiated states were assessed by analyzing the obtained X-ray diffraction patterns and calculating the deformation distortions of chemical and crystalline bonds depending on the type of irradiation. The data were obtained on a Rigaku SmartLab X-ray diffractometer.

3. Results and discussion

Fig. 2 illustrates the results of Raman spectra of the studied SiC ceramics irradiated with Ar^+ and Xe^+ ions with a fluence of $5 \times 10^{13} \text{ cm}^{-2}$ at different irradiation temperatures, the variation of which makes it possible to model radiation-induced deformation distortions and

amorphization of the damaged layer, comparable to real operating conditions. According to the data obtained, the observed positions of the main spectral lines at 770–800 cm^{-1} and 970 cm^{-1} are characteristic of the phonon modes of the A_1 , E_1 and E_2 groups, describing the structure of wurtzite with a hexagonal type of crystal structure, possessing the symmetry group C_{6v} . At the same time, the modes can split into longitudinal (LO) and transverse (TO) optical modes, which leads to the registration of the $E_1(\text{TO})$, $E_2(\text{TO})$, lines, characteristic of transverse splitting, and the $A_1(\text{LO})$ line, which characterizes longitudinal splitting. In this case, this set of modes characterizes the crystalline structure of ceramics and the degree of its ordering, describing the vibrations of the Si–Si, Si–C and C–C bonds, as well as their changes [27,28].

The absence of observed new peaks for samples exposed to irradiation at different temperatures indicates sufficient stability of ceramics to polymorphic transformations associated with a change in symmetry as a result of the interaction of incident ions with the crystal structure. At the same time, the observed changes for irradiated samples depending on the irradiation temperature are characteristic of deformation distortions of the structure, as well as partial amorphization, manifested in the broadening of spectral lines, as well as distortion of their shape, which is especially evident for samples irradiated with Xe^+ ions. In this case, irradiation with heavy Xe^+ ions at temperatures of 500–700 $^\circ\text{C}$ leads to a shift of the $E_2(\text{TO})$ peak to the region of longer wavelengths, which leads to the absorption of the $E_1(\text{TO})$ peak, as well as a shift of the $A_1(\text{LO})$ maximum to the region of shorter wavelengths, indicating an elevation in the contribution of compressive stresses in the damaged layer structure. Moreover, in contrast to the SiC ceramic samples irradiated with Ar^+ ions, for which a reduction in the intensity of the $A_1(\text{LO})$ mode is observed with a growth in the irradiation temperature, indicating disordering of the structure, irradiation with Xe^+ ions with an elevation in the irradiation temperature leads to the opposite effect, consisting in a distortion of the shape of the $E_1(\text{TO})$ and $E_2(\text{TO})$ modes, and small changes in the intensity of the $A_1(\text{LO})$ mode. Such differences in the change in the intensities of the $E_1(\text{TO})$, $E_2(\text{TO})$ and $A_1(\text{LO})$ modes in the case of a change in the type of irradiation ions can be caused by ionization processes, as well as the difference in the change in the values of ionization losses of incident ions, which cause structural disordering processes. In the case of irradiation with Ar^+ ions, the value of dE/dx_{electron} is about 6–7 keV/nm, while with irradiation with Xe^+ ions, this value of dE/dx_{electron} is about 22–23 keV/nm. As a result of the interaction of Xe^+ ions, the transferred kinetic energy during the interaction processes with electron shells is much greater than in the case of irradiation with Ar^+ ions, while the contribution to the structural disorder during irradiation with Xe^+ ions is also made by elastic interactions, the result of which are atomic displacements accompanied by the rupture of chemical bonds and the formation of vacancies, as evidenced by a more

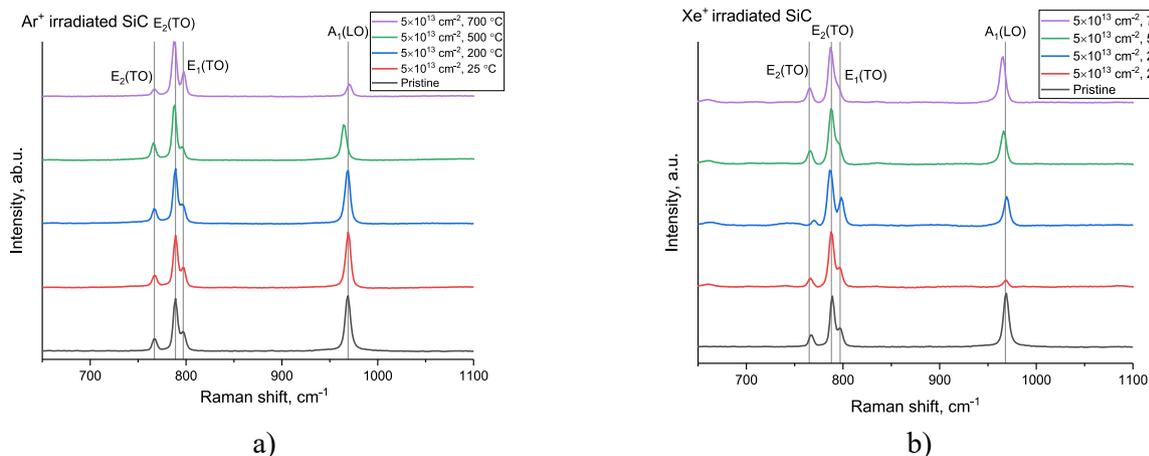


Fig. 2. Results of Raman spectroscopy of the studied SiC ceramics as a result of irradiation with heavy ions with variation of irradiation temperature: a) data of changes during irradiation with Ar^+ ions; b) data of changes during irradiation with Xe^+ ions.

pronounced shift of the $E_1(\text{TO})$, $E_2(\text{TO})$ modes, characterizing the Si–C bonds, and their shift of modes indicates the formation of chemical disorder in the structure, which manifests itself at high irradiation temperatures.

Table 1 reveals the assessment results of changes in the position of the spectral lines $E_1(\text{TO})$, $E_2(\text{TO})$ and $A_1(\text{LO})$ depending on the type and temperature of irradiation, as well as the value of their FWHM, the change of which determines the presence of amorphous inclusions in the composition of the damaged layer. As can be seen from the data presented, an alteration in the irradiation temperature, as well as the type of ions, results in various deformation changes in the shift of the maxima of the spectral line, as well as an elevation in their FWHM, caused by the processes of accumulation of short-range structural disordering, leading to partial amorphization of the damaged layer. Moreover, the analysis of the shifts of the Raman peaks $\Delta\omega$ depending on the type of ions and the irradiation temperature indicates a different nature of deformation distortions associated with the accumulation of residual mechanical stresses in the structure.

Fig. 3 reveals the assessment results of the contributions of the $E_1(\text{TO})$, $E_2(\text{TO})$ and $A_1(\text{LO})$ modes in the Raman spectra of SiC ceramic samples in the initial state and after irradiation, the analysis of which allows the assessment of the orientation effects associated with the disordering of chemical bonds, as well as structural distortions that cause the damaged layer disordering. The contribution of each mode was estimated from the areas of the spectral lines corresponding to these modes, taking into account the subtraction of background radiation.

An analysis of the value of changes in the contributions of spectral modes characteristic of transverse and longitudinal splitting associated with deformation distortion of the crystal structure showed that with a change in the irradiation temperature in the case of irradiation with Ar^+ ions, the contribution of transverse splitting increases, while with irradiation with Xe^+ ions in the case of high temperatures (500–700 °C), an equally probable influence of splitting bands on the deformation distortion of the crystal structure is observed. It should be noted that the decrease in the contribution of the $A_1(\text{LO})$ mode, the broadening and decrease in intensity of which is due to the amorphization of the damaged layer, which in the case of irradiation with Ar^+ ions appears at

Table 1
Evaluation results of spectral lines of research.

Mode	Parameter	Irradiation with Ar^+ ions				
		Pristine	25 °C	200 °C	500 °C	700 °C
$E_2(\text{TO})$, 767 cm^{-1}	Maximum center, cm^{-1}	767.09	767.10	766.93	766.05	766.95
	FWHM	4.47	5.78	5.63	5.03	4.45
$E_2(\text{TO})$, 789 cm^{-1}	Maximum center, cm^{-1}	788.91	789.10	788.77	787.81	787.74
	FWHM	4.98	5.11	4.92	4.66	5.00
$E_1(\text{TO})$, 797 cm^{-1}	Maximum center, cm^{-1}	796.16	797.39	796.71	796.41	797.77
	FWHM	5.16	4.15	5.02	3.53	3.83
$A_1(\text{LO})$, 969 cm^{-1}	Maximum center, cm^{-1}	968.79	969.17	968.53	964.80	970.43
	FWHM	6.12	5.52	5.56	5.55	4.98
Mode	Parameter	Irradiation with Xe^+ ions				
		Pristine	25 °C	200 °C	500 °C	700 °C
$E_2(\text{TO})$, 767 cm^{-1}	Maximum center, cm^{-1}	767.09	766.00	769.21	765.81	765.37
	FWHM	4.47	3.39	2.41	4.09	4.21
$E_2(\text{TO})$, 789 cm^{-1}	Maximum center, cm^{-1}	788.91	788.03	786.95	788.06	787.39
	FWHM	4.98	5.60	5.99	5.57	5.22
$E_1(\text{TO})$, 797 cm^{-1}	Maximum center, cm^{-1}	796.16	796.80	798.45	795.29	793.38
	FWHM	5.16	4.69	5.04	5.38	6.86
$A_1(\text{LO})$, 969 cm^{-1}	Maximum center, cm^{-1}	968.79	968.39	969.35	966.14	965.26
	FWHM	6.12	4.63	6.27	5.93	6.04

a temperature of 700 °C, and in the case of irradiation with Xe^+ ions, the most pronounced changes are observed at a temperature of 25 °C.

Based on the obtained data on the shifts in the positions of the spectral line maxima on the Raman spectra of the samples depending on the irradiation temperature, the values of residual mechanical stresses were calculated according to the method specified in Ref. [29]. The results are presented in Fig. 4 in the form of diagrams reflecting not only the values of residual mechanical stresses, but also their type. The overall view of the presented data on alterations in the values of residual mechanical stresses in the damaged layer revealed that the most significant changes associated with the accumulation of structural deformations and distortions in the case of samples irradiated with Ar^+ ions are observed at temperatures of 500–700 °C. It should be noted that the nature of the structural deformations determined for all the studied spectral lines characteristic of the $E_1(\text{TO})$, $E_2(\text{TO})$ and $A_1(\text{LO})$ modes indicates anisotropic distortion of chemical bonds, which is most pronounced at high temperatures. At the same time, the nature of deformation distortions in the case of temperatures of 25–500 °C has a unidirectional type of deformation, while for samples irradiated at a temperature of 700 °C, multidirectional deformation distortions, associated with both tensile and compressive residual stresses, the increase in the concentration of which is associated with the thermal effects of thermal expansion of the crystal lattice and accelerated migration of defective inclusions in the damaged layer, are observed.

In the case of irradiation with heavy Xe^+ ions, the values of residual mechanical stresses in the damaged layer are significantly greater in comparison with the observed changes for samples irradiated with Ar^+ ions, from which it can be concluded that in the case of irradiation with heavy Xe^+ ions, not only ionization processes, which cause the occurrence of thermal peaks along the trajectory of ion movement, but also thermal expansion processes, which are most pronounced at high temperatures (500–700 °C), play a role in the disordering processes. Such clearly expressed differences in deformation distortions in the damaged layer in the case of irradiation with different ions at the same temperatures can be caused by the following factors associated with the sizes of structurally altered regions that arise along the trajectory of ion movement in the damaged layer and their subsequent overlap. When irradiated with heavy Xe^+ ions, the sizes of the structurally altered regions are significantly larger than when irradiated with Ar^+ ions, which in turn results in more pronounced effects of overlapping defective inclusions, which in turn leads to more pronounced structural disorder due to a rise in the contribution of chemical disorder caused by distortions of Si–C bonds in the damaged layer (according to an assessment of changes in the shape of the $E_1(\text{TO})$, $E_2(\text{TO})$ lines).

Thus, analyzing the observed changes in the Raman spectra of the studied samples depending on the type of exposure, it can be concluded that a change in the type of ions during irradiation in the case of the same temperatures at which irradiation occurs results in differences in the deformation distortions of chemical bonds, which in turn leads to differences in the change in the distribution of electron density.

Fig. 5 reveals the simulation results of the electron density distribution in the structure of SiC ceramics in the initial state and in the case of samples exposed to irradiation with heavy ions Ar^+ and Xe^+ with a change in the irradiation temperature. The general form of the presented constructions in the case of the initial sample is characterized by an isotropic distribution of electron density, small changes in which in this case are due to structural distortions associated with the process of manufacturing ceramics, as well as imperfections of the crystal structure. In the case of irradiated samples at a temperature of 25 °C, the most pronounced alterations are observed for samples irradiated with Xe^+ ions, for which a blurring of the electron density halos, associated with deformation distortions of chemical bonds, is observed. The irradiation temperature growth at the same fluence values leads to a more intense distortion of the electron density, which indicates an adverse effect of temperature factors on the electron density distortion.

Table 2 shows the results of the assessment of the values of chemical

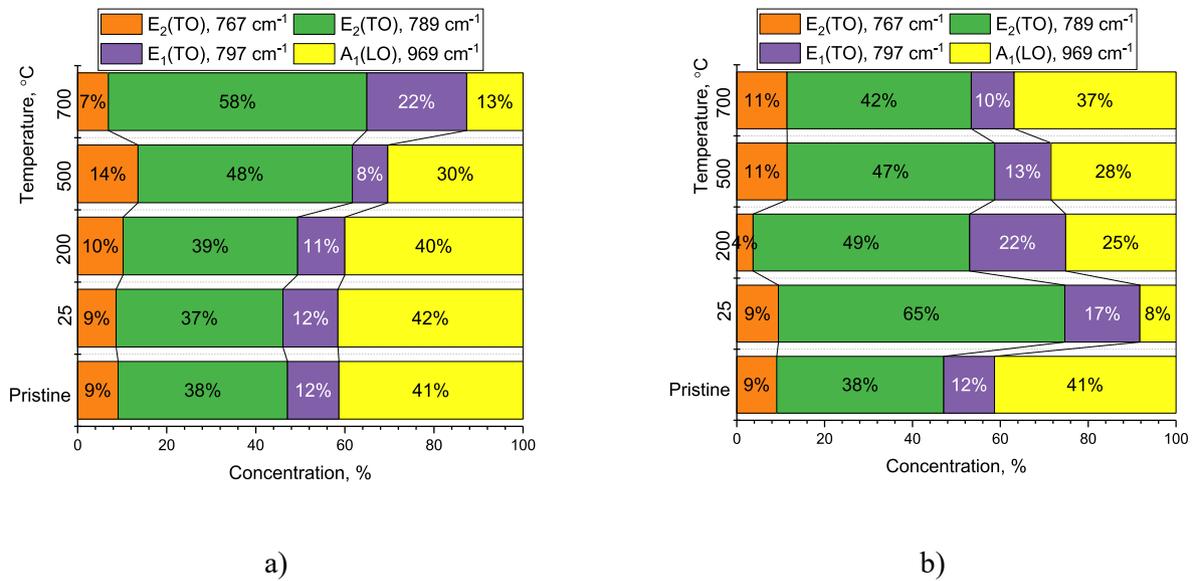


Fig. 3. Assessment results of changes in the contributions of modes indicating the influence of irradiation on the orientation effects of structural distortions in the damaged layer with variations in the irradiation temperature: a) when irradiated with Ar^+ ions; b) when irradiated with Xe^+ ions.

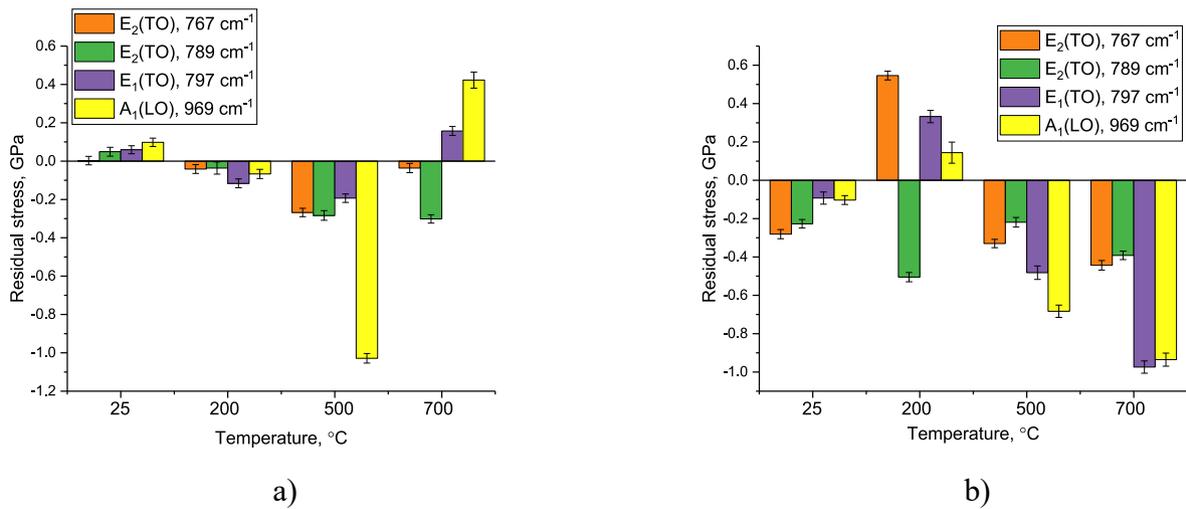


Fig. 4. Evaluation results of the values of residual mechanical stresses in the crystal structure depending on the ion irradiation type, as well as temperature variations (In this case, the physical meaning of negative values is related to the magnitude of the deformation compression of the structure as a result of external influences. A positive value reflects tensile deformation.): a) when irradiated with Ar^+ ions; b) when irradiated with Xe^+ ions.

bonds and their distortion as a result of irradiation with heavy ions with a change in irradiation temperature.

In the case of high-temperature irradiation (at temperatures of 500–700 $^{\circ}\text{C}$), as is evident from the presented changes in the electron density distribution, an elevation in the irradiation temperature leads to the formation of an anisotropy effect in the distributions, which are most pronounced in the case of high temperatures. At the same time, in the case of samples irradiated with heavy Xe^+ ions, an increase in temperature to 700 $^{\circ}\text{C}$ leads to a clearly expressed anisotropy of the electron density distribution, caused by a strong distortion of chemical bonds. The observed alterations in the electron density distributions, as well as the values of chemical bonds presented in Table 2, are in good agreement with the assessment results of changes in structural damage obtained from the analysis of the Raman spectra of the studied samples.

4. Conclusion

According to the results of the conducted studies, the influence of

temperature factors associated with thermal expansion and alterations in the amplitude of thermal vibrations of atoms in the nodes of the crystal lattice on the effects of disordering under high-dose irradiation with heavy Ar^+ and Xe^+ ions was determined. It was established that with an elevation in the irradiation temperature above 200 $^{\circ}\text{C}$, the observed structural distortions are associated with the thermal effect on the crystalline structure of the damaged layer, resulting in more pronounced distortions of crystalline and chemical bonds, as well as the formation of amorphous inclusions in the damaged layer. Analysis of the observed alterations in the electron density distribution in the crystalline structure of SiC subjected to heavy ion irradiation revealed a direct dependence of anisotropic distortions of the electron density distribution on the irradiation temperature, from which it follows that the dominant contribution to the electron density distortion is made by thermal effects, which have an adverse impact on ionization processes and cascade effects associated with changes in the distribution of electrons in the damaged layer.

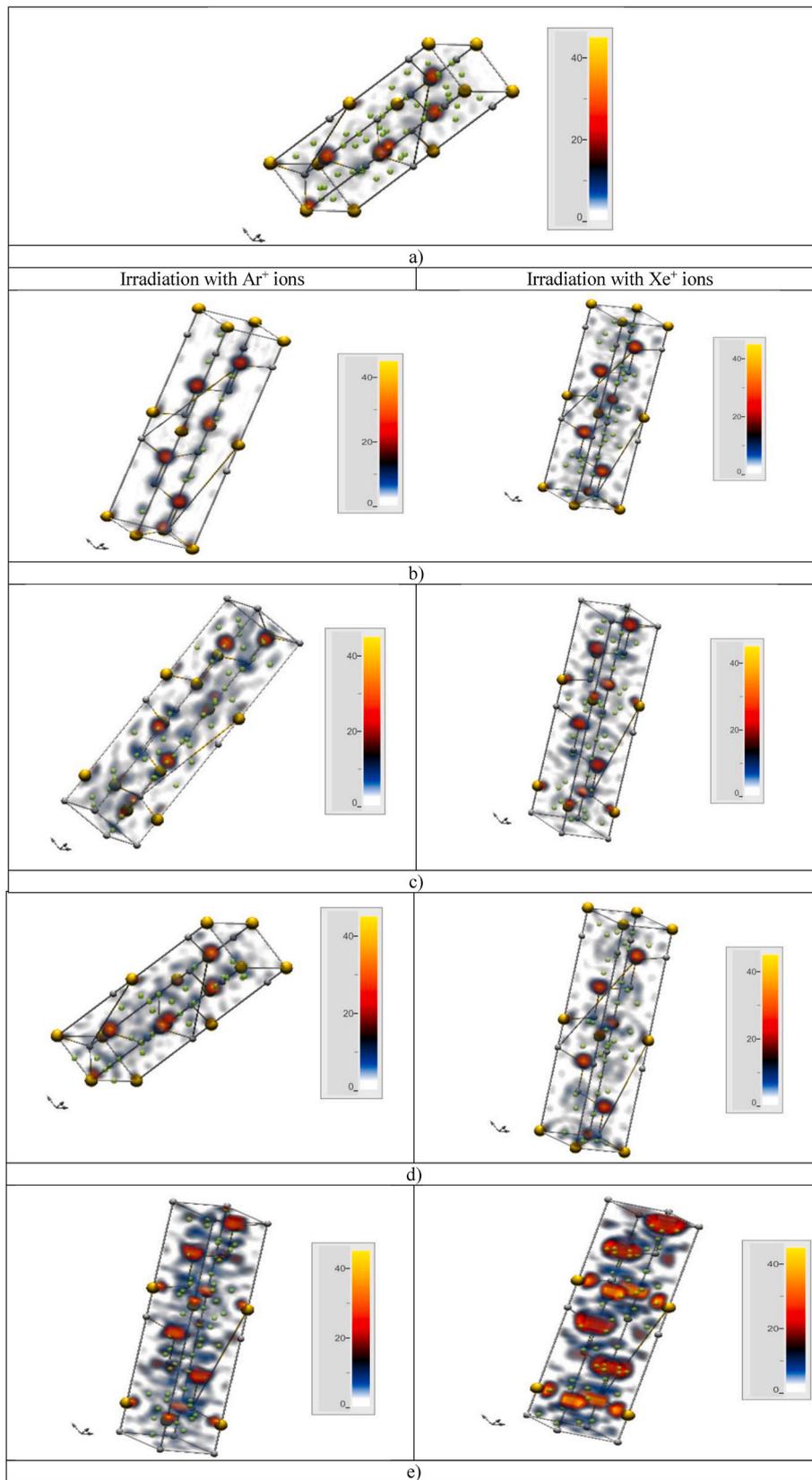


Fig. 5. Results of electron density distribution depending on variations in heavy ion irradiation conditions: a) Pristine; b) at a temperature of 25°C; c) at a temperature of 200°C; d) at a temperature of 500°C; e) at a temperature of 700°C

Table 2

Data on changes in the value of chemical bonds depending on heavy ion irradiation at temperature variations.

Type of chemical bond	Chemical bond value, Å				
	Irradiation with Ar ⁺ ions				
	Pristine	25 °C	200 °C	500 °C	700 °C
Si1–C1(x,-1+y,z)	1.88551	1.88627	1.89087	1.88599	1.89074
Si1–C1(-1+x,-1+y,z)	1.88551	1.88627	1.88846	1.88599	1.88854
Si1–C1	1.88551	1.88627	1.88846	1.88599	1.88854
Si1–C3(-x,-y,-1/2+z)	1.89658	1.89718	1.88846	1.89719	1.88854
Si2–C1	1.89356	1.89416	1.89087	1.89416	1.89528
Si2–C2	1.88751	1.88827	1.88795	1.888	1.88653
Si2–C2(-1+x,y,z)	1.88751	1.88827	1.88795	1.888	1.88653
Si2–C2(x,1+y,z)	1.88751	1.88827	1.88795	1.888	1.88653
Si3–C2	1.88902	1.88962	1.88846	1.88962	1.89007
Si3–C3(1+x,y,z)	1.88802	1.88878	1.88846	1.88851	1.89007
Si3–C3	1.88802	1.88878	1.88846	1.88851	1.89007
Si3–C3(1+x,1+y,z)	1.88802	1.88878	1.89087	1.88851	1.88621

Type of chemical bond	Chemical bond value, Å				
	Irradiation with Xe ⁺ ions				
	Pristine	25 °C	200 °C	500 °C	700 °C
Si1–C1(x,-1+y,z)	1.88551	1.88645	1.89147	1.89166	1.88659
Si1–C1(-1+x,-1+y,z)	1.88551	1.88645	1.88872	1.88906	1.88659
Si1–C1	1.88551	1.88645	1.88872	1.88906	1.88659
Si1–C3(-x,-y,-1/2+z)	1.89658	1.89739	1.88872	1.88906	1.89762
Si2–C1	1.89356	1.89437	1.89147	1.8962	1.89459
Si2–C2	1.88751	1.88846	1.88821	1.88705	1.88859
Si2–C2(-1+x,y,z)	1.88751	1.88846	1.88821	1.88705	1.88859
Si2–C2(x,1+y,z)	1.88751	1.88846	1.88821	1.88705	1.88859
Si3–C2	1.88902	1.88983	1.88872	1.89059	1.89005
Si3–C3(1+x,y,z)	1.88802	1.88897	1.88872	1.89059	1.8891
Si3–C3	1.88802	1.88897	1.88872	1.89059	1.8891
Si3–C3(1+x,1+y,z)	1.88802	1.88897	1.89147	1.88712	1.8891

CRedit authorship contribution statement

Kymbat M. Tynyshbayeva: Writing – original draft, Visualization, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Artem L. Kozlovskiy:** Writing – original draft, Visualization, Formal analysis, Data curation, Conceptualization.

Data availability statement

Not applicable.

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Declaration of competing interest

+ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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