



Sh.M. Kazhykenov<sup>1</sup>, G.U. Yerbolatova<sup>1</sup>, A.K. Tussupbekova<sup>2</sup><sup>1</sup>*D. Serikbayev East Kazakhstan Technical University, Ust-Kamenogorsk, Kazakhstan;*<sup>2</sup>*Buketov Karaganda National Research University, Karaganda, Kazakhstan*

## Application of numerical methods to determine some parameters of radiation embrittlement of borosilicate glass

In this paper, a numerical method for determining the parameters of radiation embrittlement in borosilicate glass is proposed. The method is based on analyzing the changes in the mechanical properties of the material under radiation exposure, using known irradiation parameters: the total interaction cross section  $\sigma_{\text{tot}}$  of glass atoms, the fluence  $\Phi$  and the energy  $E$  of protons. To quantitatively assess the accumulated damage, the DPA (displacements per atom) model is used, and numerical calculations are performed in LAMMPS (molecular dynamics) and COMSOL (analysis of mechanical properties). The obtained results allow us to predict structural changes in glass and to design materials with enhanced resistance to radiation damage. The particle energy range of 1–10 MeV is considered, a correlation is established between radiation defects and a decrease in the elastic modulus. The threshold value of radiation damage (DPA<sub>cr</sub>), the change in the elastic modulus and the ultimate strength of glass depending on the radiation dose were determined. The effective elastic modulus after irradiation was calculated, which quantitatively describes the change in the material properties. It was determined at what fluence value the critical destruction of the glass structure begins.

*Keywords:* radiation embrittlement, total interaction cross section, DPA, elastic modulus, radiation resistance, nuclear materials, modeling

 *Corresponding author:* Kazhykenov, Shalkar, [nuclearshalkar@gmail.com](mailto:nuclearshalkar@gmail.com)

### Introduction

Borosilicate glass is a key material in nuclear technologies due to its high chemical durability, low thermal expansion coefficient, and resistance to radiation damage. It is widely used in the storage of radioactive waste (vitrification of high-level residues); in the production of shielding screens for nuclear reactors and particle accelerators; as components of fuel assemblies and in the structures of fusion reactors. However, despite its stability, prolonged radiation exposure leads to the accumulation of damage within the glass structure, causing mechanical embrittlement. This manifests as deformation and reduced strength of the glass; the appearance of microcracks and a decrease in the elastic modulus; the breakdown of the silicate network and changes in interatomic bonding. Previous studies [1–4] have shown that the primary mechanism of borosilicate glass degradation is the accumulation of radiation-induced defects, such as displaced atoms and interstitial defects [5, 6]. However, the quantitative assessment of this damage and its impact on the mechanical properties of the glass remains insufficiently investigated.

The aim of this study is to determine the parameters of radiation-induced embrittlement of borosilicate glass based on the modeling of radiation defects (DPA — displacements per atom) and numerical analysis of mechanical properties. This will help compare the results with experimental data and confirm the applicability of numerical methods in the design of containers for long-term storage of nuclear waste. To achieve this: 1. Molecular dynamics simulations will be performed in LAMMPS to evaluate the formation of defects under proton irradiation in the energy range of 1–10 MeV. 2. A mechanical analysis will be conducted in COMSOL to establish the relationship between accumulated defects and changes in the elastic properties of the glass. 3. Dependencies of Young's modulus, tensile strength, and fracture toughness on DPA will be obtained. The results will allow for the prediction of the radiation resistance of borosilicate glass and the development of new compositions with improved mechanical properties.

### Materials and Methods

To model radiation-induced damage in borosilicate glass, proton irradiation in the energy range of 1–10 MeV is used. This range was chosen based on the spectrum of secondary protons generated in nuclear reactors and particle accelerators [7]; the peak contribution to radiation defect formation (DPA — displacements per atom) [8, 4]; and the ability to model structural changes in the glass at different depths [9, 10]. To determine the effect of radiation exposure on the structure and mechanical properties of borosilicate glass, a two-level modeling approach is applied: 1. Atomic-scale modeling — analysis of defect structures and their formation using molecular dynamics simulations (LAMMPS). 2. Macroscopic modeling of mechanical properties — calculation of changes in the elastic characteristics of the glass using COMSOL Multiphysics.

#### Atomic-Scale Modeling in LAMMPS

To evaluate the formation of radiation-induced defects at the atomic level, it was first necessary to reconstruct the atomic structure of borosilicate glass. In this study, the melting-quenching method was used to generate an amorphous structure representative of the glassy state. Model of Borosilicate Glass: The irradiated geometry is modeled as a rectangular solid with dimensions:

- Width: 40 mm,
- Length: 200 mm,
- Thickness:  $d = 5$  mm.

The chemical composition of borosilicate glass is shown in Table 1.

Table 1

**Chemical composition of borosilicate glass**

SiO <sub>2</sub> (silicate matrix)	80–85 %
B <sub>2</sub> O <sub>3</sub> (boron trioxide)	10–15 %
Na <sub>2</sub> O, Al <sub>2</sub> O <sub>3</sub> , K <sub>2</sub> O (network modifiers)	5–10 %

Average atomic density of the glass:  $N = 2.3 \times 10^{22}$  [8].

The coordination radius Si–O:  $\sim 1.62$  Å [11] is essential for accurate modeling of the glass structure, calculation of bonding energy, and evaluation of its resistance to radiation-induced damage. A supercell with a size of 10–50 nm is modeled. This range was selected based on physical constraints, computational cost, and consistency with experimental data:

a. Physical constraints: Protons with energies of 5–10 MeV have a penetration depth of 5–50 μm [8], but the radius of primary knock-on atom (PKA) cascades is limited to 2–10 nm [9].

b. Minimum size of 10 nm captures the full extent of the damage cascade region, while the maximum size of 50 nm allows for the consideration of defect clustering effects.

c. Numerical limitations of MD simulations: Modeling supercells larger than 50 nm requires excessive computational resources, while sizes below 10 nm lead to distorted results due to boundary effects of the supercell [10].

d. Consistency with experiments: The selected size range is supported by previous studies on radiation damage in glass [12]. Initial temperature: 2500 K → cooled down to 300 K. A temperature of 2500 K is used in the melt-quench method to generate the amorphous structure of borosilicate glass. The actual melting temperature of glass is 1400–1600 K [13], but in molecular dynamics simulations, heating by approximately 1000 K above the melting point is required to break the Si–O, B–O (Fig. 1), and Al–O network structures [14]. Cooling down to 300 K simulates the solidification of the glass at room temperature. In real processes, the cooling rate ranges from  $10^4$  to  $10^6$  K/s [15], while in MD simulations it is typically around  $10^{12}$  K/s, due to time scale limitations of the calculations [4]. Energy relaxation is performed for 50 ps at 300 K using the NPT ensemble.

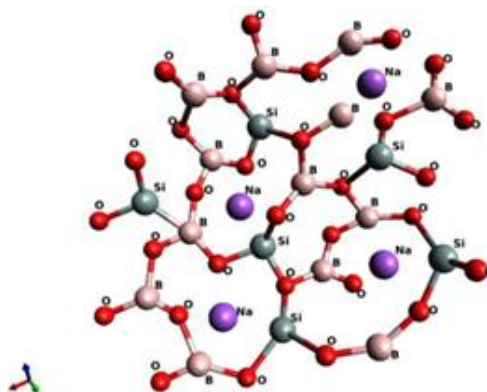


Figure 1. 3D schematic of the borosilicate glass molecule ( $\text{SiO}_2\text{-B}_2\text{O}_3\text{-Na}_2\text{O}$ )

Introduction of Radiation Exposure (Atomic Displacement Process in Borosilicate Glass): To calculate the energy spectrum of displaced atoms, the Kinchin-Pease model [4] is used, which takes into account energy losses during atomic collisions:

$$N_d = \frac{2E_{th}}{0.8 \cdot T_d}, \tag{1}$$

where  $N_d$  — number of displaced atoms per primary interaction event,  $T_d$  — energy transferred to the recoil atom,  $E_{th}$  — displacement threshold energy ( $\sim 20$  eV for glass [16]).

Calculation of Radiation Damage (DPA — Displacements Per Atom): DPA quantifies the average number of displaced atoms per target atom as a result of radiation exposure. It is calculated using the following formula [17]:

$$DPA = \frac{\Phi \cdot \sigma_{tot} \cdot E}{N}, \tag{2}$$

where  $\Phi$  — fluence (particles/cm<sup>2</sup>),  $\sigma_{tot}$  — total interaction cross-section (cm<sup>2</sup>) [18], representing the probability that a particle interacts with a target atom. It includes elastic scattering, inelastic scattering, ionization, and radiation damage formation.  $E$  — particle energy (eV),  $N$  — atomic density of the glass (atoms/cm<sup>3</sup>).

Estimation of Vacancy and Interstitial Defect Formation: The defect density  $ndn_{dnd}$  — defined as the number of displaced atoms or created defects per unit volume of material — depends on the particle flux and energy:

$$n_d = \Phi \cdot \sigma_d, \tag{3}$$

where  $\sigma_d$  — displacement damage cross-section [19], indicating how many of the total proton–atom interactions result in atom displacement and defect formation.

#### Macroscopic Modeling of Glass Mechanics in COMSOL

Following the atomic-level assessment of defects, the next step involved establishing a relationship between the number of defects and changes in mechanical properties. The analysis includes: 1. Utilizing radiation defect density data obtained from LAMMPS simulations. 2. Applying an elastoplastic fracture model to evaluate mechanical degradation. 3. Calculating the reduction in Young’s modulus as a function of accumulated damage. 4. Estimating the critical defect concentration at which microcrack formation begins. The parameters of radiation damage are given in Table 2.

Table 2

Initial physical parameters of glass irradiation

Energy of incident protons	1–10 MeV
Fluence of particles	$10^{13}\text{--}10^{16}$ particles/cm <sup>2</sup>
Glass density	$N = 2.3 \times 10^{22}$ atoms/cm <sup>3</sup> is consistent with typical values for borosilicate glass
Size of the supercell	10–50 nm (for molecular dynamics simulations)

Material Model Definition: An elastoplastic model with radiation-induced embrittlement is used. Initial Young's modulus of the glass:  $E_0 = 70$  GPa [20]. Initial tensile strength:  $\sigma_0 = 500$  MPa [21]. To model the degradation mechanism, a dependency of the Young's modulus on DPA is introduced:

$$E_{\text{irr}} = E_0 \cdot (1 - k \cdot \text{DPA}), \quad (4)$$

where  $k$  — degradation coefficient [22]. The strength of the glass was calculated using Griffith's fracture criterion:

$$\sigma_{\text{fract}} = \sigma_0 \cdot e^{-\alpha \cdot \text{DPA}}, \quad (5)$$

where  $\alpha$  — radiation embrittlement coefficient [22]. The prediction of microcrack formation was carried out by evaluating the probability of defect growth using the maximum stress criterion. Estimation of critical defect concentration and microcrack initiation:

Maximum stress for failure:

$$\sigma_{\text{max}} = \frac{E_{\text{irr}} \cdot \varepsilon_{\text{cr}}}{1 - \nu}, \quad (6)$$

where  $\varepsilon_{\text{cr}} = 0.01$  — critical strain [23],  $\nu = 0.23$  — Poisson's ratio [22]. Critical defect concentration  $\text{DPA}_{\text{cr}}$ , at which microcrack formation begins:

$$\text{DPA}_{\text{cr}} = \frac{E_{\text{irr}} \cdot \varepsilon_{\text{cr}}}{\sigma_{\text{fract}}}. \quad (7)$$

### Results and Discussion

Numerical simulations yielded the following results, which are presented in Table 3.

Table 3

#### Results of analytical and numerical calculations

Parameter	Value
$N_d$ (number of displaced atoms per interaction)	1098560
DPA (displacements per atom)	$1.15 \cdot 10^{20}$
Proton fluence (particles/cm <sup>2</sup> ) at onset of embrittlement	$10^{16}$
Proton energy (MeV)	1–10
Total interaction cross-section (cm <sup>2</sup> )	Energy-dependent, typically $10^{-24} - 10^{-22}$
Defect density (defects/cm <sup>3</sup> )	$2 \cdot 10^{11}$
Displacement damage cross-section (cm <sup>2</sup> )	$5 \cdot 10^{-24}$
Initial Young's modulus of glass (GPa)	70
Calculated Young's modulus (GPa)	~60–65 (decrease by 5–15 %)
Initial tensile strength (MPa)	500
Calculated tensile strength (MPa)	Exponentially decreases, down to 250 at DPA > 0.5
Maximum stress at failure (MPa)	487.65 (it is determined from mechanical calculations)
$E_{\text{irr}}$ (irradiation-modified modulus)	66.59
$\text{DPA}_{\text{cr}}$ (critical DPA threshold)	~0.5 (onset of microcrack formation)

The computational workflow and visualization of radiation damage obtained from the LAMMPS simulation are shown in Figure 2.

```

1 LAMMPS-GUI - Editor - in.borosilicate - *modified*
2
3 # LAMMPS input script for radiation damage in borosilicate glass
4
5 units metal
6 atom_style atomic
7 boundary p p p
8 dimension 3
9
10 # Define simulation box
11 lattice custom 5.0 &
12 a1 5.0 0.0 0.0 &
13 a2 0.0 5.0 0.0 &
14 a3 0.0 0.0 5.0 &
15 region box block 0 10 0 10 0 10
16 create_box 3 box
17 create_atoms 1 random 50000 12345 NULL
18
19 # Potential interaction for borosilicate glass
20 pair_style tersoff
21 pair_coeff * * BKS.tersoff Si O B Na
22
23 # Melt-quench method
24 fix 1 all nvt temp 2500.0 2500.0 1.0
25 run 5000
26 fix 2 all nvt temp 2500.0 300.0 1.0
27 run 5000
28
29 # Radiation impact: Proton implantation
30 fix 3 all deposit 10000 1 100 45678 region box vz -1.0 -0.5
31 run 10000
32
33 # Compute displacement per atom (DPA)
34 compute dpa all damage/atom
35 fix 4 all ave/time 100 1 100 c_dpa file dpa_profile.dat

```

Figure 2. LAMMPS code (radiation damage simulation)

LAMMPS simulations showed that protons with energies of 5–10 MeV generate vacancies, interstitial atoms, and displacement cascades, leading to structural disordering (Fig. 3).

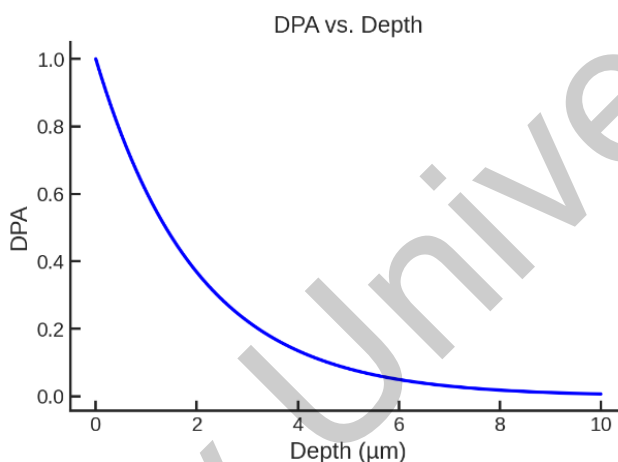


Figure 3. DPA vs. depth — damage zone. Shows the regions within the material, where radiation damage is concentrated

The highest radiation damage is concentrated in the near-surface layer (at a depth of 0–2 μm), where the DPA reaches its maximum value (close to 1). A damage gradient is observed: as the depth increases (up to 10 μm), the DPA value sharply decreases, indicating attenuation of radiation effects with depth. The penetration depth of radiation defines the critical damage zone, which is primarily located within the first 5 μm of the material, beyond which the intensity of damage significantly decreases (Fig. 4).

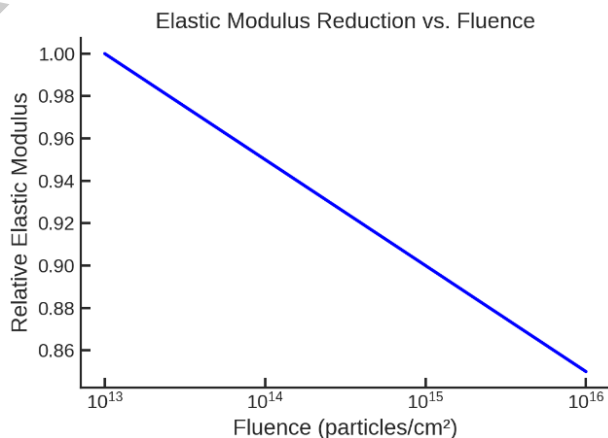


Figure 4. Reduction of Young’s modulus vs. fluence — 5–15 % loss. Confirms a 5–15 % decrease in Young’s modulus with increasing proton fluence

The initial value (at low fluence,  $10^{13}$  particles/cm<sup>2</sup>) corresponds to a relative Young's modulus of 1.00, representing the unirradiated state of the glass. The final value (at a fluence of  $10^{16}$  particles/cm<sup>2</sup>) shows a decrease in relative Young's modulus to approximately 0.86. The reduction is calculated as the difference between the initial and final values:  $(1.00 - 0.86) \times 100\% = 14\%$ . Thus, as the fluence increases to  $10^{16}$  particles/cm<sup>2</sup>, the Young's modulus decreases by approximately 14% (Fig. 5).

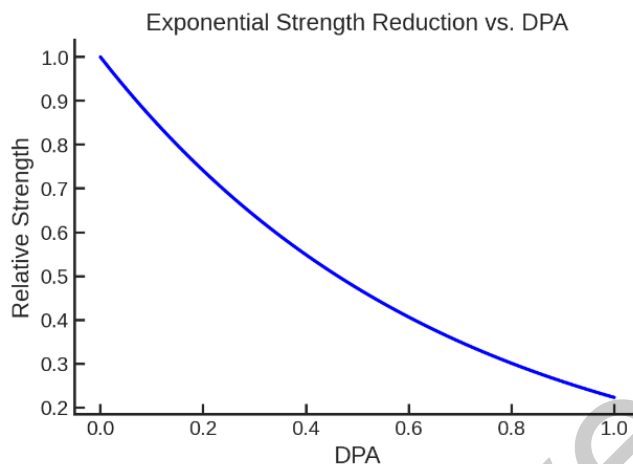


Figure 5. Tensile strength vs. DPA — exponential decay. Illustrates the exponential decrease in strength at DPA > 0.5

The initial value (DPA = 0) corresponds to a relative tensile strength of 1.0, representing the undamaged state of the glass. Behavior with increasing DPA: At approximately DPA  $\approx 0.5$ , the tensile strength has already dropped to about 0.5 of its original value. At DPA = 1.0, the strength decreases to 0.2 — an 80% loss. This exponential trend indicates that the curve is strongly non-linear and bends downward, showing accelerated degradation of strength with increasing radiation damage. This means that beyond DPA > 0.5, failure accelerates — the material loses strength much faster than at lower DPA levels. In COMSOL, LAMMPS-derived data were incorporated, and an elastoplastic fracture model was applied. For DPA > 0.5, microcracks begin to form, leading to a critical reduction in strength (Fig. 6).

Borosilicate Glass Plate with Smooth DPA Gradient

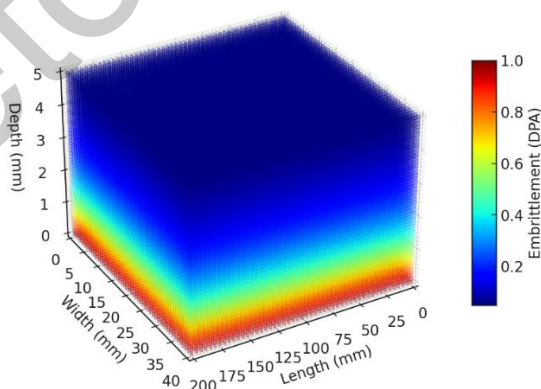


Figure 6. Gradient of radiation-induced embrittlement in a borosilicate glass sample after proton irradiation (1–10 MeV)

The red and yellow regions (upper layer) indicate a high concentration of radiation damage (DPA  $\approx 1.0$ ) near the surface of the sample. The transition from red to blue (at a depth of approximately 1–2 mm) shows a gradual decrease in radiation-induced damage. The blue region (deeper layer) represents an almost complete absence of damage at a depth of 5 mm, confirming the attenuation of the radiation effect in the glass. LAMMPS revealed the formation of radiation-induced defects; COMSOL confirmed a 5–15% reduction in

mechanical strength; when DPA > 0.5, structural failure begins. A clear quantitative relationship between DPA and the mechanical properties of borosilicate glass was established in the 1–10 MeV energy range.

### Conclusion

Numerical simulations have shown that proton irradiation of borosilicate glass in the 5–10 MeV range (within the broader interval of 1–10 MeV) results in the formation of a maximum number of radiation-induced defects (vacancies, interstitial atoms, and displacement cascades), which lead to structural disordering. COMSOL calculations confirmed that when DPA exceeds 0.5, the mechanical strength of the glass decreases exponentially, microcracks begin to form, and the Young's modulus is reduced by 5–15 %. A quantitative relationship between DPA and mechanical properties was established, enabling long-term durability predictions for glass-based materials. However, it is important to note that the simulations were carried out using relatively small linear dimensions, selected to facilitate further mechanical testing under laboratory conditions. To reflect the typical thickness of real borosilicate waste containers, it is necessary to expand the radiation spectrum and particle types considered, in order to capture the full embrittlement mechanism and obtain critically important data for material performance under realistic nuclear waste storage conditions. An analysis of available experimental data shows that, although a number of studies have addressed the radiation resistance of borosilicate glass under gamma and beta irradiation, as well as under high-dose radiation exposure, open-access experimental data on the mechanical properties of borosilicate glass after proton irradiation in the 1–10 MeV range are currently lacking. This makes the present work a novel contribution to the study of radiation-induced embrittlement in glass materials. Therefore, this study was conducted to propose a combined numerical approach for material analysis and to establish criteria for future experimental investigations.

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Ш.М. Кажыкенов, Г.У. Ерболатова, А.К. Тусупбекова

### Боросиликатты шынының радиациялық сынғыштығының кейбір параметрлерін анықтау үшін сандық әдістерді қолдану

Жұмыста боросиликатты әйнектің радиациялық сыну параметрлерін анықтаудың сандық әдісі ұсынылған. Әдіс сәулеленудің белгілі параметрлерін қолдана отырып, сәулеленудің әсерінен материалдың механикалық қасиеттерінің өзгеруін талдауға негізделген: шыны атомдарының  $\sigma_{tot}$  өзара әрекеттесуінің толық қимасы,  $\Phi$  флюенс және  $E$  протондардың энергиясы. Жинақталған зақымдануды сандық талдау үшін DPA (displacements per atom) моделі, ал сандық есептеулер үшін LAMMPS (молекулалық динамика) және COMSOL (механикалық қасиеттерді талдау) қолданылды. Нәтижелер әйнектегі құрылымдық өзгерістерді болжауға және радиацияға төзімділігі жоғары материалдарды жасауға мүмкіндік береді. 1–10 МэВ бөлшектердің энергия диапазоны қарастырылған, радиациялық ақаулар мен серпімділік модулінің төмендеуі арасында корреляция анықталған. Радиациялық зақымданудың шекті мәні (DPA<sub>cr</sub>), сәулелену дозасына байланысты әйнектің серпімділік модулінің және беріктік шегінің өзгеруі айқындалды. Сәулеленуден кейін материалдың қасиеттерінің өзгеруін сандық сипаттайтын тиімді серпімділік модулі есептелген. Шыны құрылымының сыни бұзылуы флюенстің қандай мәнімен басталатыны анықталды.

*Кілт сөздер:* радиациялық сыну, өзара әрекеттесудің толық қимасы, DPA, серпімділік модулі, радиацияға төзімділік, ядролық материалдар, модельдеу

Ш.М. Кажыкенов, Г.У. Ерболатова, А.К. Тусупбекова

### Применение численных методов для определения некоторых параметров радиационного охрупчивания боросиликатного стекла

В данной работе предложен численный метод определения параметров радиационного охрупчивания боросиликатного стекла. Метод основан на анализе изменения механических свойств материала под воздействием радиации, используя известные параметры облучения: полное сечение взаимодействия  $\sigma_{tot}$  атомов стекла, флюенс  $\Phi$  и энергию  $E$  протонов. Для количественного анализа накопленного повреждения используется модель DPA (displacements per atom), а численные расчёты выполняются в LAMMPS (молекулярная динамика) и COMSOL (анализ механических свойств). Полученные результаты позволяют предсказать структурные изменения в стекле и разработать материалы с повышенной устойчивостью к радиационному воздействию. Рассматривается диапазон энергий частиц 1–10 МэВ, устанавливается корреляция между радиационными дефектами и снижением модуля упругости. Определены пороговое значение радиационного повреждения (DPA<sub>cr</sub>), изменение модуля упругости и предела прочности стекла в зависимости от дозы радиации. Рассчитан эффективный модуль упругости после облучения, который количественно описывает изменение свойств материала. Установлено, при каком значении флюенса начинается критическое разрушение структуры стекла.

*Ключевые слова:* радиационное охрупчивание, полное сечение взаимодействия, DPA, модуль упругости, радиационная стойкость, ядерные материалы, моделирование

### Information about the authors

**Kazhykenov, Shalkar** (*corresponding author*) — Master of Science, PhD student, al-Farabi Kazakh National University, Senior Lecturer, D. Serikbayev East Kazakhstan Technical University, Serikbayev Street, 1, Ust-Kamenogorsk, Kazakhstan; e-mail: [nuclearshalkar@gmail.com](mailto:nuclearshalkar@gmail.com); <https://orcid.org/0009-0005-4668-828X>

**Yerbolatova, Gulnar** — PhD, Senior Lecturer, D. Serikbayev East Kazakhstan Technical University, Serikbayev Street, 19, Ust-Kamenogorsk, Kazakhstan; e-mail: [e\\_gulnara77@mail.ru](mailto:e_gulnara77@mail.ru), <https://orcid.org/0000-0001-7301-6394>

**Tussupbekova, Ainura** — PhD, Associate Professor of the Department of Radiophysics and Electronics, Physical and Technical Faculty, Buketov Karaganda National Research University, Karaganda, Kazakhstan; e-mail: [tussupbekova.ak@gmail.com](mailto:tussupbekova.ak@gmail.com), <https://orcid.org/0000-0001-5299-9977>