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## Research Article

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# Significant effect of neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) into mechanical and structural characteristics of lithium borate glass systems for superior radiation-shielding performance

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## Abstract

Because of their remarkable structural flexibility, comparatively low melting temperature, and easily adjustable physical properties, borate glasses have attracted a lot of scientific interest and are attractive candidates for a variety of multipurpose applications. In this work,  $\text{Nd}_2\text{O}_3$ -containing borate glasses were created using the melt-quenching method with the composition  $47\text{B}_2\text{O}_3\text{--}27\text{SiO}_2\text{--}11\text{Bi}_2\text{O}_3\text{--}11\text{Li}_2\text{O}\text{--}(4\text{--}x)\text{Na}_2\text{O}\text{--}x\text{Nd}_2\text{O}_3$ , where  $x = 0, 1, 2, 3$ , and  $4$  mol%, to investigate how the structural, mechanical, and radiation shielding properties are affected by the substitution of  $\text{Nd}_2\text{O}_3$ . The experimental density elevated from  $3.594$  to  $3.878$   $\text{gm.cm}^{-3}$  as  $\text{Nd}_2\text{O}_3$  gradually replaced  $\text{Na}_2\text{O}$ . Furthermore, the molar volume increased slightly from  $29.484$  to  $30.155$   $\text{cm}^3.\text{mol}^{-1}$ , indicating simultaneous densification and structural rearrangement. The average B-B distance increased marginally from  $0.2904$  to  $0.2965$  nm, whereas the local field strength increased from  $96.59 \times 10^{30}$  to  $2.41 \times 10^{30}$   $\text{cm}^{-2}$ , reflecting enhanced ionic interactions. Further addition of  $\text{Nd}_2\text{O}_3$  induced conversion of trigonal  $\text{BO}_3$  units into tetrahedral  $\text{BO}_4$  units, with increasing the fraction ( $N_4$ ) of  $\text{BO}_4$  from  $0.499$  for the undoped glass to  $0.651$  at  $4$  mol% based glass. Increased packing density, stronger Nd-O bonding, and greater bond dissociation energy all contributed to the continual improvement in elastic and mechanical properties of glass samples, according to theoretical calculations. According to theoretical radiation shielding qualities, the half-value layer and mean free path decreased while the linear and mass attenuation coefficients increased increasing  $\text{Nd}_2\text{O}_3$  concentration. For advanced radiation protection applications, the Nd-4 composition demonstrated the highest effective atomic number, electron density, and overall gamma-ray attenuation performance, demonstrating that  $\text{Nd}_2\text{O}_3$  substitution successfully improves the structural integrity and radiation shielding capacity of lithium borate glass.

**Keywords:** Applied Physics A; Lithium-Borate Glass; Structural properties; Mechanical behaviour; Radiation shielding performance.

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## **1. Introduction**

Because of its exceptional structural flexibility and variety of practical qualities, glass one of the earliest manmade materials ever created by humans remains essential to modern science and technology. Glass does not have a distinct melting point; instead, it undergoes a glass transition and has an uneven atomic structure without long-range periodicity. Additionally, because of its amorphous nature, its structure may be continuously altered by compositional changes, allowing for the fine-tuning of its mechanical, chemical, optical, electrical, and physical properties to suit a variety of applications [1–4]. Because it combines the advantageous qualities of both silicate and borate glass networks, borosilicate glass holds a special place among the many oxide glass families. Silica greatly enhances the mechanical integrity, thermal stability, and chemical durability of borate glass without compromising the superior glass-forming capacity of borate systems. Because of its exceptional thermal shock resistance, comparatively low thermal expansion, high optical transparency, and superior chemical resistance, borosilicate glass can be used in laboratory equipment, optical windows, laser hosts, nuclear waste stabilization, biomedical devices, and electrical insulating materials [3,5]. Furthermore, the coexistence of silicon-oxygen and boron-oxygen polyhedra largely controls the structure of borosilicate glass. The exceptional durability of silicate-based glass is usually attributed to silicon's formation of highly stable  $\text{SiO}_4$  tetrahedra, which are joined by oxygen atoms to form a rigid three-dimensional network. The tertiary  $\text{BO}_3$  and tetrahedra  $\text{BO}_4$  structural units, on the other hand, include boron, and the relative concentration of these units is largely dependent on the composition of the glass. Density, molar volume, thermal stability, modulus of elasticity, optical behavior, and ion transport properties are all significantly impacted by the boron anomaly, which is the conversion of  $\text{BO}_3$  units to  $\text{BO}_4$  units following the addition of changed oxides. The capacity of borosilicate glass to support a variety of modified and intermediate oxides is one of its main advantages. To alter the structure and functional performance of the glass network, heavy metal oxides, alkali oxides, alkaline earth oxides, and rare earth element oxides can be added. Nearly all physical attributes are impacted by the interaction between these oxides and the glass-forming lattice, which changes the concentration of bonding and non-bonding oxygen atoms as well as the lattice structure. As a

result, creating multifunctional glass systems effectively requires accurate structural design [1,3,6,7]. Because of its high atomic number, high ionic polarity, and comparatively low melting point, bismuth oxide ( $\text{Bi}_2\text{O}_3$ ) has attracted a lot of attention.  $\text{Bi}_2\text{O}_3$  may function as a lattice modifier or an intermediate oxide, depending on the composition of the glass. Density, dielectric constant, refractive index, nonlinear optical response, and gamma-ray absorption efficiency all often rise with its introduction. Additionally, glass containing bismuth shows outstanding transparency in the visible and infrared spectrums [8–11]. The transport characteristics of oxide glass are significantly influenced by common alkali modifiers such as sodium oxide ( $\text{Na}_2\text{O}$ ) and lithium oxide ( $\text{Li}_2\text{O}$ ). They increase the mobility of alkali ions across the glass matrix and create non-bridging oxygen atoms by breaking certain Si–O–Si and B–O–B connections. As a result, density, molar volume, glass transition temperature, dielectric characteristics, and ionic conductivity are all greatly impacted by these modifiers. Additionally, compared to monovalent glass systems, the simultaneous presence of sodium and lithium ions can cause the mixed alkali effect, which dramatically modifies the ion transport and dielectric behaviour [3,5,12–14]. Because  $\text{Nd}^{3+}$  ions show strong electron transitions in the near-infrared (NIR) region, which improve optical characteristics, neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) is one of the most often utilized rare-earth element oxides. Through its interaction with oxygen atoms, neodymium modifies the internal structure of the glass lattice, changing the degree of lattice bonding and the distribution of the  $\text{BO}_3$  and  $\text{BO}_4$  building blocks. Numerous characteristics, such as density, molar volume, oxygen packing density, elastic properties, electrical activity, and thermal stability, are indicative of these structural changes. Thus, a useful method for examining the connection between composition, structure, and characteristics in borosilicate glass is to gradually replace sodium oxide with neodymium oxide [15–18]. Understanding how structural alterations affect the structure of the glass requires characterizing the structure. The lattice structure and general cohesiveness of the glass can be inferred from measurements of density, molar volume, oxygen packing density, oxygen molar volume, and bond packing density. While Fourier transform infrared spectroscopy (FTIR) offers detailed information about the various structural units, such as  $\text{BO}_3$ ,  $\text{BO}_4$ ,  $\text{SiO}_4$ , and Bi–O bonds, as well as the relative proportions of bridging and non-bridging oxygen within the glass lattice, X-ray diffraction (XRD) is used to confirm the amorphous nature of the prepared glass [19,20]. Glass's suitability for use in capacitors, insulators, electronic devices, sensors, and solid electrolytes is largely determined by its electrical properties. Charge transfer in alkali-containing glass usually happens when mobile ions move across open locations in the glass

lattice. Temperature, chemical composition, and the amount of space available for ion mobility all have a significant impact on this process. Charge transfer processes and electrical relaxation phenomena in glass systems are frequently studied using methods including AC conductivity, dielectric constant, dielectric loss, modulus of elasticity, and impedance spectroscopy [21–26]. The radiation shielding capabilities of borosilicate glass have received a lot of interest lately because of its prospective uses in industrial radiography, nuclear facilities, medical diagnostics and radiotherapy, and radioactive waste management. Glass materials' ability to protect is largely determined by their effective atomic number, density, and chemical makeup. Because of the high atomic number and density of bismuth, the inclusion of heavy metal oxides, especially  $\text{Bi}_2\text{O}_3$ , greatly enhances gamma radiation absorption, making bismuth-containing glass an eco-friendly substitute for conventional lead-based shielding materials [27–30]. Furthermore, by raising the effective atomic number and electron density while also altering the lattice structure of the glass, rare-earth element oxides like  $\text{Nd}_2\text{O}_3$  may improve radiation absorption qualities. Nevertheless, there hasn't been much research done on how  $\text{Nd}_2\text{O}_3$  substitution affects multi-component borosilicate glass's ability to filter gamma rays [31–34]. Based on these considerations, this study aims to investigate the following glass system:  $47\text{B}_2\text{O}_3\text{--}27\text{SiO}_2\text{--}11\text{Bi}_2\text{O}_3\text{--}11\text{Li}_2\text{O--}(4\text{--}x)\text{Na}_2\text{O--}x\text{Nd}_2\text{O}_3$ , where  $x = 0, 1, 2, 3$ , and  $4$  mol%. The purpose of this work is to investigate how the structural, electrical, and gamma-ray shielding characteristics of this borosilicate glass system are affected when sodium oxide is gradually replaced with neodymium oxide. This was accomplished by focusing on how important radiation shielding parameters, such as mass attenuation coefficient, line attenuation coefficient, effective atomic number, effective electron density, half-value layer, tenth-value layer, mean free path, and radiation shielding efficiency, relate to changes in the internal glass lattice. The ultimate objective is to create a multipurpose borosilicate glass with enhanced gamma-ray shielding capabilities and advantageous structural and electrical characteristics for use in nuclear radiation, industrial, and medical settings.

## 2-Experimental procedures

## 2.1 Glass preparation

A glass formulation with the formula  $47\text{B}_2\text{O}_3 + 27\text{SiO}_2 + 11\text{Bi}_2\text{O}_3 + 11\text{Li}_2\text{O} + (4-X)\text{Na}_2\text{O} + X\text{Nd}_2\text{O}_3$  ( $X=0, 1, 2, 3$ , and  $4$ ) was made using high-purity oxide and carbonate powders of  $\text{B}_2\text{O}_3$ ,  $\text{SiO}_2$ ,  $\text{Na}_2\text{CO}_3$ ,  $\text{Bi}_2\text{O}_3$ ,  $\text{Li}_2\text{O}$ , and  $\text{Nd}_2\text{O}_3$ . This was accomplished by quickly cooling the molten substance at ambient temperature and in the air. A precision electronic balance was used to measure the particle size (See Figure 1(b)). After gathering and grinding the measured raw powders in an agate mortar, they were moved to different ceramic crucibles and heated to  $500\text{ }^\circ\text{C}$  for an hour in an electric furnace to eliminate impurities such moisture and carbonates. After that, the temperature was raised to  $1200\text{ }^\circ\text{C}$  for four hours at a fast-heating rate of  $20\text{ }^\circ\text{C}$  per minute until glass was produced. uniform. Once a clear liquid was obtained, all crucibles were continuously stirred to guarantee glass homogeneity. The liquid was then quickly cooled to room temperature using stainless steel plates.

## 2.2 Glass characterizations

X-ray powder diffraction was implemented by using a  $\text{D}_8$  Advance with DAVINCI design (Bruker, Germany). The sample's density ( $\rho$ ) was measured and calculated using Archimedes' principle and xylene liquid as follows  $\rho = \frac{W_a}{W_a - W_b} \times \rho_L$ , where  $w_a$  is the weight of the sample in air,  $w_b$  is the weight of the sample in liquid, and  $\rho_L$  is the liquid density. Furthermore, the molar volume ( $V_m$ ) of the measured samples can be calculated using the equation  $V_m = \frac{M}{\rho}$ , where  $M$  is the average molecular weight of the glass sample. The vibrational properties and structure of the crushed powder glasses utilizing a spectrometer (Nicolet-TM iS50-Thermo Scientific) through a wavenumber range ( $400\text{--}4000\text{ cm}^{-1}$ ). Additionally, the bond compression and Makishima-McKenzie models were used to theoretically calculate the mechanical parameters of the glass samples. Lastly, XCOM and EpiXS apps were used to theoretically assess the radiation shielding attenuation.

## 3-Results& decision

### 3.1 X-ray diffraction (XRD)

A representative glass picture and X-ray diffraction (XRD) patterns for three formulations are displayed in Figure 1(a):  $47\text{B}_2\text{O}_3 + 27\text{SiO}_2 + 11\text{Bi}_2\text{O}_3 + 11\text{Li}_2\text{O} + (4-X)\text{Na}_2\text{O} + X\text{Nd}_2\text{O}_3$  ( $X=0, 1, 2, 3$ , and  $4\text{ mol\%}$ ) in a glass matrix. These patterns validate the amorphous characteristics of the glass under investigation and show the short-range ordering of borosilicate structures doped with  $\text{Nd}_2\text{O}_3$ . The amorphous character of the glass system is further supported by the fact that none of the three formulations' diffraction curves exhibit any clear Bragg reflections. A broad, diffuse protrusion centered at around  $2\theta = 25^\circ\text{--}35^\circ$

characterizes the patterns, showing the glass matrices' short-range atomic ordering. The position and shape of the amorphous protrusions regularly change as the concentration of  $\text{Nd}_2\text{O}_3$  rises at the cost of  $\text{Na}_2\text{O}$ . In particular, as more  $\text{Na}_2\text{O}$  is substituted with  $\text{Nd}_2\text{O}_3$ , there is a noticeable shift of the primary protrusion towards lower  $2\theta$  angles. The average interatomic distances within the glass crystal lattice have expanded, as indicated by this change. The replacement of smaller  $\text{Na}^+$  ions with larger  $\text{Nd}^{3+}$  ions is primarily responsible for this expansion.[35,36]

It's interesting to note that the protrusions in the **Nd -4** sample got substantially more prominent and thinner. In the short term, this structural improvement suggests a more orderly environment. The lack of crystalline peaks indicates that the rapid molten cooling method was successful in turning all of the investigated  $\text{Nd}_2\text{O}_3$  concentrations into glass. These findings support the stability of the amorphous phase in spite of the high concentration of  $\text{Nd}^{3+}$  ions and are completely consistent with other data on comparable borosilicate systems.

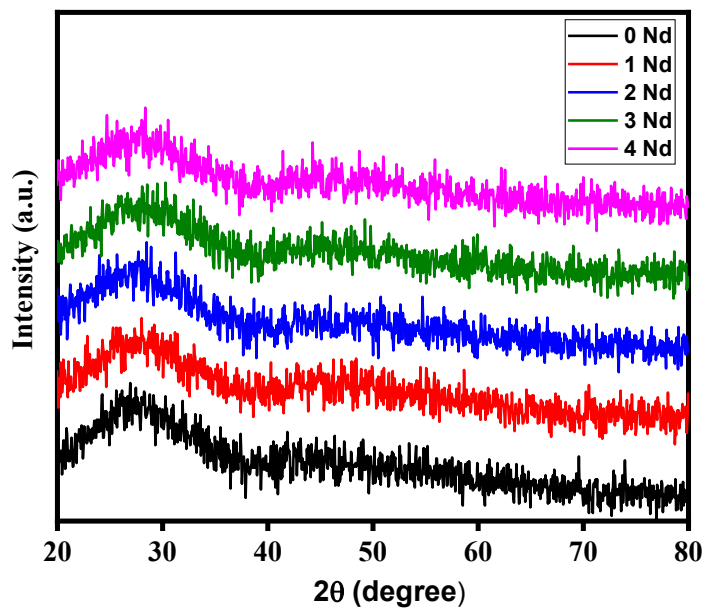


Figure 1(a): X-ray diffraction of the glass structures under study

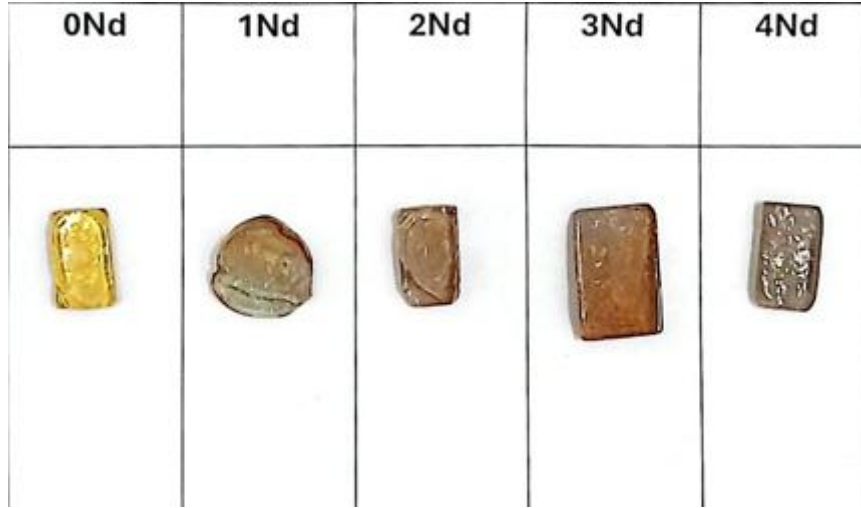


Figure 1(b): The color gradient of the glasses under study

### 3.2. Density, Molar Volume, and Structural Parameter Analysis

The computed structural and physical parameters shown in Table 1 offer important information on how the glass network structure is affected by the slow addition of neodymium oxide ( $\text{Nd}_2\text{O}_3$ ). The following relationship was used to compute the glass's density ( $\rho$ ) in accordance with Archimedes' principle:  $\rho = \frac{W_a}{W_a - W_l} \rho_l$  while the molar volume ( $V_m$ ) was determined from  $V_m = \frac{M_w}{\rho}$ . [35–37] The density ( $\rho$ ) of the investigated glasses increases gradually from 3.594 to 3.878 g/cm<sup>3</sup> with increasing  $\text{Nd}_2\text{O}_3$  content (as seen in Figure 2(a)). Since  $\text{Nd}_2\text{O}_3$  has a greater molecular weight (336.4822 g/mol) than  $\text{Na}_2\text{O}$  (61.979 g/mol), this behavior is mainly explained by the substitution of sodium oxide ( $\text{Na}_2\text{O}$ ) with neodymium oxide ( $\text{Nd}_2\text{O}_3$ ). Additionally,  $\text{Nd}_2\text{O}_3$  has a far higher intrinsic density (about 7.24 g/cm<sup>3</sup>) than  $\text{Na}_2\text{O}$  (about 2.27 g/cm<sup>3</sup>). As a result, the addition of  $\text{Nd}_2\text{O}_3$  raises the glass matrix's total mass per unit volume, gradually increasing the bulk density. Furthermore, as stated in the FTIR section, FTIR examination reveals a structural transfer from [BO3] trigonal units to [BO4] tetrahedral units, which enhances network connectivity and further densifies the glass structure [35–37]. The molar volume ( $V_m$ ) increases slightly but steadily from 29.484 to 30.156 cm<sup>3</sup>/mol in spite of the density rise. This pattern suggests that the increase in mass is greater than the equivalent rise in volume. The expansion in molar volume suggests that the incorporation of  $\text{Nd}^{3+}$  ions modify the spatial arrangement of the glass network, creating additional free volume and inducing slight structural expansion. The average distance between boron atoms (dB–B), which gradually increases from 0.2903 to 0.2965 nanometers, supporting

this view, shows a slight gap between the building blocks of nearby borates[37–41]. Furthermore, the concentration of  $\text{Nd}^{3+}$  ions ( $N_{\text{Nd}^{3+}}$ ), calculated from  $N_{\text{Gd}^{3+}} = \text{mol\% of Nd} \frac{\rho N_A}{M_w}$ , increases progressively with increasing  $\text{Nd}_2\text{O}_3$  content. As a consequence, both the inter-ionic distance ( $R_i = (1/N)^{1/3}$ ) and the polaron radius  $r_p = (\frac{1}{2})(\frac{\pi}{6N})^{1/3}$  decrease systematically due to the closer packing of  $\text{Nd}^{3+}$  ions within the glass network. The reduction in these parameters enhances the electrostatic interactions among neighboring ions and results in a pronounced increase in the local field strength (F), which is given by  $F = \frac{Z}{r_p^2}$  [42], which increases from  $9.659 \times 10^{29}$  to  $2.41 \times 10^{30} \text{ cm}^{-2}$ . This relationship are schematically summarized in Figure 2(b)

In the end, these results show that  $\text{Nd}_2\text{O}_3$  doping drives a strong structural reconfiguration. The conversion of  $[\text{BO}_3]$  units to  $[\text{BO}_4]$  and spatial reconfiguration to meet the significant mass and steric demands of the  $\text{Nd}^{3+}$  ions show that the network experiences simultaneous topological tightening. This dynamic interaction between increased local field strength, increased cross-link density, and heavy-metal substitution offers a comprehensive mechanism controlling the significant changes in the physical and structural properties of the matrix.

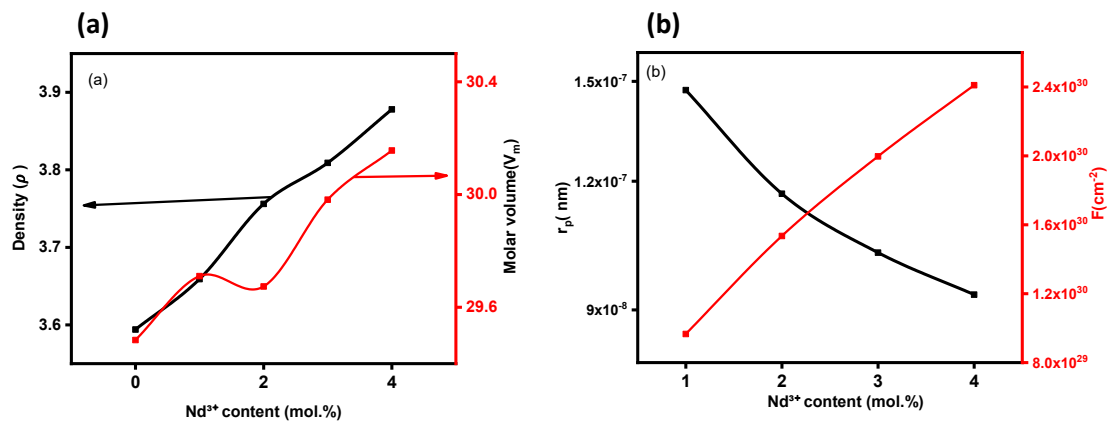


**Figure 2 .**(a) Schematic representation of the correlations between density ( $\rho$ ) and molar volume ( $V_m$ ) and (b) ionic radius ( $r_p$ ) and local field strength (F) with increasing  $\text{Nd}_2\text{O}_3$  content in the glass under study.

Table 1: Density ( $\rho$ ), molar volume ( $V_m$ ), average boron-boron separation ( $d_{B-B}$ ), the inter-ionic distance ( $R_i$ ), concentration of  $\text{Nd}^{3+}$  ions ( $N_{\text{Nd}^{3+}}$ ), Polaron radius of B ( $r_p$ ) and field strength of Bi (F)

| Sample<br>(mol. %) | $\rho$ (Th)<br>(g/cm <sup>3</sup> ) | $\rho$ (Exp)<br>(g/cm <sup>3</sup> ) | $V_m$<br>(cm <sup>3</sup> /mol) | $d_{B-B}$<br>(nm) | $R_i$<br>(nm) | $N_{\text{Nd}^{3+}}$<br>( $\times 10^{20}$ /cm <sup>3</sup> ) | $r_p$<br>( $\times 10^{-7}$<br>nm) | $F$<br>( $\times 10^{30}$ cm <sup>-2</sup> ) |
|--------------------|-------------------------------------|--------------------------------------|---------------------------------|-------------------|---------------|---------------------------------------------------------------|------------------------------------|----------------------------------------------|
| <b>Nd -0</b>       | 3.273                               | 3.594                                | 29.484                          | 0.2904            | -             | 0                                                             | -                                  | -                                            |
| <b>Nd -1</b>       | 3.322                               | 3.659                                | 29.710                          | 0.2920            | 1.7023        | 2.026                                                         | 1.471                              | 96.59                                        |
| <b>Nd -2</b>       | 3.372                               | 3.756                                | 29.763                          | 0.2929            | 1.3506        | 4.058                                                         | 1.166                              | 1.534                                        |
| <b>Nd -3</b>       | 3.422                               | 3.809                                | 29.981                          | 0.2949            | 1.1839        | 6.025                                                         | 1.022                              | 1.997                                        |
| <b>Nd -4</b>       | 3.472                               | 3.878                                | 30.155                          | 0.2965            | 1.0777        | 7.099                                                         | 0.931                              | 2.41                                         |

### 3.3. FTIR Spectral Analysis and Structural Evolution

The structural characteristics of a neodymium-doped borosilicate glass system were investigated using Fourier transform infrared (FTIR) spectroscopy, and the impact of gradually substituting neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) for sodium oxide ( $\text{Na}_2\text{O}$ ) on the glass's local structure was assessed. Because the observed absorption bands derive from the fundamental vibrational modes of the building blocks that comprise the glass lattice, FTIR spectroscopy is one of the most dependable methods for examining short-range order in amorphous materials. As a result, variations in the location, strength, and form of these absorption bands offer important insights into the structural reorganizations brought about by the structural alterations. The nominal composition of the glass system under study is as follows:  $47\text{B}_2\text{O}_3 + 27\text{SiO}_2 + 11\text{Bi}_2\text{O}_3 + 11\text{Li}_2\text{O} + (4-x)\text{Na}_2\text{O} + x\text{Nd}_2\text{O}_3$  where  $x = 0, 1, 2, 3$ , and  $4$  mol%, corresponding to the samples **Nd-0**, **Nd-1**, **Nd-2**, **Nd-3**, and **Nd-4**, respectively. By recognizing the distinctive vibrational modes connected to various structural units, Fourier transform infrared (FTIR) spectroscopy is a potent and popular method for examining the short-range structural order of glass lattices. The produced glass's FTIR spectra were recorded at room temperature in the  $500\text{--}1600\text{ cm}^{-1}$  spectral range, which is where the structural borate clusters' fundamental vibrational bands are usually seen. The amorphous nature of the glassy state and the existence of several structural borate units are reflected in the resultant spectra, which are displayed in Figure 3 and show broad and overlapping absorption bands. After baseline correction and normalization, the experimental spectra were subjected to Gaussian decoding in order to better understand the structural changes brought about by  $\text{Nd}_2\text{O}_3$  inclusion. The broad absorption

bands were able to be divided into distinct component bands that corresponded to certain vibrational modes thanks to this process. Table 2 summarizes the recovered peak positions and their structural designations, while Figure 4 displays the decomposed spectra [2,43].

Vibrations involving Bi-O bonds and bending vibrations related to oxygen atoms connected to the silicate structure are the main causes of the low-frequency absorption region, which spans from roughly 500 to 600  $\text{cm}^{-1}$ . This absorption band's existence attests to bismuth oxide's ( $\text{BiO}_3$ ) structural involvement in the glass matrix. The structural function of bismuth oxide, which is typically regarded as an intermediate oxide, depends on the composition of the glass and the coordination environment surrounding it [44]. The absorption band with the highest intensity is seen between 1100 and 1200  $\text{cm}^{-1}$ . The asymmetric stretching vibrations of the B-O bonds in the tetra-coordinated  $\text{BO}_4$  units are the main cause of this wide band [45,46]. The asymmetric stretching vibrations of the Si-O-Si bonds also contribute to this region because borate and silicate network components coexist. The interconnectedness of the silicate and borate sublattices inside the glass formations under study is reflected in this overlap of vibrational modes. The asymmetric stretching vibrations of the B-O bonds in the  $\text{BO}_3$  ternary units are responsible for another sizable absorption region that spans roughly from 1300 to 1500  $\text{cm}^{-1}$  [47]. A distinctive structural trait of borosilicate glass, simultaneous inspection of the beams associated with  $\text{BO}_3$  and  $\text{BO}_4$  reveals the presence of boron in several coordination contexts. Within the spectral region of 3200–3600  $\text{cm}^{-1}$ , two faint absorption bands were seen at about 1630  $\text{cm}^{-1}$ . These bands represent the stretching vibration of hydroxyl groups and the bending vibration of water molecules, respectively. They have been extensively documented in oxide glass systems and are usually linked to moisture absorbed during sample preparation or storage under conventional laboratory settings [2,43,45,46].

While maintaining the overall amorphous nature of the borosilicate lattice, the stepwise substitution of neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) for sodium oxide ( $\text{Na}_2\text{O}$ ) causes significant changes in the local structural environment of the glass system under study. The addition of  $\text{Nd}_2\text{O}_3$  does not produce new crystalline phases or change the basic structural framework of the glass, as seen in Figure 5, where the overall spectral profile is almost constant for all investigated formulations (from Nd-0 to Nd-4). Instead, the small alterations in the local bonding environment brought about by the addition of  $\text{Nd}^{3+}$  ions are reflected in the observed spectrum variations. Generally regarded as a classic lattice modifier, sodium oxide ( $\text{Na}_2\text{O}$ ) weakens the cohesiveness of the glass lattice by breaking bridging oxygen bonds and changing the

arrangement of positions surrounding the glass-forming units. On the other hand, trivalent rare-earth ions ( $\text{Nd}^{3+}$ ), which have a larger ionic charge and a stronger electrostatic field than sodium ions ( $\text{Na}^+$ ), are introduced by neodymium oxide ( $\text{Nd}_2\text{O}_3$ ). As a result, substituting neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) for sodium oxide ( $\text{Na}_2\text{O}$ ) modifies the short-range arrangement within the amorphous lattice and the distribution of oxygen atoms surrounding the building blocks. The stability of the borate-silicate framework structure throughout the synthesis series is confirmed by the fact that the major absorption band, which is situated in the  $1100\text{--}1200\text{ cm}^{-1}$  region, continues to be the dominating feature in all examined samples. However, a closer look of the spectra shows that this broadband's form changes slightly qualitatively when the concentration of  $\text{Nd}_2\text{O}_3$  increases. These differences could be explained by localized structural changes brought about by the addition of  $\text{Nd}^{3+}$  ions to the glass matrix surrounding the  $\text{BO}_4$  tetrahedra and Si-O-Si links. In a similar vein, all examined structural bands exhibit the large absorption region ascribed to the  $\text{BO}_3$  structural units. Following the addition of rare-earth elements, boron maintains several coordination states, as evidenced by the co-occurrence of the  $\text{BO}_3$  and  $\text{BO}_4$  bands. The Fourier transform infrared (FTIR) spectroscopy results show that  $\text{Nd}_2\text{O}_3$  influences the local structural environment without significantly changing the borate lattice because there were no sudden changes in the spectral signature. In every sample examined, the faint absorption bands seen about  $1630\text{ cm}^{-1}$  and in the  $3200\text{--}3600\text{ cm}^{-1}$  region were still identifiable. Water molecules and hydroxyl groups, which are commonly present in oxide glass exposed to atmospheric conditions, are responsible for these bands. The spectra showed no discernible structural dependence, suggesting that the structural evolution linked to neodymium incorporation is not dominated by moisture-related absorption. Fourier transform infrared (FTIR) spectra generally show that localized structural rearrangements are induced while the distinctive borosilicate glass structure is preserved when sodium oxide ( $\text{Na}_2\text{O}$ ) is gradually replaced with neodymium oxide ( $\text{Nd}_2\text{O}_3$ ). The principal absorption zones' preservation shows that the glass structures under study maintain structural homogeneity over the whole concentration range. These findings show that neodymium ions can be successfully incorporated into the glass structures under study without causing crystallization or major structural disruption. As a result, the produced glass system is a viable option for additional optical and photonic applications using rare-earth element-doped glass materials since it retains its structural integrity within the range of investigated structures.

To quantitatively evaluate the structural evolution of the borate network, the fractions of tetrahedrally coordinated boron ( $N_4$ ) and trigonal boron ( $N_3$ ) were estimated from the relative areas of the deconvoluted FTIR bands according to the following relations:

$$N_4 = \frac{A_{BO_4}}{A_{BO_4} + A_{BO_3}}$$

$$N_3 = \frac{A_{BO_3}}{A_{BO_4} + A_{BO_3}}$$

where  $A_{BO_4}$  and  $A_{BO_3}$  represents the total integrated areas of the bands assigned to tetrahedral  $[BO_4]$  and trigonal  $[BO_3]$  units, respectively. As listed in **Table 3** The  $N_4$  ratio increases significantly from 0.499 for Nd-0 to 0.651 for the Nd-4 sample, respectively, accompanied by a similar decrease in  $N_3$  from 0.501 to 0.439. This behavior indicates that  $Nd_2O_3$  incorporation facilitates the transformation of trigonal  $[BO_3]$  units into tetrahedral  $[BO_4]$  units, thereby increasing the degree of network polymerization and the connectivity of the borate framework [48–51].

Overall, FTIR research reveals that the addition of  $Nd_2O_3$  causes significant modifications in the borate glass structure by redistributing boron coordination states, which leads to a more tightly bound glass lattice and an increase in tetrahedral boron units. The observed variations in the physical, optical, and radiation-shielding characteristics of the examined glass are fundamentally explained by these structural alterations [52,53].

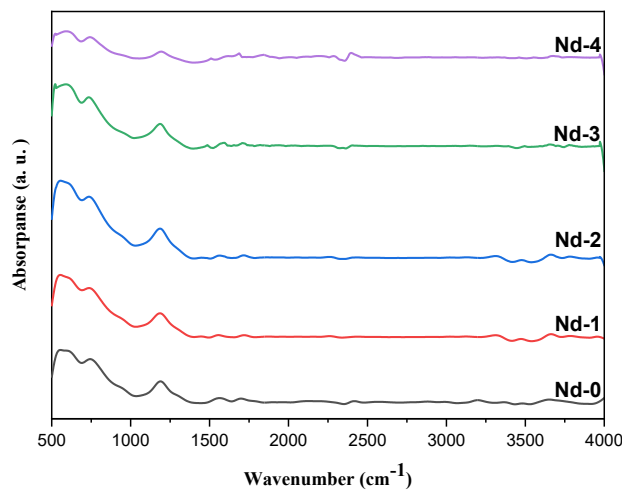


Figure 3. FTIR spectra of the glass under study.

Table 2. FTIR band assignments of glass under study.

| Peak position (cm <sup>-1</sup> ) | Assignment                                                                                                     | Structural origin                                        |
|-----------------------------------|----------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|
| 500–600                           | Bi-O stretching vibration with O-Si-O bending contributions                                                    | Silicate structural units and BiO <sub>3</sub> polyhedra |
| 646–716                           | Bending vibrations of B–O bonds in borate groups                                                               | Borate structural units                                  |
| 850                               | B–O stretching vibrations of tetrahedral borate units [BO <sub>4</sub> ]                                       |                                                          |
| 960–1050                          | B–O stretching vibrations in tetrahedral borate groups containing non-bridging oxygens                         | [BO <sub>4</sub> ] units                                 |
| 1100–1200                         | Tetrahedral BO <sub>4</sub> units with overlapping Si-O-Si asymmetric stretching and asymmetric B-O stretching | [BO <sub>4</sub> ]                                       |
| 1300–1500                         | Asymmetric stretching vibrations of B–O bonds in trigonal borate units                                         | [BO <sub>3</sub> ]                                       |

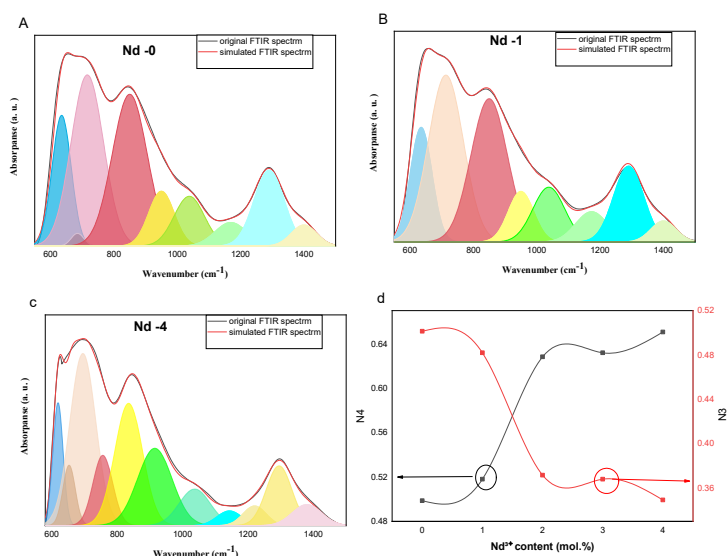


Figure 4. Gaussian decoding of FTIR spectra of glass under study.

**Table 3.** Deconvoluted FTIR peak positions ( $X_C$ ), integrated areas ( $A$ ), and structural fractions ( $N_4, N_3$ ) of the glass under study.

| Peak No. | Nd-0                  |                  | Nd-1                  |                  | Nd-2                  |                  | Nd-3                  |                  | Nd-4                  |                  |
|----------|-----------------------|------------------|-----------------------|------------------|-----------------------|------------------|-----------------------|------------------|-----------------------|------------------|
|          | $X_C \text{ cm}^{-1}$ | $A \text{ a.u.}$ | $X_C \text{ cm}^{-1}$ | $A \text{ a.u.}$ | $X_C \text{ cm}^{-1}$ | $A \text{ a.u.}$ | $X_C \text{ cm}^{-1}$ | $A \text{ a.u.}$ | $X_C \text{ cm}^{-1}$ | $A \text{ a.u.}$ |
| 1        | 635                   | 113.79           | 635                   | 113.79           | 630                   | 63.61            | 617                   | 50.93            | 619                   | 67.135           |
| 2        | 685                   | -15.984          | 716                   | 269.84           | 680                   | 191.45           | 665                   | 147.9            | 653                   | 40.36            |
| 3        | 716                   | 248.735          | 850                   | 243.835          | 750                   | 96.04            | 735                   | 190.15           | 695                   | 240.86           |
| 4        | 850                   | 240.385          | 960                   | 59.68            | 840                   | 244.32           | 835                   | 168.06           | 756                   | 74.53            |
| 5        | 950                   | 62.285           | 1050                  | 80.88            | 940                   | 70.78            | -                     |                  | 835                   | 184.6            |
| 6        | 1038                  | 66.889           | 1169                  | 44.53            | 1030                  | 73.68            | 920                   | 105.35           | 915                   | 143.95           |
| 7        | 1169                  | 31.852           | 1290                  | 105.726          | 1140                  | 33.62            | 1026                  | 86.77            | 1037                  | 61.42            |
| 8        | 1290                  | 100.437          | 1400                  | 23.467           | 1225                  | 29.43            | 1145                  | 32.53            | 1220                  | 25.779           |
| 9        | 1400                  | 22.414           | -                     | -                | 1290                  | 71.75            | 1219                  | 32.03            | 1295                  | 80.45            |
| 10       | -                     | -                | -                     | -                | 1363                  | 32.74            | 1290                  | 63.09            | 1380                  | 35.082           |
| $N_4$    | 0.499                 |                  | 0.518                 |                  | 0.628                 |                  | 0.632                 |                  | 0.651                 |                  |
| $N_3$    | 0.501                 |                  | 0.482                 |                  | 0.372                 |                  | 0.368                 |                  | 0.439                 |                  |

### 3.4. Mechanical properties

#### 3.4.1 The theoretically computed parameters

The bond compression model and the Makishima-McKenzie model are two theoretical models that are crucial for determining the moduli of elasticity in glass from both a scientific and practical standpoint.[54,55] Applying these models to borate-based glass is tricky since the coordination number of boron changes from 3 to 4 when different modifiers are added to the borate network. A model to explain how much pure glass oxides deviate from microscopic symmetry was put up by Bridge [56].

This model takes into account the atomic geometry of the oxides, including bond length and coordination number. Bridge found that the average entanglement density per formula unit rises in tandem with the first-order tensile strength constant. The following relationship was used to determine the average entanglement density, or  $n_c$  [56][57]:

$$n_c = \frac{1}{\eta'} \sum_i x_i (n_c) i (N_c) i \quad (1)$$

Where  $n_c$  represents the number of cross-links per cation unit, which is equal to the number of bonds minus 2,  $N_c$  represents the quantity of cations in each glass formula unit, and  $\eta'$  represents the total amount of cations in each unit of glass formula, as seen in [58]:

$$\eta' = \sum_i x_i (N_c) i \quad (2)$$

The average ring size and the predicted volumetric elasticity modulus are two crucial factors that must be considered in order to complete the structural engineering picture. One can compute the predicted volumetric elasticity modulus using the following expression [59] :

$$K_{BC} = \frac{N N_A \sum_i x_i n_i r_i^2 f b_i}{9 V_m} \quad (3)$$

where  $f$  is the first-order tensile strength constant,  $r$  is the bond length,  $n_i$  is the number of lattice bonds per unit volume, and  $x$  is the mole fraction of the oxide component. The following formula can be used to determine the tensile strength constant [60]:

$$f = 5.28 \left[ \frac{x_a x_b}{r^2} \right]^{3/4} + 30 \quad (4)$$

where  $r$  is measured in nanometres,  $X_a$  and  $X_b$  are the electronegativity of the anion and cation, respectively, and  $N$  is the bond order (1, 2, or 3). If the electronegativity of the cations of the previously described and modified atoms falls within the same limited range, the latter

equation can be used. For a three-dimensional multi-component oxide glass, the average bond expansion constant  $F\%$  is as follows [61]:

$$F_b = \frac{\sum_i x_i n_i f_i}{\sum_i x_i f_i} \quad (5)$$

where  $n$  is the alkali metals' and boron's coordination number. The link between the computed volume factor and the number of network bonds per unit volume,  $n_i$ , as follows [62]:

$$n_i = \frac{n_f N_A \rho}{M} \quad (6)$$

here  $\rho$  is the density,  $n_f$  is the number of network bonds per formula unit,  $N_A$  is Avogadro's number, and  $M$  is the molecular weight (grams of an atom), which is calculated by multiplying the mole fraction of the components by their molecular weights [61]:

The moduli of elasticity of glass can be calculated using a model based on the bond dissociation energy and the constituent ionic radii. Makishima and Mackenzie adopted this model [63,64]:

Based on the chemical makeup of the glass, the packing density of the atoms ( $V_t$ ), and the bond energy per unit volume or dissociation energy ( $G$ ), they developed a quasi-empirical formula that may be used to compute Young's modulus and Poisson's ratio. Glass's Young's modulus ( $E$ ), volume modulus ( $K_m$ ), and Poisson's ratio ( $\mu_m$ ) were computed theoretically using:

$$E = 2V_t \sum_i G_i x_i \quad (7)$$

$$K_m = \lambda V_t E \quad (8)$$

$$\mu_m = \frac{1}{2} - \frac{1}{7.2V_t} \quad (9)$$

$$V_t = \left(\frac{1}{V_m}\right)_t \sum_i V_i x_i \quad (10)$$

where  $V_m$  is the molar volume,  $x_i$  is the mole fraction of component  $i$ , and  $\lambda$  is the slope obtained from the experimental value of the volume factor, which is the product of the packing density and the experimentally determined Young's modulus. The following relation provides the packing factor  $V_i$  for  $AmOn$  oxide, having  $A$  and  $O$  ions with Pauling radii ( $A$ )  $R_A$  and  $RO$ :

$$V_i = \left(\frac{4P}{3}\right) N_A [mR_A^3 + nR_O^3] \left(\frac{m^3}{mol}\right) \quad (11)$$

Where  $R_A$  and  $RO$  represent the ionic Pauling radii of the metals and oxygen, respectively. **Table 4** presents data for several glass parameters under investigation. This study focuses specifically on the properties of a glass system doped with gadolinium oxide ( $Nd_2O_3$ ), which

contains high-field-intensity cations as lattice components. The interfacial sites in the glass lattice exhibit the presence of gadolinium oxide ( $\text{Gd}_2\text{O}_3$ ), which has a lower coordination number than barium oxide ( $\text{Na}_2\text{O}$ ).

However, replacing sodium oxide ( $\text{Na}_2\text{O}$ ) with neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) reduces elasticity and increases hardness and mechanical properties. A more cohesive and interconnected glass lattice is formed when atomic bonds are created between oxygen atoms due to rearrangements and coordination changes, particularly in sodium oxide ( $\text{Na}_2\text{O}$ ) and boron oxide ( $\text{B}_2\text{O}_3$ ) upon the addition of neodymium oxide ( $\text{Nd}_2\text{O}_3$ ). The incorporation of oxygen atoms into the structural lattice is facilitated by this process. As a result, the crystal lattice experiences considerable compression, which lowers the interatomic distances. By increasing the number of bonds per unit volume, this compression raises the system's packing density. Lastly, there is a large increase in bond strength ( $F$ ) and dissociation energy ( $G_i$ ), which directly improves the glass system's mechanical properties. When neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) is substituted for sodium oxide ( $\text{Na}_2\text{O}$ ) the glass lattice undergoes substantial structural changes, mainly due to changes in the coordination number and the redistribution of oxygen atoms [65]. This improves the cohesion of the crystal lattice by converting non-bonding oxygen atoms into bonding atoms. In addition, neodymium-oxygen ( $\text{Nd-O}$ ) interactions are strengthened, and the structural order is improved due to the increased field strength of neodymium ions ( $\text{Nd}^{3+}$ ) compared to sodium ions ( $\text{Na}^+$ ). As a result, there are more bonds per unit volume and less free volume due to lattice compression. Increased packing density, dissociation energy ( $G_i$ ), and bond strength ( $F$ ) are the results of this structural condensation, and they all work together to significantly improve elastic moduli and the glass system's overall mechanical performance [65]. The high field strength of neodymium ions ( $\text{Nd}^{3+}$ ) improves network cohesion at low concentrations and increases packing density at high concentrations despite partial dissociation. The increased density with increasing  $\text{Nd}_2\text{O}_3$  content is attributed to the increased atomic mass of neodymium, improved packing efficiency resulting from the formation of  $\text{BO}_4$  units, and a decrease in free volume within the crystal lattice. According to the Makishima-McKenzie model, the increased dissociation energy ( $G_i$ ) is supported by this increase in packing density and bonding strength. Consequently, as the  $\text{Gd}_2\text{O}_3$  concentration increases, elasticity parameters such as Young's modulus, volume modulus, and shear modulus exhibit a consistent upward trend. At greater  $\text{Nd}_2\text{O}_3$  concentrations, however, minor alterations in the FTIR spectra show the beginning of structural deformation. Partial lattice dissociation due to increased modifier ion input is suggested by the emergence or mild stability of NBO-bound bands. Some B-O-B bonds are

also broken. The mechanical characteristics are still becoming better in spite of this partial dissociation. The prevalence of strong Nd–O bonds and the ongoing increase in packing density, which surpasses the weakening impact of the freshly created NBOs, can account for this seeming paradox. Additionally, the addition of bismuth ( $\text{Bi}^{3+}$ ) and lithium ( $\text{Li}^{+}$ ) ions increases bond polarity and improves local structural stability, resulting in an overall increase in crystal lattice stiffness, according to low-frequency Fourier transform infrared spectroscopy (FIR) (around  $400\text{--}500\text{ cm}^{-1}$ ). To sum up, integrated FIR spectroscopy, density analysis, and mechanical property studies verify that the addition of  $\text{Nd}_2\text{O}_3$  causes: conversion of low concentrations from  $\text{BO}_3$  units to  $\text{BO}_4$  units; at higher concentrations, NBO bonds decrease and then partially increase; higher dissociation energy and greater packing density; and mechanical properties continue to improve despite slight structural dissociation. These findings show that the glass system changes from a relatively open crystal lattice dominated by the modifier to a more cohesive, stiffer, and mechanically robust structure as the  $\text{Nd}_2\text{O}_3$  level increases [66,67]. Stronger lattice bonding and better packing density not only boost the glass's mechanical strength but also raise its overall density, which is a critical component in photon absorption. Thus, better radiation shielding performance is anticipated as a result of the previously mentioned structural and mechanical advancements.

**Table 4:** Average cross-linking density NB; number of lattice bonds per unit volume nfa; Longitudinal elastic modulus (Lbc)elasticity moduli calculated according to the bond compression model: volume modulus (Kbc); Young's modulus (Ebc); Poission's ratio( $\sigma_{bc}$ )Elasticity moduli calculated according to the Makishima-McKenzie model: Young's modulus ( $Y_m$ ); volume modulus ( $K_m$ ); shear modulus ( $S_m$ ); packing density ( $V_{to}$ ) and Dissociation energy ( $D_{to}$ ) for the glass  $47\text{B}_2\text{O}_3\text{--}27\text{SiO}_2\text{--}11\text{Bi}_2\text{O}_3\text{--}11\text{Li}_2\text{O}\text{--}(4\text{--}x)\text{Na}_2\text{O}\text{--}x\text{Nd}_2\text{O}_3$ ,  $x = 0, 1, 2, 3$ , and  $4\text{ mol}\%$ [68].

| Code        | $N_B$<br>$\times 10^{28}$<br>$m^3$ | $n_{fa}$ | $Lbc$   | $Kbc$  | $Ebc$  | $\sigma_{bc}$ | $Y_m$<br>$K_m$ | $S_m$  | $D_{to}$<br>$\times 10^6$ | $V_{to}$ |
|-------------|------------------------------------|----------|---------|--------|--------|---------------|----------------|--------|---------------------------|----------|
|             |                                    |          | GPa     | GPa    |        |               | GPa            | GPa    | KJm <sup>3</sup>          |          |
| <b>Nd-0</b> | 0.858                              | 2.236    | 144.309 | 86.596 | 91.949 | 0.229         | 84.386         | 32.333 | 61.722                    | 0.684    |
| <b>Nd-1</b> | 0.859                              | 2.27     | 144.741 | 86.716 | 92.077 | 0.228         | 86.596         | 33.140 | 62.831                    | 0.689    |
| <b>Nd-2</b> | 0.869                              | 2.353    | 144.997 | 86.834 | 92.968 | 0.226         | 98.616         | 37.425 | 67.482                    | 0.729    |
| <b>Nd-3</b> | 0.874                              | 2.378    | 145.19  | 87.109 | 92.979 | 0.225         | 99.145         | 37.638 | 68.008                    | 0.731    |
| <b>Nd-3</b> | 0.878                              | 2.412    | 146.208 | 87.538 | 93.515 | 0.224         | 101.641        | 38.539 | 69.117                    | 0.735    |

### 3.5. Radiation protection

#### 3.5.1. XCOM and EpiXS programs

The computations in the XCOM program are based on the proximity of the beam and are easier to utilize. While the sample composition is part of the input, the output of XCOM shows the mass attenuation coefficient ( $\mu/\rho$ ). This applies to the EpiXS software as well. On the other hand, the EpiXS program provides a fast way to compute more than ten parameters. This online tool is easy to use and navigate [69].

#### 3.5.2. Methodology

Studies have consistently shown that when radiation travels through or along a material, its effects are lessened. Numerous factors pertaining to absorption and scattering mechanisms impact this reduction. By looking at the calculated attenuation factors, we may decide if a material is appropriate for radiation shielding applications. The Lambert-Beer law can be used to determine the linear attenuation coefficient (LAC), which is the main factor for calculating the residual attenuation factors.

$$I = I_i \exp(-\mu x) \quad (12)$$

Where "I<sub>o</sub>" stands for the measured gamma-ray intensity without the sample, whereas "I" is the measured intensity following the gamma-rays' passage through the sample. The symbol x (in cm) represents the sample thickness. These data can be used to precisely calculate the

samples' experimental mass attenuation coefficient (MAC), represented as ( $\mu/\rho$ ), using the corresponding formulae.

$$\mu_{mass} = \frac{\mu}{\rho} \left( \frac{cm^2}{g} \right) \quad (13)$$

$$\frac{\mu}{\rho} = \left( \frac{1}{\rho x} \right) \ln \left( \frac{I_0}{I} \right) \quad (14)$$

The following formula provides the total molecular cross section,  $\sigma_m$ [70]

$$\rho_m = \left( \frac{\mu}{\rho} \right) \left( \frac{M}{N_A} \right) \quad (15)$$

Here, Avogadro's number ( $N_A$ ) and ( $M$ ) represent the molecular weight. The following formula can be used to determine the total atomic cross section ( $\sigma_a$ ) from ( $\sigma_m$ ).

$$\rho_a = \frac{\rho_m}{\sum(I \times n_i)} \quad (16)$$

The following relation illustrates how the total atomic and electronic cross sections may be obtained using the effective atomic number ( $Z_{eff}$ ):

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad (17)$$

The following relation[71–73] can be used to compute the electron density ( $N_e$ ):

$$N_e = \frac{N_A}{M} (Z_{eff} \sum(I \times n_i)) \quad (18)$$

The thickness of material needed to cut the initial radiation intensity in half is known as the half-value layer (HVL). The following formula can be used to compute it:

$$HVL = \frac{0.693}{\mu} \quad (19)$$

The mean free path (MFP, in cm) is computed using the mass attenuation coefficient  $\mu$ .

$$\lambda = \frac{1}{\mu} \quad (20)$$

The G-P fitting is used to compute (EABF) [74].

$$C = \frac{C_1(\log Z_2 - \log Z_{eq}) + C_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1} \quad (21)$$

$$B(E, X) = 1 + \left( \frac{b-1}{K-1} \right) (K^x - 1), \text{ for } K \neq 1 \quad (22)$$

$$B(E, X) = 1 + (b-1)x, \text{ for } K = 1 \quad (23)$$

where:

$$K(E, x) = cx^a + d \frac{\tanh\left(\frac{x}{x_K} - 2\right) - \tanh(-2)}{1 - \tanh(-2)} \text{ for } x \leq 40 \text{ mfp} \quad (24)$$

### 3.5.3. Radiation shielding investigation

#### I. Linear attenuation coefficient ( $\mu_L$ ) and mass attenuation coefficient $\mu_m$

The mass attenuation coefficient ( $\mu_m$ ) is influenced by both the photon energy and the material composition. **Fig. 5** and **Fig. 6** demonstrate the high agreement between the  $\mu_m$  values derived from EpiXS and the XCOM program for all samples. Based on the data supplied, the relative deviation ( $R_d\%$ ), computed as  $R_d\% = [(x - y)/y] \times 100$ , was negligible. **Fig. 5** and **Fig. 6** display the trends for the linear attenuation coefficient ( $\mu_m$ ) and mass attenuation coefficient ( $\mu_L$ ), respectively.  $\mu_L$  and  $\mu_m$  were found to decrease with increasing photon energy.

Furthermore, it was shown that when the ratio of ( $\text{Nd}_2\text{O}_3$ ) to BaO increased, both the mass attenuation coefficient ( $\mu_m$ ) and the linear attenuation coefficient ( $\mu_L$ ) increased. This might be the result of a sample ( $\text{Nd}_2\text{O}_3$ ) having a larger molecular weight and density than a sample ( $\text{Na}_2\text{O}$ ). Additionally, Nd's atomic numbers are higher than Na's[75]. As a result, sample Nd-4 demonstrated the best degree of protection of all the samples examined. The attenuation capabilities are represented quantitatively by the MAC values. The investigated glass's improved radiation-shielding efficacy is demonstrated by its MAC values, which show that it can significantly reduce radiation transmission.

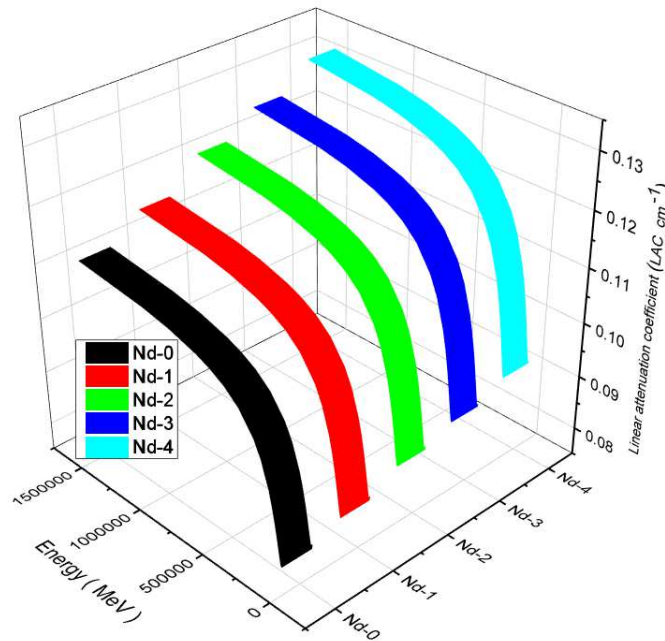


Fig. 5: The LAC variation for the considered glass samples versus the incident gamma photon energies (See text for more details).

Table 5: Mass attenuation coefficients (MAC) calculated by using XCOM and EpiXS techniques for the sample Nd-0 and Nd-1

| Energy  | Nd-0          |                |                   | Nd-1          |                |                  |
|---------|---------------|----------------|-------------------|---------------|----------------|------------------|
|         | MAC from XCOM | MAC from EpiXS | Dev% XCOM & EpiXS | MAC from XCOM | MAC from EpiXS | Dev% XCOM& EpiXS |
| 15000   | 0.02243       | 0.022385       | 0.202407          | 0.022627      | 0.02267        | -0.18791         |
| 16000   | 0.02234       | 0.022294       | 0.204118          | 0.022547      | 0.02259        | -0.19212         |
| 18000   | 0.02222       | 0.022181       | 0.177768          | 0.02245       | 0.02249        | -0.18008         |
| 20000   | 0.02217       | 0.022135       | 0.160126          | 0.022419      | 0.02246        | -0.18388         |
| 22000   | 0.02218       | 0.022143       | 0.166366          | 0.022441      | 0.02248        | -0.17527         |
| 24000   | 0.02223       | 0.022195       | 0.156995          | 0.022505      | 0.02254        | -0.15484         |
| 26000   | 0.0223        | 0.022264       | 0.163229          | 0.022585      | 0.02262        | -0.1565          |
| 28000   | 0.02238       | 0.022346       | 0.153262          | 0.022677      | 0.02271        | -0.14487         |
| 30000   | 0.02248       | 0.022442       | 0.16726           | 0.022783      | 0.02282        | -0.1617          |
| 40000   | 0.02302       | 0.02299        | 0.130321          | 0.023368      | 0.0234         | -0.13504         |
| 50000   | 0.02359       | 0.023556       | 0.143281          | 0.023962      | 0.02399        | -0.11505         |
| 60000   | 0.0241        | 0.024075       | 0.10332           | 0.024503      | 0.02453        | -0.11048         |
| 80000   | 0.02499       | 0.024961       | 0.115246          | 0.02542       | 0.02545        | -0.11749         |
| 100000  | 0.02569       | 0.025668       | 0.084858          | 0.026149      | 0.02617        | -0.08024         |
| 150000  | 0.02695       | 0.026933       | 0.064935          | 0.027448      | 0.02747        | -0.08082         |
| 200000  | 0.02778       | 0.027759       | 0.075594          | 0.028295      | 0.02831        | -0.05475         |
| 300000  | 0.02882       | 0.028797       | 0.080847          | 0.029356      | 0.02937        | -0.04835         |
| 400000  | 0.02945       | 0.029428       | 0.074703          | 0.030001      | 0.03002        | -0.06429         |
| 500000  | 0.02987       | 0.029854       | 0.054905          | 0.030435      | 0.03045        | -0.04959         |
| 600000  | 0.03019       | 0.030168       | 0.074528          | 0.030755      | 0.03077        | -0.0481          |
| 800000  | 0.03061       | 0.030598       | 0.039856          | 0.031194      | 0.03121        | -0.05159         |
| 1000000 | 0.0309        | 0.030881       | 0.061489          | 0.031482      | 0.0315         | -0.05619         |
| 1500000 | 0.03131       | 0.031301       | 0.028745          | 0.03191       | 0.03192        | -0.03102         |

Table 6: Mass attenuation coefficients (MAC) calculated by using XCOM and EpiXS techniques for the sample Nd-2 and Nd-3 and Nd-4

| Energy | Nd-2          |                |                   | Nd-3          |                |                  |
|--------|---------------|----------------|-------------------|---------------|----------------|------------------|
|        | MAC from XCOM | MAC from EpiXS | Dev% XCOM & EpiXS | MAC from XCOM | MAC from EpiXS | Dev% XCOM& EpiXS |
| 15000  | 0.02291       | 0.02287        | 0.173723          | 0.02316       | 0.023113       | 0.202936         |
| 16000  | 0.02284       | 0.022799       | 0.180385          | 0.02309       | 0.023051       | 0.169337         |
| 18000  | 0.02276       | 0.022719       | 0.181898          | 0.02302       | 0.022988       | 0.140313         |
| 20000  | 0.02274       | 0.022703       | 0.163149          | 0.02303       | 0.022987       | 0.186279         |
| 22000  | 0.02278       | 0.022738       | 0.183933          | 0.02308       | 0.023036       | 0.192374         |
| 24000  | 0.02285       | 0.022815       | 0.152735          | 0.02316       | 0.023125       | 0.150691         |
| 26000  | 0.02294       | 0.022906       | 0.149956          | 0.02326       | 0.023227       | 0.143594         |
| 28000  | 0.02305       | 0.023009       | 0.180043          | 0.02338       | 0.02334        | 0.171514         |
| 30000  | 0.02316       | 0.023124       | 0.156736          | 0.0235        | 0.023464       | 0.151915         |
| 40000  | 0.02378       | 0.023747       | 0.139613          | 0.02416       | 0.024125       | 0.143626         |
| 50000  | 0.0244        | 0.024369       | 0.128689          | 0.02481       | 0.024775       | 0.141878         |
| 60000  | 0.02496       | 0.024931       | 0.117788          | 0.02539       | 0.025358       | 0.124852         |
| 80000  | 0.0259        | 0.025879       | 0.080695          | 0.02636       | 0.026338       | 0.08346          |
| 100000 | 0.02665       | 0.02663        | 0.076173          | 0.02713       | 0.027111       | 0.071876         |
| 150000 | 0.02798       | 0.027963       | 0.060758          | 0.0285        | 0.028478       | 0.07614          |
| 200000 | 0.02885       | 0.02883        | 0.068977          | 0.02939       | 0.029366       | 0.083021         |
| 300000 | 0.02993       | 0.029915       | 0.050785          | 0.03049       | 0.030474       | 0.053132         |

|         |         |          |          |         |          |          |
|---------|---------|----------|----------|---------|----------|----------|
| 400000  | 0.03059 | 0.030573 | 0.054266 | 0.03116 | 0.031146 | 0.044608 |
| 500000  | 0.03104 | 0.031016 | 0.076675 | 0.03162 | 0.031598 | 0.071157 |
| 600000  | 0.03136 | 0.031343 | 0.054528 | 0.03195 | 0.031931 | 0.06072  |
| 800000  | 0.03181 | 0.03179  | 0.063188 | 0.0324  | 0.032386 | 0.04321  |
| 1000000 | 0.0321  | 0.032084 | 0.05109  | 0.0327  | 0.032685 | 0.045872 |
| 1500000 | 0.03253 | 0.032519 | 0.032893 | 0.03314 | 0.033128 | 0.035003 |

| Energy  | Nd-4          |                |                   |
|---------|---------------|----------------|-------------------|
|         | MAC from XCOM | MAC from EpiXS | Dev% XCOM & EpiXS |
| 15000   | 0.0234        | 0.023356       | 0.188889          |
| 16000   | 0.02334       | 0.023303       | 0.158098          |
| 18000   | 0.02329       | 0.023257       | 0.14255           |
| 20000   | 0.02331       | 0.023271       | 0.166023          |
| 22000   | 0.02337       | 0.023333       | 0.157895          |
| 24000   | 0.02347       | 0.023435       | 0.148274          |
| 26000   | 0.02358       | 0.023548       | 0.137405          |
| 28000   | 0.02371       | 0.023671       | 0.162801          |
| 30000   | 0.02384       | 0.023805       | 0.146812          |
| 40000   | 0.02454       | 0.024504       | 0.147922          |
| 50000   | 0.02521       | 0.025181       | 0.11543           |
| 60000   | 0.02581       | 0.025786       | 0.092987          |
| 80000   | 0.02682       | 0.026797       | 0.085757          |
| 100000  | 0.02761       | 0.027591       | 0.068091          |
| 150000  | 0.02901       | 0.028994       | 0.056877          |
| 200000  | 0.02992       | 0.029901       | 0.062834          |
| 300000  | 0.03105       | 0.031033       | 0.055072          |
| 400000  | 0.03174       | 0.031719       | 0.067108          |
| 500000  | 0.0322        | 0.032179       | 0.065839          |
| 600000  | 0.03254       | 0.032518       | 0.066687          |
| 800000  | 0.033         | 0.032982       | 0.054242          |
| 1000000 | 0.0333        | 0.033286       | 0.041141          |
| 1500000 | 0.03375       | 0.033738       | 0.037037          |

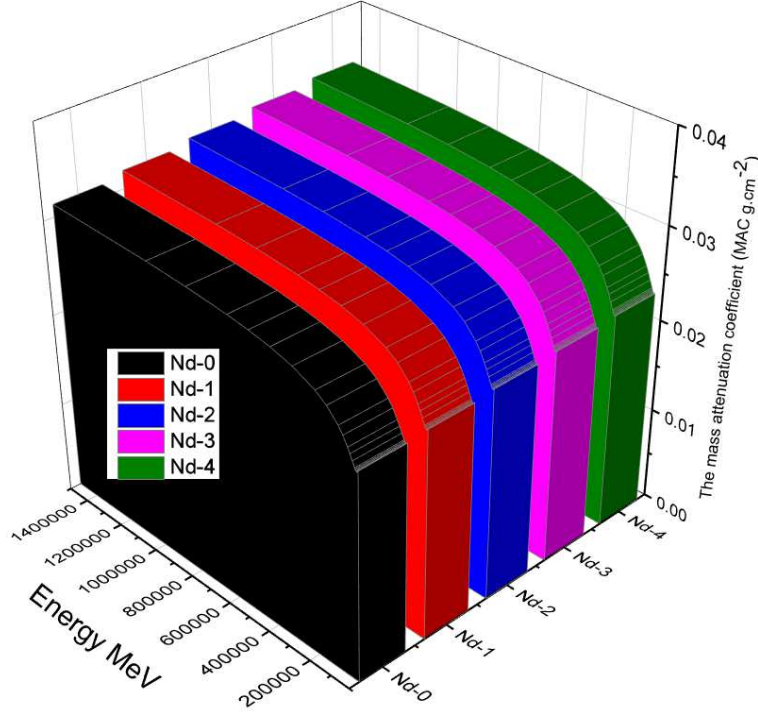


Fig. 6: The MAC variation for the considered glass samples versus the incident gamma photons.

## II. Effective atomic numbers $Z_{\text{eff}}$ and effective electron densities $N_e$

A sample's ability to function as a radiation shield is significantly influenced by its atomic number ( $Z$ ). The atomic number ( $Z$ ) of a material is known to affect its interaction with photons. For example,  $Z^2$  is required for pair formation,  $Z$  is associated with Compton scattering, and  $Z^4$  affects photoelectric absorption. A material's radiation shielding effectiveness can be assessed by calculating the effective atomic number ( $Z_{\text{eff}}$ ) using the effective atomic cross-section ( $\sigma_a$ ).

Sample Nd-4 is expected to be the best option among all the samples examined in the study, as **Fig. 7** illustrates. The reported  $Z_{\text{eff}}$  values can be explained by the considerable variation in photon interactions with the materials.  $Z_{\text{eff}}$  is thus linked to the quantity of elements and the positions of their atomic numbers in the materials under study [76].  $N_e$  is an important material attribute since it displays the total number of electrons present per unit mass of the material being studied. The  $N_e$  parameter for each glass sample shows a consistent relationship with photon energy, as the effective atomic number  $Z_{\text{eff}}$ , as seen in **Fig. 8**. This indicates that sample Nd-4 provides the best shielding efficacy of all the samples being studied. **Table 7** additionally includes  $Z_{\text{eff}}$  and  $N_e$  values.

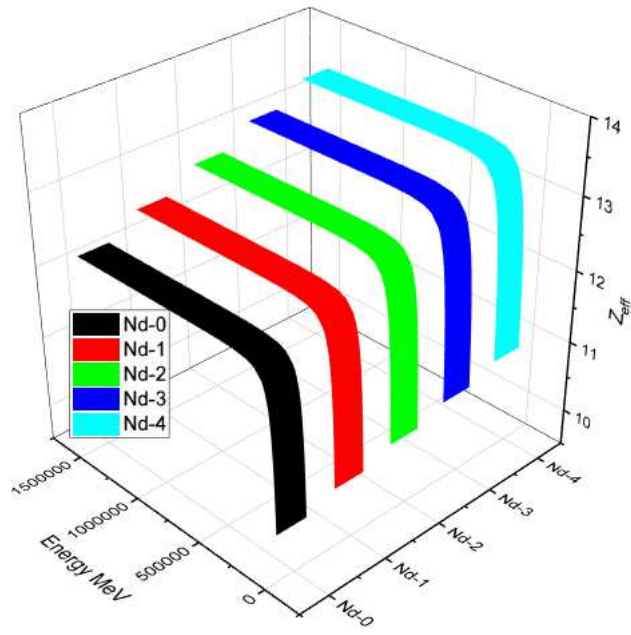


Fig. 7: Variation of effective atomic number  $Z_{eff}$  versus the photon energy for the considered glass samples.

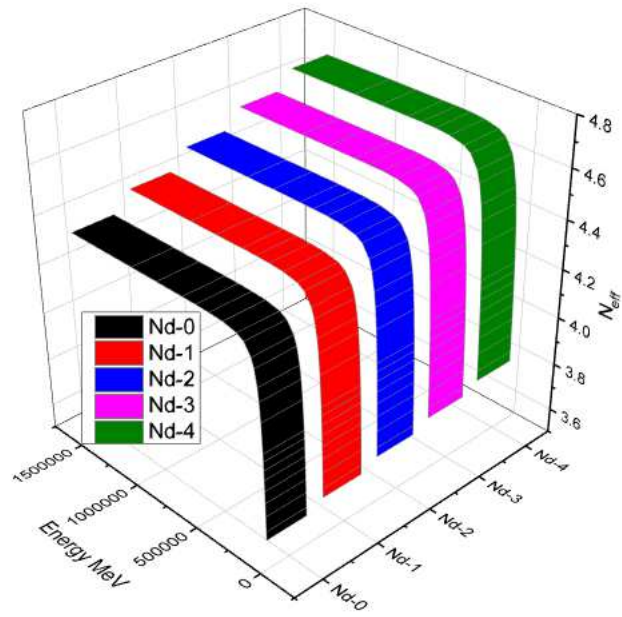


Fig. 8: Variation of effective electron  $N_e$  versus photon energy for the considered glass samples.

Table 7:  $Z_{eff}$  and  $N_e$  values vis-à-vis the energies for the considered glass samples.

| Energy  | $Z_{eff}$ |        |        |        |        | $N_e * E + 23$ |       |       |       |       |
|---------|-----------|--------|--------|--------|--------|----------------|-------|-------|-------|-------|
|         | Nd-0      | Nd-1   | Nd-2   | Nd-3   | Nd-4   | Nd-0           | Nd-1  | Nd-2  | Nd-3  | Nd-4  |
| 15000   | 10.132    | 10.286 | 10.441 | 10.597 | 10.755 | 3.614          | 3.648 | 3.682 | 3.716 | 3.750 |
| 16000   | 10.229    | 10.388 | 10.549 | 10.711 | 10.874 | 3.649          | 3.685 | 3.720 | 3.756 | 3.791 |
| 18000   | 10.404    | 10.574 | 10.744 | 10.916 | 11.090 | 3.711          | 3.750 | 3.789 | 3.828 | 3.866 |
| 20000   | 10.558    | 10.736 | 10.916 | 11.097 | 11.279 | 3.766          | 3.808 | 3.850 | 3.891 | 3.932 |
| 22000   | 10.696    | 10.881 | 11.069 | 11.257 | 11.448 | 3.815          | 3.860 | 3.904 | 3.948 | 3.991 |
| 24000   | 10.818    | 11.010 | 11.205 | 11.400 | 11.598 | 3.859          | 3.905 | 3.952 | 3.998 | 4.043 |
| 26000   | 10.927    | 11.126 | 11.326 | 11.528 | 11.731 | 3.898          | 3.946 | 3.995 | 4.042 | 4.090 |
| 28000   | 11.025    | 11.229 | 11.435 | 11.643 | 11.852 | 3.933          | 3.983 | 4.033 | 4.083 | 4.132 |
| 30000   | 11.112    | 11.322 | 11.532 | 11.745 | 11.959 | 3.964          | 4.016 | 4.067 | 4.118 | 4.169 |
| 40000   | 11.446    | 11.673 | 11.903 | 12.133 | 12.366 | 4.083          | 4.141 | 4.198 | 4.255 | 4.311 |
| 50000   | 11.661    | 11.900 | 12.141 | 12.384 | 12.628 | 4.160          | 4.221 | 4.282 | 4.343 | 4.403 |
| 60000   | 11.808    | 12.055 | 12.305 | 12.555 | 12.808 | 4.212          | 4.276 | 4.340 | 4.403 | 4.465 |
| 80000   | 11.990    | 12.248 | 12.507 | 12.767 | 13.030 | 4.277          | 4.344 | 4.411 | 4.477 | 4.543 |
| 100000  | 12.094    | 12.357 | 12.622 | 12.888 | 13.156 | 4.314          | 4.383 | 4.452 | 4.520 | 4.587 |
| 150000  | 12.214    | 12.484 | 12.755 | 13.028 | 13.302 | 4.357          | 4.428 | 4.499 | 4.569 | 4.638 |
| 200000  | 12.262    | 12.535 | 12.808 | 13.084 | 13.361 | 4.374          | 4.446 | 4.517 | 4.588 | 4.658 |
| 300000  | 12.295    | 12.569 | 12.845 | 13.123 | 13.401 | 4.386          | 4.458 | 4.530 | 4.602 | 4.672 |
| 400000  | 12.305    | 12.580 | 12.856 | 13.134 | 13.414 | 4.389          | 4.462 | 4.534 | 4.606 | 4.677 |
| 500000  | 12.306    | 12.581 | 12.858 | 13.136 | 13.416 | 4.390          | 4.463 | 4.535 | 4.606 | 4.678 |
| 600000  | 12.306    | 12.581 | 12.858 | 13.136 | 13.416 | 4.390          | 4.463 | 4.535 | 4.606 | 4.677 |
| 800000  | 12.303    | 12.578 | 12.854 | 13.132 | 13.412 | 4.389          | 4.461 | 4.534 | 4.605 | 4.676 |
| 1000000 | 12.299    | 12.574 | 12.851 | 13.128 | 13.408 | 4.388          | 4.460 | 4.532 | 4.604 | 4.675 |
| 1500000 | 12.291    | 12.566 | 12.842 | 13.119 | 13.398 | 4.385          | 4.457 | 4.529 | 4.601 | 4.671 |

### III. The half-value layer HVL, the tenth value layer TVL, and the mean free path ( $\lambda$ )

Figs. 9 and 10 provided us with the HVL and MFP ( $\lambda$ ). They exhibit the same behavior as each sample. These parameters' values increase together with energy values. The characteristics decrease as the samples' ( $Nd_2O_3$ ) content rises. This might be because (Nd) generates a higher density while having a bigger atomic number (Z) than (Na). We can deduce that an increase in ( $Nd_2O_3$ ) rather than ( $Na_2O$ ) causes a decrease in HVL and the mean free path ( $\lambda$ ) values. In the end, this offers us efficient defense[77]

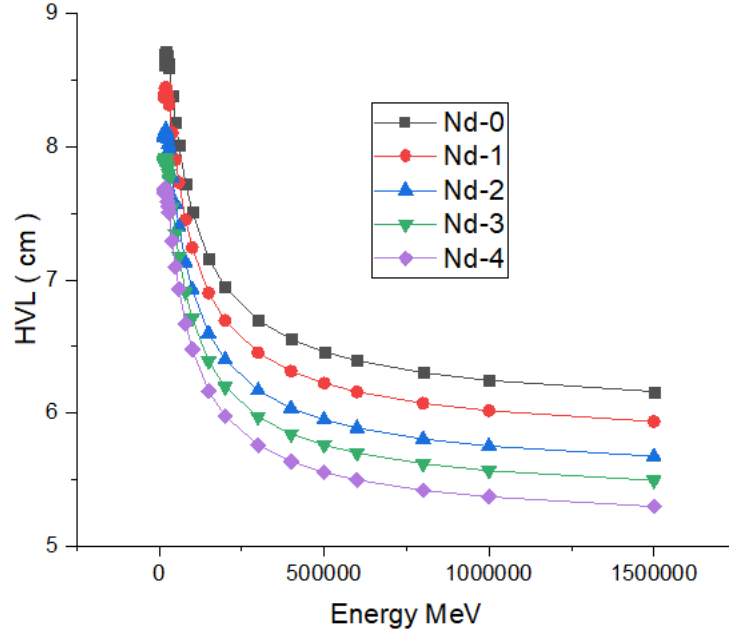


Fig. 9: The HVL for the considered glass samples versus various Gamma photon energies.

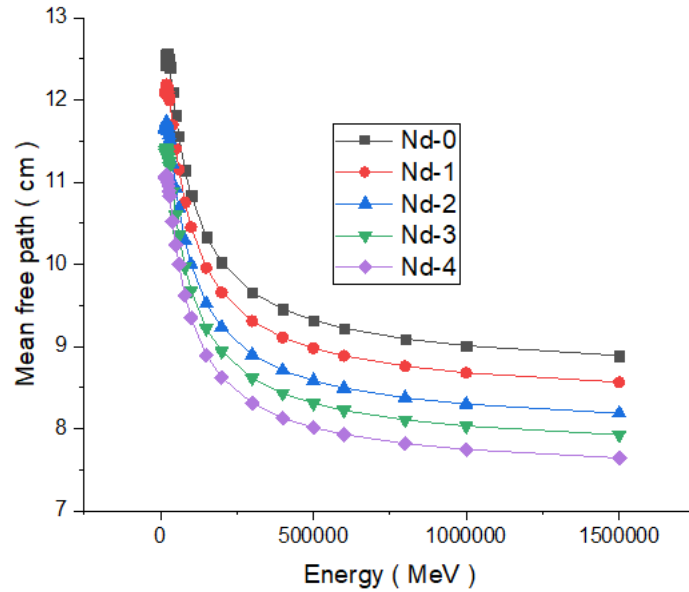


Fig. 10: Variation of the mean free path (MFP) versus photon energy for the considered glass samples.

**Fig. 11** compares the concentration of Neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) and the half-value layer (HVL) at a certain energy level. Neodymium oxide ( $\text{Nd}_2\text{O}_3$ ) concentrations at various energy levels are therefore compared with the half-value layer (HVL).

Interestingly, sample Nd-4 outperformed the others as a shield; this was explained by the fact that Nd has a higher atomic number ( $Z=60$ ) than Na ( $Z=11$ ). As a result, the density is greater.

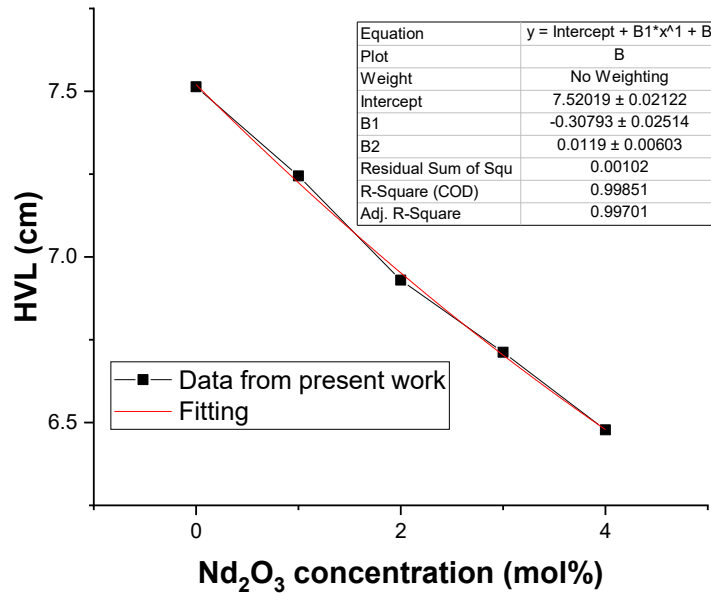


Fig. 11: Fitting of the HVL versus the concentration for the considered glass samples.

### 3.5.4. Predictions

It is necessary to ascertain the necessary half-section thickness and the essential glass thinness, which are affected by the Neodymium level. Consequently, we used a concentration and thickness of Neodymium that were suitable for the half-application. The half-thickness for any given concentration can be calculated using the formula in **Fig. 11**, or vice versa.

### 3.5.5. Exposure build-up factors

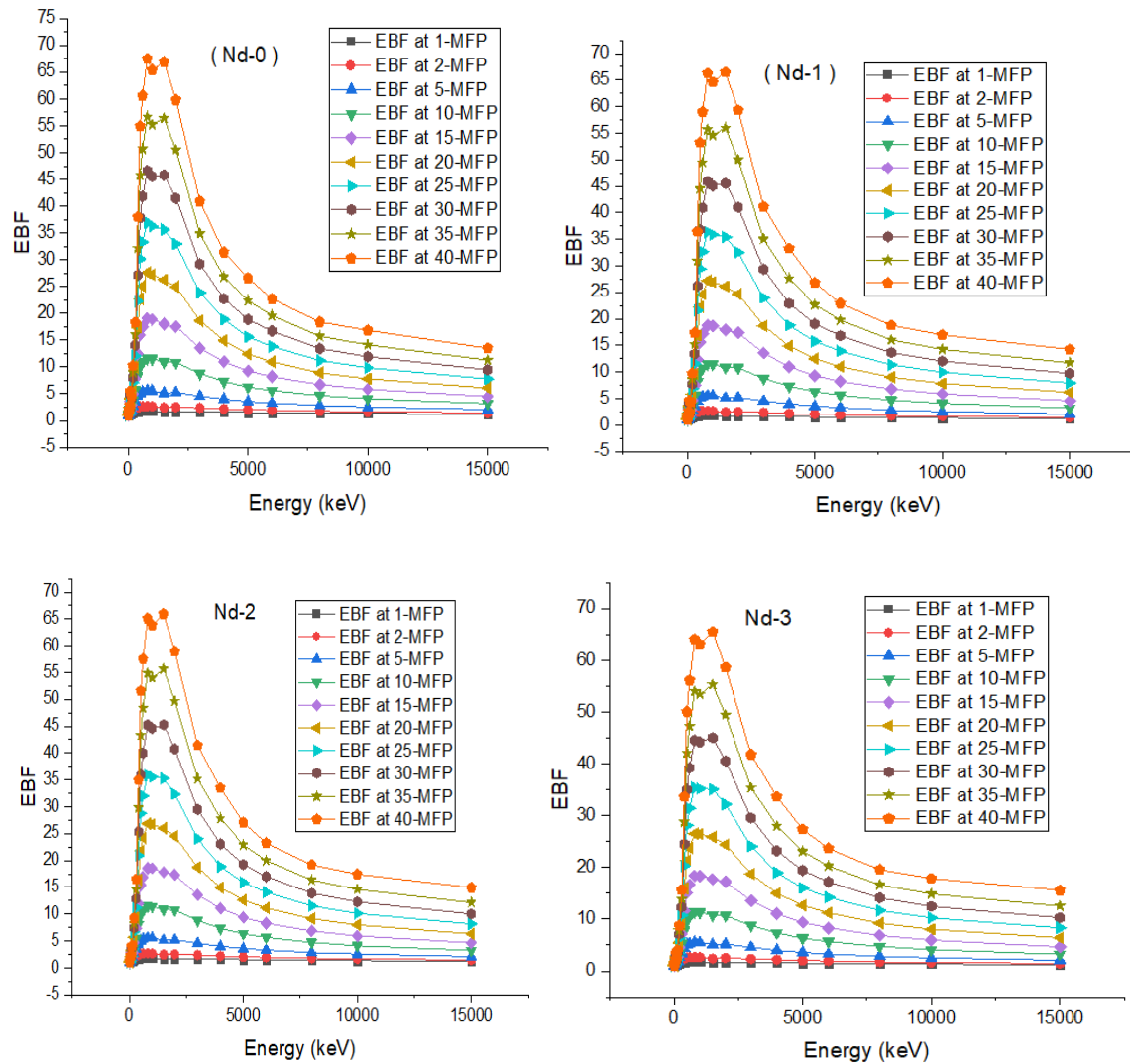
The exposure accumulation characteristics are one of the primary criteria used to evaluate samples as radiation shields. It provides parameters for the accumulation or absorption of gamma rays within the sample layers. Two parameters are used: the number of photons that will gather in space after passing through the sample's thickness is predicted by the exposure buildup factor (EBF). The quantity of photons gathered within the layers of the sample is the factor EABF.

The behaviour of EBF and EABF as seen in **Figs. 12 and 13** is examined in the current study. We may conclude that EBF and EABF exhibit consistent behaviour across all samples. Photon energy and penetration into the material's depth also have an impact on them. Furthermore, photoelectric absorption which occurs when a photon uses all of its energy to remove one electron from the sample is the reason why EBF and EABF values are low at low energies.

However, the EBF and EABF values significantly rise in the Compton scattering energy range. This is due to the fact that the photon not only uses a portion of its energy to extract one electron from the

sample, but it also uses the leftover energy to drive other events within the sample. Lastly, EBF and EABF show low values in the energy range (pair formation). This is due to the fact that 100% of the photon energy is used to create electron-positron particles. As the depth values of the sample increased, so did the EBF and EABF results.

Ultimately, it was shown that the EBF and EABF values somewhat increased when the concentration of ( $\text{Nd}_2\text{O}_3$ ) rose in the samples rather than ( $\text{Na}_2\text{O}$ ). This is due to the fact that Zeq readings rise in direct proportion to the samples'  $\text{Nd}_2\text{O}_3$  content.



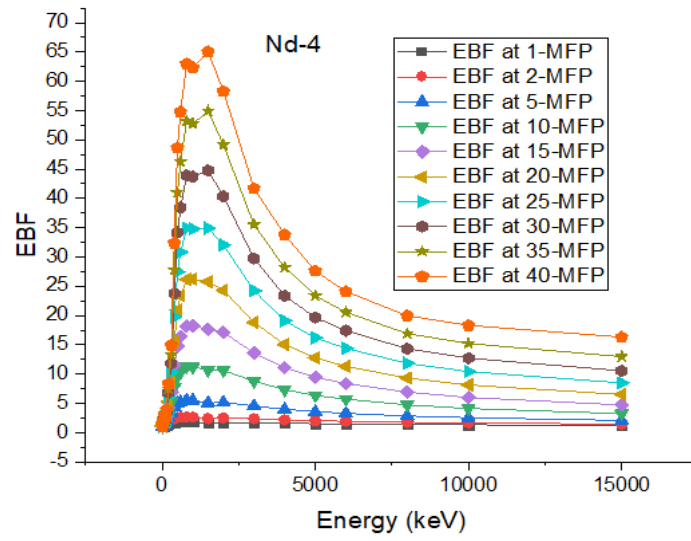
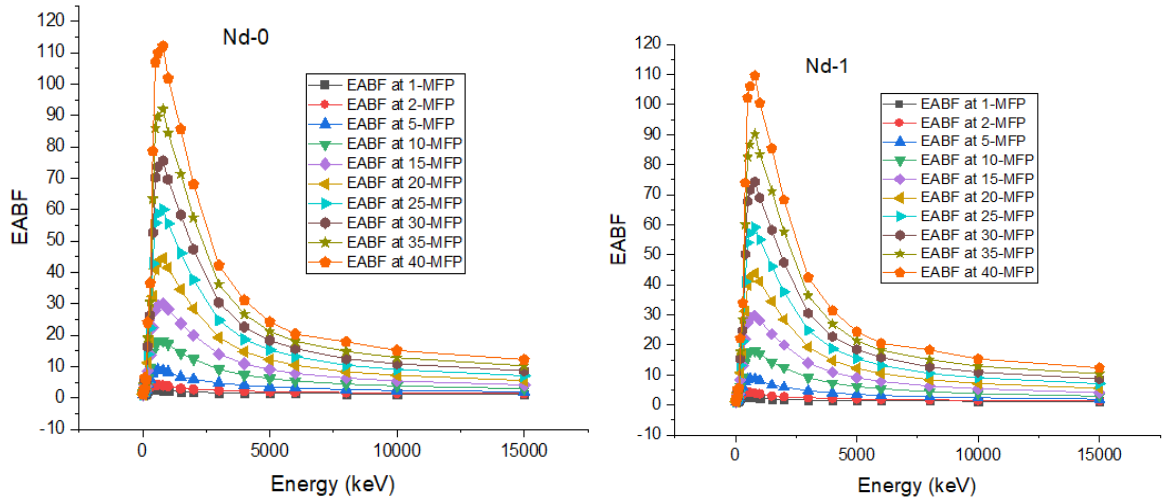


Fig. 12: EBF for (Nd-0), (Nd-1), (Nd-2), (Nd-2), (Nd-3), and (Nd-4) glasses with varying  $\text{Nd}_2\text{O}_3$  doping.



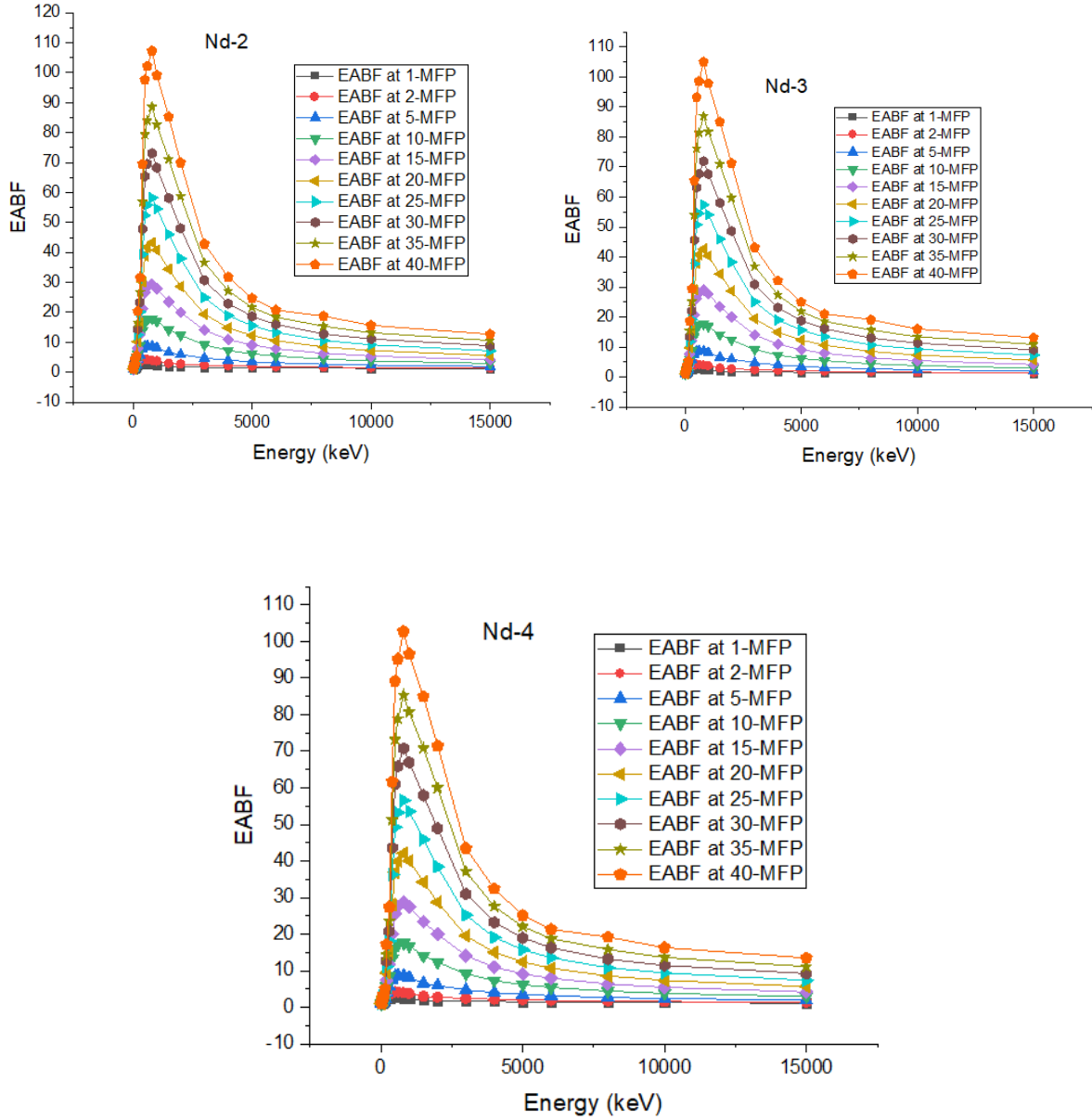


Fig. 13: EABF for (Nd-0), (Nd-1), (Nd-2), (Nd-2), (Nd-3), and (Nd-4) glasses with varying  $\text{Nd}_2\text{O}_3$  doping.

### 3.5.6. Comparison to some other works

As shown in **Table 8**, the comparison was made with studies conducted in the same field. This leads us to the following conclusion:

The study's findings about the protective properties of the glass samples may bridge a knowledge gap. The conclusions are further supported by their consistency with the body of current literature. When compared to other shielding materials, the final results demonstrate that the manufactured glass has a high shielding efficiency [78].

*Table 8: Comparison of MAC (cm<sup>2</sup>/g) and HVL (cm) of present glass with other glasses and concrete[78]*

| Samples and concrete | MAC (cm <sup>2</sup> /g) |           | HVL cm  |          |          |
|----------------------|--------------------------|-----------|---------|----------|----------|
|                      | 662 keV                  | 1173 keV  | 662 KeV | 1173 KeV | 1332 KeV |
| Nd-0                 | 0.0791591                | 0.0579666 | 2.43639 | 3.32713  | 3.5628   |
| Nd-1                 | 0.0792309                | 0.057949  | 2.39094 | 3.26902  | 3.50086  |
| Nd-2                 | 0.0793026                | 0.0579314 | 2.32709 | 3.18556  | 3.41176  |
| Nd-3                 | 0.0793744                | 0.0579138 | 2.29263 | 3.14219  | 3.36559  |
| Nd-4                 | 0.0794461                | 0.0578962 | 2.24981 | 3.08722  | 3.30698  |
| LCP4                 | 0.076                    | 0.057     | 2.009   | 2.686    | 2.885    |
| Ordinary             | 0.0778                   | 0.0592    | 3.87    | 5.-9     | 5.43     |
| Barite               | 0.0780                   | 0.0565    | 2.54    | 3.5      | 3.75     |
| Ferrite              | 0.0777                   | 0.0589    | 1.98    | 2.62     | 2.79     |
| Chromate             | 0.0751                   | 0.0569    | 2.82    | 3.72     | 3.97     |

## 4. Conclusion

A systematic investigation of the  $47\text{B}_2\text{O}_3\text{--}27\text{SiO}_2\text{--}11\text{Bi}_2\text{O}_3\text{--}11\text{Li}_2\text{O}\text{--}(4\text{--}x)\text{Na}_2\text{O}\text{--}x\text{Nd}_2\text{O}_3$ , where  $x = 0, 1, 2, 3$ , and  $4$  mol%.) glass system demonstrated that replacing  $\text{Na}_2\text{O}$  with  $\text{Nd}_2\text{O}_3$  effectively tailors the structure and significantly enhances the multifunctional performance of lithium borate glass. The addition of  $\text{Nd}_2\text{O}_3$  induces simultaneous densification and structural reorganization of the glass network, alongside with increasing in local field strength from  $96.59 \times 10^{30}$  to  $2.41 \times 10^{30} \text{ cm}^{-2}$ , yielding improvement of the theoretically predicted elastic and mechanical properties. Radiation shielding calculations further demonstrated that increasing  $\text{Nd}_2\text{O}_3$  content improved the mass and linear attenuation coefficients while reducing the half-value layer and mean free path over the investigated photon energy range. The excellent agreement between XCOM and EpiXS calculations validates the reliability of the obtained shielding parameters. Among all investigated compositions, Nd-4 exhibited the best overall performance owing to its higher density and the larger atomic number of Neodymium, producing the highest effective atomic number, electron density, and gamma-ray attenuation efficiency. These findings demonstrate that  $\text{Nd}_2\text{O}_3$  substitution is an effective strategy for developing mechanically robust, structurally stable, and highly efficient lithium borate glass for advanced gamma-radiation shielding applications.

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## Data availability

No datasets were generated or analysed during the current study.

## Conflict of 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.

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