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Studies of the Mechanical and Neutron Shielding Efficiency of Dy^{3+}-Doped $MgO–SrO–B_2O_3$ Glass Systems

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ABSTRACT
This study investigates the influence of dysprosium oxide doping on the mechanical and fast neutron removal cross-section of borate glass systems with the composition. The elastic behavior of the glass was assessed using the Makishima–Mackenzie theoretical model. Calculations of dissociation energy and packing density revealed that both properties increased as the Dy_2O_3 concentration rose from 0.2 to 1 mol%. Specifically, dissociation energy increased from 43.329 to 43.465 kJ/cm³, and packing density grew from 0.398 to 0.478 cm³/mol. This consistent upward trend indicates that adding Dy_2O_3 enhances the structural density and bond strength within the glass network, leading to improved rigidity and compactness of the glass structure. Also, all elastic mechanical moduli (such as Young's, Bulk, Shear, and Longitudinal) increase with increasing the quantity of Dy3+ ions in the glass lattice. For the fast neutron shielding, materials with lower density and lighter atomic mass are generally more efficient. As a result, the S1 glass sample, with a lower density of 2.42 g/cm³, exhibited superior fast neutron attenuation compared to the denser S4 sample, which had a density of 2.52 g/cm³. Among all tested samples, S1 recorded the highest effective removal cross-section (ΣR) at 0.115 cm⁻¹, whereas S4 showed the lowest value at 0.104 cm⁻¹. The increase in B_2O_3 content contributed to the improvement in ΣR. Therefore, glass system will be served as promising candidate for radiation protection related applications.

Keywords:
Radiation,
Shielding,
Borate,
Glass,
Dysprosium,
Fast neutron.

INTRODUCTION

Borate glass matrices are the materials mostly used in many different fields, because they have the ability to accommodate many different impurities, so they have a variety of properties depending on the nature of additives/impurities. Glasses have dual properties because they are transparent to visible light and they can attenuate gamma rays, thereby allowing their use as transparent radiation shields (Salama, et al. 2019). Glass materials have attracted many researchers' interests and have been used as a potential inorganic material for diverse applications such as optical fiber, optoelectronic devices, optical switch devices, radiation shielding because of their excellent physical chemistry characters (An et al, 2021). Conventionally, different types of materials such as concrete, ceramic, lead, and alloy are utilized for radiation protection. Although these materials are low in cost and can be molded in desired shape and size, they have several limitations, e.g., concrete is opaque and needs a large area for installing. But the usage of concrete has several drawbacks due to its density and structural strength, which decreases with the water content, thereby directly affecting the calculated shielding parameters (Salama, et al. 2019). Another standard shielding material, compounds based on lead, possess toxic impacts on the health of humankind and the environment. This drawback due to lead compounds needs great concern for hygiene (Mhareb, et al. 2020). Therefore, the current research has moved towards studying and building glass shields with high density and sufficient transparency to replace other typical shield alternatives composed of lead, ceramic, polymers, alloys, and concrete. The glass characteristics should determine its efficient use in a specific application (Sayyed et al. 2021).

According to (Abou Hussein et al, 2021) studying the effect of ionizing radiation on matters becomes with an urgent consideration for researchers because of the harmful and destructive effects of ionizing radiation on humans and environment. Lead and concrete are common effective ways to shield ionizing radiation to their safe limit that does not approximately affect matters. However, an alternative material can be used to achieve the same target, such as glass. In the recent days, glass materials have surprising attention in nuclear and radiation field as radiation shielding material, dosimeter materials, and in the scintillation devices for testing dangerous radiations. Radiation by (Abouhaswa et al 2020) is energy traveling through space, having some wave, and some particle characteristics. It can be categorized into 2- different kinds, ionizing and non-ionizing, which depend on the amount of energy present. Ionizing radiation can cause damage to matter, as it is capable of detaching electrons from atoms, and can be especially harmful to living tissue. This type of radiation mainly comes from the nuclei of atoms. Unstable nuclei often emit excess energy as radiation in the form of gamma photons. Gamma radiations represent energy transmitted in a wave without the movement of a medium. Gamma photons have relatively high energy and accordingly can move through the human body. Radiation has many advantageous applications, ranging from dental and medical fields to uses in agriculture, industry, and power generation Due to their high penetrating strength, gamma photons can damage internal organs and bone marrow. Accordingly, it is essential to minimize the hazard of the photons by using shielding materials. Lead has been commonly utilized in the radiation shielding fields in the past. Lead has great mechanical and physical features which makes it an effective shielding material. However, the toxicity of lead and the harm it can cause to the environment and humans can be lethal. Lead also may produce small particles in the form of aerosols that may be swallowed or breathed in by humans and animals.

Radiation leakage can create serious effects on living organisms. Due to wide applications of the radiation in human daily activities, safety demand is increasing for proper radiation shielding day by day. For this reason, researchers are trying to obtain new shielding materials for high energetic electromagnetic radiation such as X-and gamma rays which have been used in many different areas including radiology, elemental analysis, food irradiation, industry and medicine etc. (Şakar, et al. 2019). The aim of this research is to evaluate the mechanical and fast neutron removal cross-section of strontium magnesium borate glasses doped with dysprosium ion.

MATERIALS AND METHODS

The methodology employed in this research is to achieve its stated objectives. The preparation and analysis of samples follow established standard procedures. The strontium magnesium borate glasses doped with dysprosium ion were synthesized using the melt-quenching technique. The mechanical properties such as (Young's (Y), bulk (B), shear (S), and longitudinal (L)) and Poisson's ratio (σ) were determined using Makishima–Mackenzie model (Mhareb, et al. 2020). Neutron shielding was determined using the Phy-X/PSD computational software (Şakar, et al. 2019).

Materials

The materials to be used in this research work include Phy-X/PSD software version, XCOM software, and a laptop computer (HP-2560) with a 64-bit operating system, 8.00BG RAM, and window 10 installed.

Sample preparation

Four samples of strontium magnesium borate glasses doped with dysprosium ion with chemical form (70 - x)B_2O_3–20SrO–10MgO–xDy_2O_3 (where x =0.2, 0.5, 0.7 and 1.0 mol%) glasses were prepared by using a conventional method of melt quenching by (Ichoja, et al., 2019). In this work, two different mixed alkaline earth borate glasses were produced by utilizing the melt-quenching method. High-purity chemicals from Sigma-Aldrich were used in the present work. These chemicals include boric acid (H3BO3; 99.99%), strontium carbonate (SrCO3; 99.99%), magnesium carbonate ($MgCO_3$; 99.99%) and dysprosium (III) oxide (Dy_2O_3; 99.99%). Each * 20 g of the batch composition was weighed separately on an electronic balance with an accuracy of 1 mg and thoroughly mixed for 2 h in an electric milling machine to obtain homogenous mixture. Finally, optically transparent and air bubble-free glasses were obtained. The glass samples were then crushed into fine powder for XRD and FTIR measurements.

Table 1: Four samples of strontium magnesium borate glasses doped with dysprosium ion with chemical form (70 - x)B_2O_3–20SrO–10MgO–xDy_2O_3 (where x =0.2, 0.5, 0.7 and 1.0 mol%) glasses

S/N	Glass Code	B_2O_3	SrO	MgO	Dy_2O_3	Density (g/cm^3)
1	S1	69.8	20	10	0.2	2.42
2	S2	69.5	20	10	0.5	2.45
3	S3	69.3	20	10	0.7	2.47
4	S4	69.0	20	10	1.0	2.52

Phy-X / PSD Software

The Photon shielding and Dosimetry (Phy-X/PSD) database, accessible at http: //phy-x.net/PSD enables calculation of gamma and neutron attenuation parameter for series of element. These parameters include: Linear Attenuation Coefficient, (LAC), Mass Attenuation Coefficient, (MAC), Effective Atomic Number, (Zeff), Half Value Layer, (HLV) Tenth Value Layer, (TVL), Mean Free Path, (MFP) and Removal Cross-Section. Moreover, the energy range of this work is calculated by the software between 15 KeV and 15 MeV. Meanwhile, it needs to choose the mole fraction, weight fraction, density of the materials, and radiation energy (15 KeV-15 MeV or 1 KeV-100 GeV) for assessing the ability of radiation shielding (An et al., 2021). The software also includes some commonly known radioactive sources (Na - 22, Fe - 55, Co - 60, Cd - 109, I - 131, Ba - 133, Cs - 137, Eu - 152, and Am 241) and their corresponding energies, as well as certain distinctive (K-shell) X-ray energies of Cu, Rb, Mo, Ag, Ba, and Tb elements that the user can choose from (Şakar et al., 2019).

To begin, it is essential to accurately define the composition of the material that will be used in the calculations. The software allows users to input the material composition in two different formats: mole fraction or weight fraction. Once the desired format is selected, users must ensure that the sum of the mole or weight fractions equals 100% or 1, and if necessary, normalize the values before entering them into the program. Furthermore, the density of the material in its phase state (in g/cm³) is required for calculating various shielding parameters, including LAC, HVL, TVL, MFP, Ceff, and FNRCS. Additionally, users must enter the material label in the designated box to proceed with the calculations.

The software has predefined two energy ranges: 15 keV to 15 MeV, which is relevant to the ANSI database and used for calculating the Exposure Air-Borne Fraction (EABF) and Exposure Buildup Factor (EBF), and 1 keV to 100 GeV. Additionally, the software includes a library of well-known radioactive sources, such as 22Na, 55Fe, 60Co, 109Cd, 131I, 133Ba, 137Cs, 152Eu, and 241Am, along with their corresponding energies. The software also provides a selection of characteristic X-ray energies obtained from secondary sources, including the K-shell energies of various elements like Cu, Rb, Mo, Ag, Ba, and Tb. Users can easily select and utilize these predefined energy ranges and radioactive sources to facilitate their calculations and analyses.

The Makishima-Mackenzie (M-M) model was adopted for calculating the mechanical properties of the fabricated glasses. The mechanical parameters such as elastic moduli (Young's (Y), bulk (B), shear (S), and longitudinal (L)) and Poisson's ratio (ϭ) of the glasses are computed from the following relation (Dong et al., 2023).

The total packing density, $V_t = \frac{1}{V_m}\sum_i (V_i x_i)$ (1)

Total dissociation energy,

G_i (kJ/cm³) $G_t = \sum_i (G_i x_i)$ (2)

Where V_m stands for molar volume, V_i and G_i are respective packing density factor and dissociation energy of oxide and x_i is the mole fraction of glass oxide.

$$Y = 2V_t G_t \quad (3)$$

$$B = 2.4V_t^2 G_t \quad (4)$$

$$S = \frac{3YB}{9B-Y} \quad (5)$$

$$L = B + \frac{4}{3}S \quad (6)$$

$$ϭ = 0.5 - \left(\frac{1}{7.2V_t}\right) \quad (7)$$

RESULTS AND DISCUSSION

The mechanical properties and neutron attenuation properties of strontium magnesium borate glasses doped with dysprosium ion glass systems were theoretically evaluated over an energy range of 0.015 to 15 MeV. The mechanical properties such as (Young's (Y), bulk (B), shear (S), and longitudinal (L)) and Poisson's ratio (ϭ) were determined using Makishima–Mackenzie model. Key radiation shielding parameters to be calculated include: Mass Attenuation Coefficient (MAC) and Linear Attenuation Coefficient (LAC). The neutron shielding for various glass compositions were compared to identify the most effective formulation for shielding, particularly against gamma radiation.

Physical properties of strontium magnesium borate glasses

The ability of a material to shield against gamma radiation is primarily influenced by how dense it is, the denser the material, the better it can attenuate or block the high-energy rays. Figure 1 and Table 2 show a clear pattern: as the concentration of Dy_2O_3 (dysprosium oxide) in the glass increases from 0.2 mol% to 1.0 mol%, the material becomes significantly denser, going from 2.42 g/cm³ to 2.52 g/cm³. This increase happens because dysprosium atoms are much heavier than boron atoms. When dysprosium replaces boron in the glass structure, the mass per unit volume increases, making the glass better at absorbing gamma radiation.

Table 2: Four samples of strontium magnesium borate glasses doped with dysprosium ion with chemical form (70 - x)B_2O_3–20SrO–10MgO–xDy_2O_3 (where x =0.2, 0.5, 0.7 and 1.0 mol%) glasses

S/N	Glass Code	B_2O_3	SrO	MgO	Dy_2O_3	Density (g/cm^3)	Molar volume (cm^3 mol^{-1})
1	S1	69.8	20	10	0.2	2.42	45.21
2	S2	69.5	20	10	0.5	2.45	44.98
3	S3	69.3	20	10	0.7	2.47	44.96
4	S4	69.0	20	10	1.0	2.52	44.63

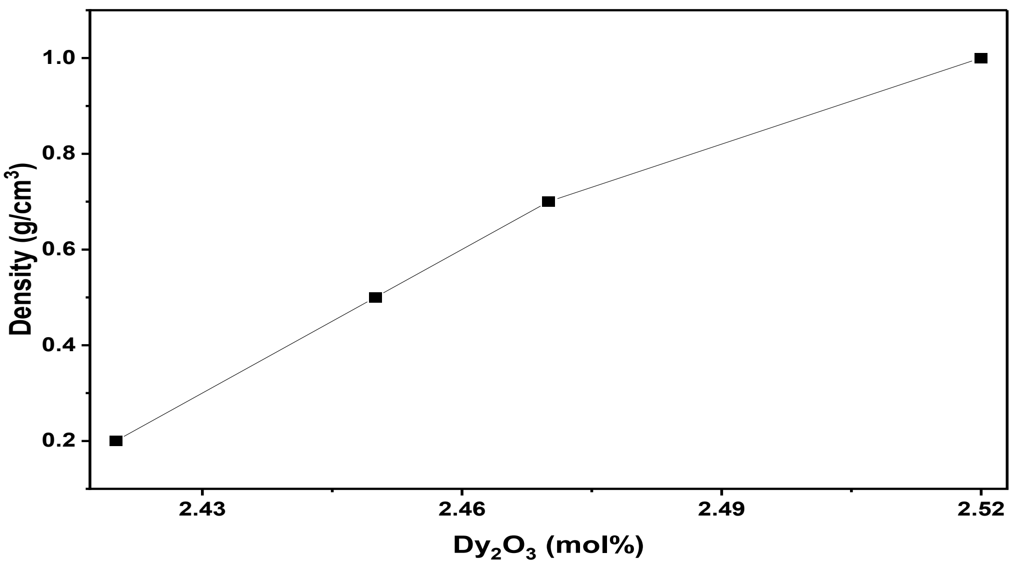

Figure 1: Variation of density with Dy_2O_3 content in the glasses

Mechanical features

For a material to be considered for radiation shielding applications it must possess high strength, stiffness, rigidity and toughness to withstand mechanical stress (Dong et al., 2023). A higher elastic modulus in glass signifies a greater ability to resist bending or deformation, which is crucial in environments exposed to radiation. These mechanical qualities enable the material to remain stable and effective as a radiation shield, thus positioning it as a valuable material for use in nuclear technologies.

The density values of the S1–S4 glass samples are shown in Table 2. As B_2O_3 was progressively replaced by Dy_2O_3, the density (ρ) of the glasses increased steadily from 2.42 to 2.52 g/cm³. This rise in density is due to the substitution of boron (a lighter element) with the much heavier dyprosium atoms. Additionally, the molar volume (V_m) of the glasses gradually decreased from 38.429 to 37.197 cm³/mol as the Dy_2O_3 content rose from 0.2 to 1.0 mol%.

Table 3: Mechanical parameters of glass system are (70 - x)B_2O_3–20SrO–10MgO–xDy_2O_3 (where x =0.2, 0.5, 0.7 and 1.0 mol%)

Sample code	G_i (kJ/cm^3)	V_t (cm^3/mol)	Y (GPa)	B (GPa)	S (GPa)	L (GPa)	б
S-1	43.329	0.398	34.49	16.47	14.98	36.40	0.15
S-2	43.331	0.455	39.43	21.53	16.50	43.48	0.19
S-3	43.332	0.467	40.47	22.68	16.83	45.53	0.20
S-4	43.465	0.478	41.55	23.83	17.18	46.68	0.21

The elastic properties of the glass were evaluated using Makishima–Mackenzie theory. The packing density (PD) was first calculated as the ratio of the sum of the products of each constituent's packing factor (V_i) and mole fraction (x_i) to the total molar volume (V_m). Furthermore, the total dissociation energy per unit volume (G_t) of the glasses was computed by summing the contributions of the dissociation energies of each individual oxide component, proportionate to their content in the glass.

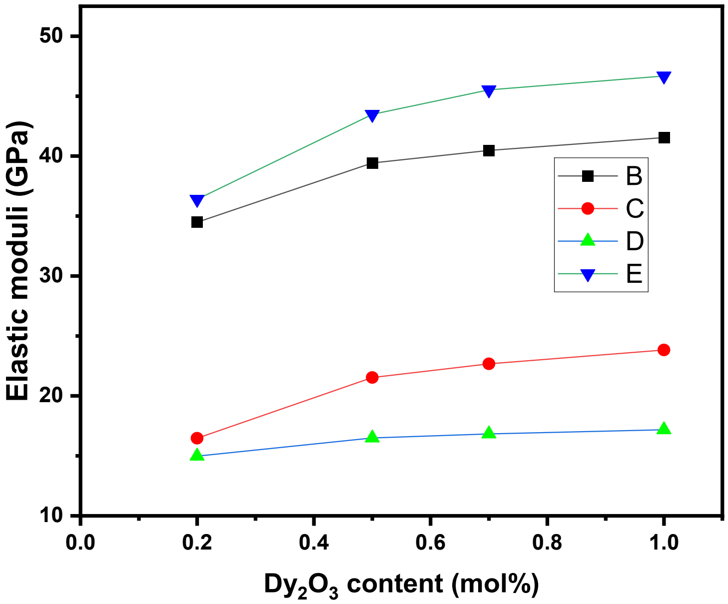

Figure 2: Variation of elastic moduli of glasses with Dy_2O_3 content using Makishima-Mackenzie model

The dissociation energy and packing density values were computed and are illustrated in Table 3. As the concentration of Dy_2O_3 increased from 0.2 to 1 mol%, both parameters exhibited a noticeable rise. Specifically, the dissociation energy grew from 43.329 to 43.465 kJ/cm³, and the packing density increased from 0.398 to 0.478 cm³/mol. This trend suggests that the incorporation of Dy_2O_3 enhances both the structural compactness and the bond strength within the glass network.

The total molar volume (V_t) and total dissociation energy (G_t) values were used in equation (3) to calculate Young's modulus (Y) for S1–S4 glass samples. Equation (4) gave the bulk modulus (B), while equations (5) and (6) yielded the shear modulus (S) and longitudinal modulus (L), respectively. The results are in Table 3 and Figure 2, where B represents Young's modulus (Y), C represents bulk modulus (B), D represents shear modulus (S), and E represents longitudinal modulus (L). Notably, Young's modulus (Y) increased with more dysprosium oxide (Dy_2O_3), from 34.49 GPa in S1 to 41.55 GPa in S4, likely due to higher dissociation energy and packing density.

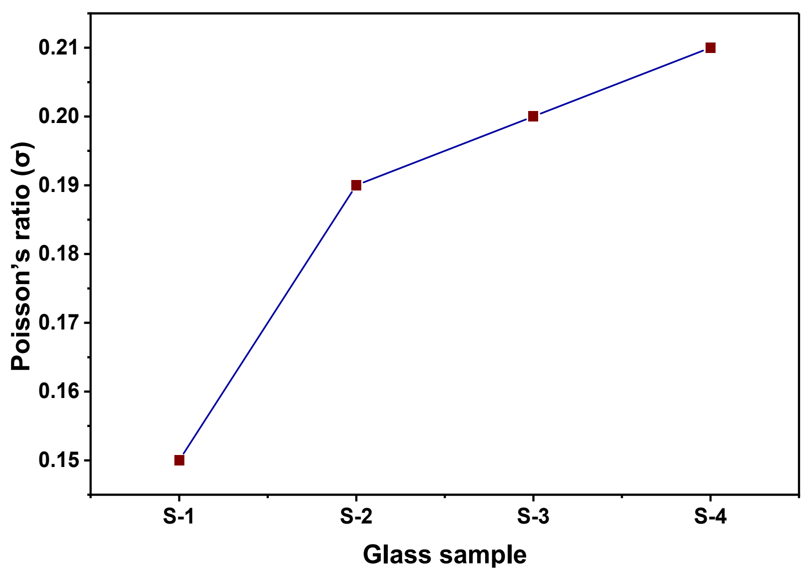

Figure 3: Variation of Poisson's ratio of the glasses with Dy_2O_3 content using Makishima-Mackenzie model

Similarly, the bulk modulus (B) improved from 16.47 GPa for S1 to 23.83 GPa for S4. The shear modulus (S) rose from 14.98 GPa to 46.68 GPa, and the longitudinal modulus (L) increased from 36.40 GPa to 96.204 GPa across the same sample range. Additionally, Poisson's ratio (σ) was determined using equation (7), with its values also listed in Table 3 and plotted in Figure 3. The Poisson's ratio increased slightly from 0.15 to 0.15 between S1 and S4, indicating a subtle enhancement in the material's ductility.

The overall improvement in the elastic moduli observed in these glasses may be attributed to a reduction in non-bridging oxygen (NBO) and structural vacancies as the Dy_2O_3 concentration increases, leading to a more tightly bonded and mechanically stable glass network (Rammah et al., 2020).

Previous studies have reported that earth (RE^{3+}) ions doped glasses improved the mechanical of the glasses. (Alharshan et al., 2024) examined the impact of doping Eu^{+3} to borate glasses. Based on results, all elastic and mechanical moduli—namely Young's, bulk, shear, and elongation moduli—were found to increase with higher concentrations of Eu^{3+} ions in the glass matrix. Specifically, the Young's modulus (Y) values for the glass samples were 34.512, 36.089, 36.504, 36.730, and 37.114 GPa for Eu molar ratios of 0, 0.25, 0.5, 0.75, and 1, respectively, corresponding to the sample codes Eu-0.0, Eu-0.25, Eu-0.5, Eu-0.75, and Eu-1.0. Increasing the Eu_2O_3 content also led to a rise in micro-hardness, from 2.050 to 2.146 GPa. Similarly, Poisson's ratio exhibited a gradual increase, recorded as 0.273, 0.275, 0.277, 0.277, and 0.278 for the same series of samples.

Fast neutron removal cross-section (FNRCS) (Σ_R)

The fast neutron removal cross-section (FNRC, denoted as ΣR in cm^{-1}) is a fundamental parameter used to assess how effectively a material can shield against fast neutrons, which are high-energy neutrons typically with energies above 0.5 MeV. This parameter represents the probability per unit path length that a fast neutron will be removed from a neutron beam either by being scattered to lower energies, absorbed through nuclear reactions, or through a combination of both mechanisms. A higher ΣR value indicates greater neutron attenuation capability, meaning the material is more effective at reducing neutron penetration. FNRC is particularly important in applications involving nuclear reactors, radiation shielding, and nuclear waste storage, where managing neutron radiation is critical for safety and performance.

Table 4: The fast neutron removal cross-sections (Σ_R) of the borate glasses

Glass Code	Density (g/cm^3)	(FNRCS) (Σ_R)
S-1	2.42	0.115
S-2	2.45	0.111
S-3	2.47	0.108
S-4	2.52	0.104

The theoretical values of the fast neutron removal cross-section (ΣR), expressed in cm^{-1}, were determined for the S1–S4 glass samples, as illustrated in Fig. 4 and summarized in Table 4. The results revealed a gradual decrease in ΣR as B_2O_3 was progressively replaced by Dy_2O_3 in the glass composition. This substitution, involving the replacement of a low atomic number (low-Z) component (B_2O_3) with a higher atomic number (high-Z) component (Dy_2O_3), led to an increase in both the density and molar mass of the glass samples. Generally, denser glass materials exhibit superior gamma-ray shielding properties. However, for fast neutron shielding, materials with lower density and lighter atomic mass tend to be more effective. Consequently, the glass sample labeled S1, with a lower density of 2.42 g/cm^3, demonstrated better fast neutron attenuation compared to the denser S4 sample, which has a density of 2.52 g/cm^3. Among the samples, S1 showed the highest ΣR value of 0.115 cm^{-1}, while S4 recorded the lowest at 0.104 cm^{-1}.

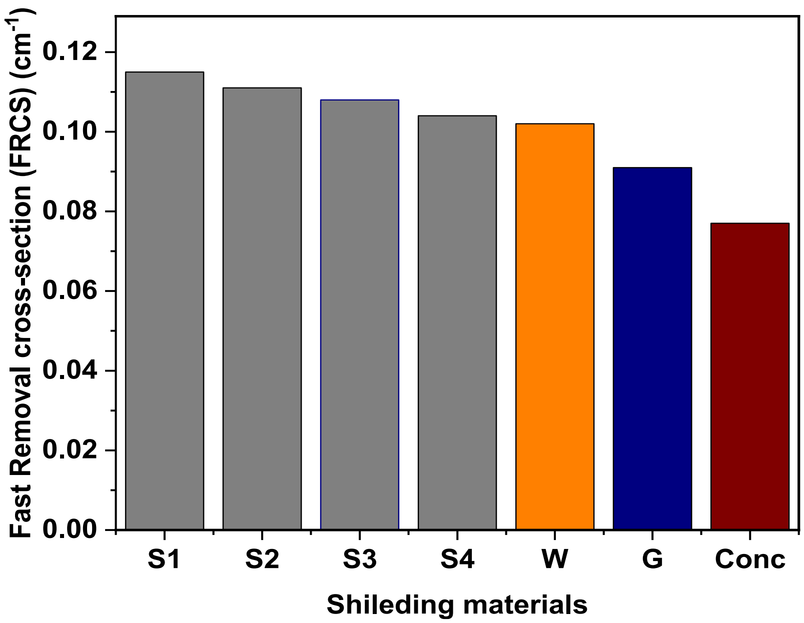

Figure 4: Comparison of FNRCS (Σ_R) of borate glass sample with previously studied shielding materials

Figure 4 also includes a comparative analysis of ΣR values for the fabricated S1–S4 glasses against common reference materials such as water (W), granite (G), and ordinary concrete (Conc.). The ΣR values of the prepared glasses were found to be superior to those of the reference materials, with water, granite, and concrete exhibiting ΣR values of 0.102, 0.091, and 0.077 cm^{-1}, respectively (Sayyed,2021).

The improved neutron shielding efficiency of S1 is due to the contribution of B_2O_3, which decreases the material's density and atomic number, thereby enhancing the likelihood of neutron capture and scattering within the glass matrix.

CONCLUSION

Theoretical assessments were conducted on the mechanical and neutron shielding properties of strontium magnesium borate glasses doped with dysprosium ions, across an energy spectrum ranging from 0.015 to 15 MeV. The elastic properties of the glass were evaluated using Makishima–Mackenzie theory. The dissociation energy and packing density values were computed. As the concentration of Dy_2O_3 increased from 0.2 to 1 mol%, both parameters exhibited a noticeable rise. Specifically, the dissociation energy grew from 43.329 to 43.465 kJ/cm³, and the packing density increased from 0.398 to 0.478 cm³/mol. This trend suggests that the incorporation of Dy_2O_3 enhances both the structural compactness and the bond strength within the glass network.

An enhanced density from 2.42 to 2.52 g cm^{-3} and reduced molar volume from 45.21 to 44.63 (cm3 mol−1) are the outcome of increasing the concentration of Dy^{3+} in glasses. Also, all elastic-mechanical moduli (such as Young's, Bulk, Shear, and Longitudinal) increase with increasing the quantity of Dy^{3+} ions in the glass lattice.

For fast neutron shielding, materials with lower density and lighter atomic mass tend to be more effective. Consequently, the glass sample labeled S1, with a lower density of 2.42 g/cm³, demonstrated better fast neutron attenuation compared to the denser S4 sample, which has a density of 2.52 g/cm³. Among the samples, S1 showed the highest ΣR value of 0.115 cm^{-1}, while S4 recorded the lowest at 0.104 cm^{-1}. The effective removal cross-section (ΣR) indicated enhanced neutron attenuation with increasing B_2O_3 content, further emphasizing the multifunctional potential of these materials. The findings provide valuable insights for the development of high-performance glass materials for advanced applications in radiation protection.

Future research can further develop these findings by exploring the potential for large-scale production and assessing how the material performs under various application-specific conditions. This could include evaluating long-term stability, environmental durability, cost-effectiveness, and integration into real-world systems such as nuclear shielding, medical radiation protection, or space technology. Additionally, optimizing the composition for targeted performance improvements could lead to the development of customized glass systems tailored to specific industrial or scientific needs.

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