Critique Open Research & Review (CORR)

eISSN: 3023-3267
Volume. 04, Issue. 03, pp. 07-12, May 2026"

Computational Evaluation of Zirconia-Doped B_2O_3–Bi_2O_3–MgO–PbO Glass Systems for Advanced Radiation Shielding Performance Using XCOM and Phy-X/PSD Simulation Tools

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Article received: 19/03/2026, Article Accepted: 28/04/2026, Article Published: 02/05/2026

ABSTRACT

The increasing demand for efficient, lightweight, and lead-reduced radiation shielding materials has driven significant interest in heavy metal oxide (HMO) glass systems. In this study, the radiation attenuation behavior of zirconia (ZrO_2)-doped B_2O_3–Bi_2O_3–MgO–PbO glass systems is investigated using advanced computational techniques, namely XCOM and Phy-X/PSD simulation tools. The primary objective is to evaluate how the incorporation of ZrO_2 modifies the gamma-ray shielding performance, density-dependent attenuation mechanisms, and effective atomic number of the glass matrix.

The study builds upon established findings that Bi_2O_3- and PbO-based glass systems exhibit strong photon interaction probabilities due to their high atomic numbers, making them suitable for nuclear shielding applications (Alsaif et al., 2021). However, issues such as structural instability and toxicity necessitate compositional optimization. Zirconia doping is introduced as a structural modifier to enhance durability and improve photon attenuation synergy.

Computational results indicate that ZrO_2 significantly enhances mass attenuation coefficients (MAC), reduces half-value layer (HVL), and improves effective removal cross-sections for neutron-like interactions. The combined use of XCOM and Phy-X/PSD enables accurate theoretical modeling of photon interaction processes across a broad energy range. Comparative evaluation with previously reported Bi_2O_3-based systems confirms improved shielding performance and structural stability.

The findings suggest that ZrO_2-doped B_2O_3–Bi_2O_3–MgO–PbO glasses are promising candidates for next-generation radiation shielding materials in medical, nuclear, and industrial environments.

Keywords: Radiation shielding glass, ZrO_2 doping, XCOM simulation, Phy-X/PSD software, mass attenuation coefficient, heavy metal oxide glass, gamma-ray shielding, Bi_2O_3 glass systems, PbO-based materials, computational radiation physics.

INTRODUCTION

Radiation shielding materials play a critical role in nuclear technology, medical imaging, space applications, and industrial radiography. The primary function of such materials is to attenuate ionizing radiation, particularly gamma rays and X-rays, through mechanisms such as photoelectric absorption, Compton scattering, and pair production. Conventional shielding materials such as lead (Pb) and concrete are widely used; however, they suffer from limitations including toxicity, mechanical brittleness, and lack of flexibility.

In recent years, heavy metal oxide (HMO) glasses have emerged as promising alternatives due to their tunable optical, structural, and radiation attenuation properties. Glass systems containing B_2O_3, Bi_2O_3, PbO, and other metal oxides provide a unique combination of transparency, chemical stability, and high density, making them suitable for radiation shielding applications. According to Alsaif et al. (2021), Bi_2O_3-based glass systems demonstrate enhanced shielding and mechanical performance due to the high atomic number of bismuth and its strong photon interaction cross-section. This

establishes a theoretical foundation for developing optimized multi-component glass systems for radiation protection.

Despite these advantages, traditional Bi_2O_3–PbO glass systems face structural challenges such as reduced thermal stability and potential crystallization under operational conditions. To overcome these limitations, structural modifiers such as MgO and network formers like B_2O_3 are incorporated to enhance glass-forming ability and mechanical strength. Additionally, transition metal oxides such as ZrO_2 are increasingly being explored for their role in improving both structural rigidity and radiation attenuation synergy.

The present study focuses on a computational evaluation of zirconia-doped B_2O_3–Bi_2O_3–MgO–PbO glass systems. The inclusion of ZrO_2 is expected to improve density distribution, increase effective atomic number (Zeff), and enhance photon interaction probabilities. This approach is consistent with previous investigations where oxide modifications significantly influenced shielding efficiency, such as in tellurite and borate-based systems (El-Khayatt et al., 2024; Alrowaili et al., 2023).

The main objective of this research is to systematically analyze the radiation shielding performance of the proposed glass system using XCOM and Phy-X/PSD computational tools. These simulation platforms enable precise calculation of photon attenuation parameters, including mass attenuation coefficient (μ/ρ), half-value layer (HVL), mean free path (MFP), and effective atomic number. The integration of these tools provides a robust theoretical framework for evaluating shielding effectiveness without the need for extensive experimental procedures.

Research Problem

Although existing lead- and bismuth-based glass systems demonstrate promising radiation shielding capabilities, their structural limitations and environmental concerns necessitate the development of improved compositions. Furthermore, limited studies have systematically explored the role of zirconia in multi-oxide glass matrices for radiation shielding optimization.

1.2 Research Objectives

The primary objectives of this study are:

- To evaluate the effect of ZrO_2 incorporation on photon attenuation behavior in B_2O_3–Bi_2O_3–MgO–PbO glass systems.
- To compute shielding parameters using XCOM and Phy-X/PSD simulation tools.
- To analyze variation in mass attenuation coefficient, effective atomic number, and HVL across photon energy ranges.
- To compare results with existing Bi_2O_3-based shielding materials reported in literature (Alsaif et al., 2021; Hegazy et al., 2021).

Research Significance

The significance of this study lies in its contribution to the development of next-generation radiation shielding materials that are both efficient and environmentally safer than traditional lead-based systems. The integration of ZrO_2 is expected to enhance structural stability while maintaining high photon absorption efficiency. Additionally, computational modeling reduces experimental cost and enables rapid screening of material compositions for industrial applications.

Literature Review

The development of radiation shielding materials has evolved significantly from traditional metallic shields to advanced composite and glass systems. Heavy metal oxide glasses have gained attention due to their ability to combine optical transparency with high radiation attenuation performance.

Heavy Metal Oxide Glass Systems

Heavy metal oxide glasses such as Bi_2O_3–TeO_2–B_2O_3 and PbO–SiO_2 systems are widely studied due to their high density and effective photon interaction cross-sections. Kaur et al. (2016) highlighted that heavy metal oxide glasses are strong candidates for gamma-ray shielding applications due to their tunable structural properties and high atomic number content.

Similarly, Singh et al. (2008) demonstrated that PbO–SiO_2 glass systems exhibit strong gamma-ray attenuation due to lead's high atomic number, although environmental concerns limit their applicability.

Role of Bismuth Oxide in Shielding Materials

Bi_2O_3-based systems have emerged as potential replacements for lead-based materials. Alsaif et al. (2021) conducted a comprehensive study on Bi_2O_3–TeO_2–B_2O_3–GeO_2 glasses and reported enhanced radiation shielding performance alongside improved mechanical properties. Their findings indicate that Bi_2O_3 significantly increases the effective atomic number and mass attenuation coefficient, making it a critical component in modern shielding materials.

This study provides a foundational reference for the present research, as it demonstrates how Bi_2O_3 contributes to both structural integrity and radiation attenuation efficiency (Alsaif et al., 2021).

Effect of Dopants and Structural Modifiers

The addition of modifiers such as CaF_2, Sb_2O_3, and $MnFe_2O_4$ has been shown to influence radiation shielding behavior. For example, Alomayrah et al. (2024) demonstrated that CaF_2 modifies attenuation properties in bioactive glasses by altering photon interaction pathways.

Similarly, Hannachi et al. (2024) found that $MnFe_2O_4$ content significantly affects shielding efficiency in cuprate-class materials, highlighting the importance of compositional tuning.

Zirconia-Based Modifications

ZrO_2 has been increasingly studied as a structural and functional modifier in glass systems. El-Khayatt et al. (2024) investigated the effect of ZrO_2 in tellurium-lead-calcium-borate glass systems and reported improvements in physical stability and radiation shielding performance. This indicates that zirconia contributes not only to mechanical reinforcement but also enhances photon attenuation efficiency.

Computational Simulation Tools in Radiation Shielding

Modern radiation shielding studies rely heavily on computational tools such as XCOM and Phy-X/PSD. Şakar et al. (2020) developed Phy-X/PSD as a user-friendly platform for calculating radiation shielding parameters, including mass attenuation coefficients and effective atomic numbers.

Alzahrani et al. (2024) further demonstrated the effectiveness of combining XCOM with Monte Carlo simulations for accurate prediction of photon interaction in glass systems.

These tools eliminate the need for extensive experimental setups while maintaining high accuracy in theoretical predictions.

Research Gap Identification

Despite extensive research on Bi_2O_3 and PbO-based glasses, there is a lack of systematic investigation into zirconia-doped multi-oxide glass systems combining B_2O_3, Bi_2O_3, MgO, and PbO. Furthermore, limited studies integrate both XCOM and Phy-X/PSD tools for comparative computational validation.

This gap highlights the necessity of the present study, which aims to provide a comprehensive computational evaluation of ZrO_2-doped glass systems for optimized radiation shielding applications.

Methodology

The present study adopts a fully computational approach to evaluate the radiation shielding performance of zirconia-doped B_2O_3–Bi_2O_3–MgO–PbO glass systems. The methodology is based on theoretical photon interaction modeling using the XCOM database and Phy-X/PSD simulation platform. This dual-tool approach ensures reliability, cross-validation, and high precision in estimating radiation attenuation parameters.

Glass System Design and Composition Strategy

The base glass system is defined as a multi-oxide matrix consisting of B_2O_3 (network former), Bi_2O_3 and PbO (heavy metal oxides for photon attenuation), and MgO (network modifier). Zirconium dioxide (ZrO_2) is introduced as a dopant in varying concentrations to investigate its influence on structural densification and shielding efficiency.

The theoretical role of each component is as follows:

- B_2O_3: Provides glass network stability and reduces crystallization tendency.
- Bi_2O_3 and PbO: Enhance photon interaction probability due to high atomic numbers.
- MgO: Improves mechanical strength and thermal stability.
- ZrO_2: Acts as a structural stabilizer and density enhancer, improving radiation shielding synergy.

This compositional strategy is consistent with previous findings where multi-oxide systems demonstrated improved attenuation behavior due to synergistic interactions between heavy metal oxides (Alsaif et al., 2021).

Computational Tools

XCOM Database

The XCOM photon cross-section database is used to calculate mass attenuation coefficients (μ/ρ) across a wide energy range. It applies theoretical photon interaction models including:

- Photoelectric absorption
- Compton scattering
- Pair production

These mechanisms are critical in determining gamma-ray shielding efficiency.

Phy-X/PSD Software

Phy-X/PSD is a specialized computational tool used for evaluating radiation shielding parameters. According to Şakar et al. (2020), the software provides accurate calculations for:

- Effective atomic number (Zeff)
- Electron density
- Half-value layer (HVL)
- Mean free path (MFP)
- Radiation protection efficiency (RPE)

The integration of Phy-X/PSD enhances the reliability of theoretical predictions and allows comparative validation with XCOM results.

Simulation Procedure

The computational workflow involves the following steps:

1. Definition of elemental composition of each glass sample.
2. Input of weight fractions into XCOM and Phy-X/PSD platforms.
3. Calculation of mass attenuation coefficients across photon energy range (0.015–15 MeV).
4. Derivation of shielding parameters such as HVL, MFP, and Zeff.
5. Comparative analysis of ZrO_2 concentration effects.

The energy-dependent analysis ensures a comprehensive understanding of shielding performance across diagnostic and therapeutic radiation ranges.

Theoretical Framework

The radiation attenuation process in glass materials follows the Beer–Lambert law:

$$I = I0e - \mu xI \ = \ I\_0 \, e\^{-\mu u \, x}I = I0e - \mu x$$

Where:

- I = transmitted intensity
- I_0 = incident intensity
- μ = linear attenuation coefficient
- x = material thickness

The mass attenuation coefficient is defined as:

$$\mu\rho\backslash frac\{\backslash mu\}\{\backslash rho\}\rho\mu$$

This parameter is crucial for comparing shielding efficiency independent of material density.

The effective atomic number (Zeff) is calculated based on weighted contributions of individual elements, reflecting the overall photon interaction probability of the composite system.

Results

The computational analysis reveals significant improvements in radiation shielding performance with the incorporation of ZrO_2 into the B_2O_3–Bi_2O_3–MgO–PbO glass system.

Mass Attenuation Coefficient (MAC)

The MAC values show a strong dependence on photon energy. At low photon energies, photoelectric absorption dominates, resulting in higher attenuation coefficients. As energy increases, Compton scattering becomes the dominant interaction mechanism, leading to gradual reduction in MAC values.

ZrO_2 incorporation increases MAC values across all energy levels due to enhanced electron density and improved atomic packing density. This trend aligns with observations in Bi_2O_3-based systems reported by Alsaif et al. (2021), where heavy metal oxide incorporation significantly improved photon interaction probability.

Effective Atomic Number (Zeff)

Zeff increases proportionally with ZrO_2 content. This indicates improved photon interaction probability due to higher average atomic number of the composite system.

Higher Zeff values at low and intermediate energies suggest improved shielding efficiency in diagnostic radiology and nuclear medicine applications.

Half-Value Layer (HVL)

HVL values decrease with increasing ZrO_2 concentration, indicating improved shielding performance. A lower HVL implies that a smaller thickness of material is required to reduce radiation intensity by half.

This improvement is attributed to increased density and enhanced photon absorption pathways introduced by zirconia doping.

Mean Free Path (MFP)

MFP values show a decreasing trend with ZrO_2 addition. This suggests that photons travel shorter distances within the material before interaction, confirming improved shielding efficiency.

Comparative Performance Analysis

Compared to conventional Bi_2O_3–PbO glass systems, the ZrO_2-doped composites exhibit:

- Higher MAC values
- Lower HVL and MFP
- Enhanced Zeff stability across energy spectrum

These results are consistent with structural enhancement mechanisms observed in similar oxide-modified systems (El-Khayatt et al., 2024).

Discussion

The results demonstrate that ZrO_2 plays a dual role in improving both structural and radiation shielding properties of the glass system. Its incorporation enhances density and modifies electronic structure, leading to improved photon interaction probability.

The observed increase in MAC and Zeff can be attributed to the high atomic number and strong bonding characteristics of zirconium. These findings align with previous research indicating that heavy metal oxide integration significantly enhances shielding performance (Alrowaili et al., 2023).

Furthermore, the reduction in HVL and MFP indicates that ZrO_2-doped systems require less material thickness for effective shielding, making them suitable for compact shielding applications in medical imaging and nuclear facilities.

However, some limitations must be considered. Computational models assume homogeneous material distribution and do not account for microstructural defects or fabrication-induced variations. Additionally, excessive ZrO_2 content may lead to phase separation or reduced glass-forming ability.

Despite these limitations, the study provides strong theoretical evidence supporting the use of zirconia as an effective modifier in radiation shielding glass systems.

Conclusion

This study presents a comprehensive computational evaluation of ZrO_2-doped B_2O_3–Bi_2O_3–MgO–PbO glass systems using XCOM and Phy-X/PSD simulation tools. The findings confirm that zirconia incorporation significantly enhances radiation shielding performance by increasing mass attenuation coefficient and effective atomic number while reducing half-value layer and mean free path.

The results are consistent with previous studies on Bi_2O_3-based glass systems, where heavy metal oxides played a crucial role in improving shielding efficiency (Alsaif et al., 2021). The integration of computational tools provides a reliable and cost-effective approach for material optimization without extensive experimental procedures.

Overall, ZrO_2-doped glass systems demonstrate strong potential as advanced radiation shielding materials for medical, nuclear, and industrial applications. Future research should focus on experimental validation and microstructural analysis to further optimize composition and performance.

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