Analysis of key factors on the neutron shielding performance for various boron-containing compounds

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Abstract

Boron-containing compounds have gained significant attention as effective additives for enhancing the performance of composite materials. This study systematically investigates the key factors influencing the neutron shielding efficiency of various boron compounds, including mass density, boron content, and boron number density (atoms/nm3), to establish guidelines for their optimal selection in radiation shielding applications. The effective removal cross-section (ΣR) for fast neutrons was evaluated using Phy-X and NXcom software, while the macroscopic cross-section (Σ) for thermal neutrons was calculated via Monte Carlo N-Particle (MCNP) simulations and manual computations. The results demonstrate that mass density and boron number density are the dominant factors for fast neutron shielding, with ΣR values ranging from 0.082 cm−1 (KBH4) to 0.225 cm−1 (WB2). For thermal neutrons, boron number density is the primary determinant of shielding performance, with Σ values reaching 4070.34 cm−1 for GdB6, 474.67 cm−1 for ZrB12, and 447.37 cm−1 for B4C. Notably, GdB6 exhibits exceptional thermal neutron shielding due to the high absorption cross-section of 157Gd. The findings provide critical insights for designing advanced shielding materials, emphasizing the synergistic effects of density and boron number density to optimize neutron attenuation.

Full Text

Preamble

Analysis of key factors on the neutron shielding performance for various boron-containing compounds∗ Zhi-Cheng Qian,1 Zhi-Hong Zhang,1, † Jin-Sen Xie,2,

3, ‡ Jun Cai Wang,1 De-Feng Chen,1 Chang-Yuan Li İD ,1 Jian-Hua İD ,1 Xian-Wei Guo,1 and Hui-Quan Li1 1Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China 2School of Nuclear Science and Technology, University of South China, Hengyang 421001, China 3Key Lab of Advanced Nuclear Energy Design and Safety, Ministry of Education, Hengyang 421000, China Boron-containing compounds have gained significant attention as effective additives for enhancing the per- formance of composite materials. This study systematically investigates the key factors influencing the neutron shielding efficiency of various boron compounds, including mass density, boron content, and boron number density (atoms/nm3), to establish guidelines for their optimal selection in radiation shielding applications. The effective removal cross-section (ΣR) for fast neutrons was evaluated using Phy-X and NXcom software, whereas the macroscopic cross-section (Σ) for thermal neutrons was calculated via Monte Carlo N-Particle (MCNP) sim- ulations and manual computations. The results demonstrate that mass density and boron number density are the dominant factors for fast neutron shielding, with ΣR values ranging from 0.082 cm−1 (KBH4) to 0.225 cm−1 (WB2). For thermal neutrons, the boron number density is the primary determinant of shielding performance, with Σ values of 4070.34 cm−1 for GdB6, 474.67 cm−1 for ZrB12, and 447.37 cm−1 for B4C. Notably, GdB6 exhibits exceptional thermal neutron shielding owing to the high absorption cross-section of 157Gd. These find- ings provide critical insights for designing advanced shielding materials, emphasizing the synergistic effects of density and boron number density to optimize neutron attenuation.

Keywords: Boron-containing compounds, Neutron shielding properties, Shielding impact factors

INTRODUCTION

The widespread application of nuclear technology and equipment has driven significant advancements in neutron- shielding materials development. Among the various shield- ing elements, boron has emerged as a particularly effective component owing to its exceptionally high neutron absorp- tion cross-section [1–6] and cost-effectiveness. However, the practical implementation of boron for neutron shielding requires its incorporation into bulk materials, as elemental boron alone cannot meet the structural and functional re- quirements of shielding applications [7, 8]. To address this challenge, researchers have extensively investigated the in- tegration of various boron compounds into different matrix materials. Commonly used boron compounds include boron carbide (B4C), boron oxide (B2O3), titanium boride (TiB2), tungsten diboride (W2B5/WB), boron nitride (BN), and boric acid (H3BO3). These compounds have been successfully in- corporated into concrete matrices [9–11], composites [12–17], reactive sintered borides [18], glass systems [19, 20], and ceramics [21, 22]. These composite materials combine the neutron absorption capability of boron with the struc- tural integrity and radiation stability of host materials. When boron forms compounds with transition metals or rare earth ele-

ments, the resulting materials exhibit enhanced macro- scopic neutron capture cross-sections and exceptional refrac- tory properties [23]. This improvement is attributed to the synergistic effects between boron and metal atoms, which not ∗ This work was supported by the Key Laboratory of Advanced Nuclear En- ergy Design and Safety, Ministry of Education (No. KLANEDS202317). † Corresponding author, zhangzhihong@sinap.ac.cn ‡ Corresponding author, jinsen_{xie}@usc.edu.cn only increase the neutron absorption efficiency but also en- hance the thermal stability and mechanical strength.

Some boron metal compounds, especially metal borides such as borated steels (Fe2B and FeB), hafnium diboride (HfB2), and europium hexaborides (EuB6), exhibit out- standing characteristics, including exceptional hardness and strength, high melting points, and robust chemical stabil- ity. These materials have been evaluated for use as neutron- absorbing pellets in control rods of nuclear reactors [24]. Nu- merous studies have focused on the processing, structure, and properties of boron compounds and boron-containing com- posites, driven by the demand for high-performance mate- rials [25–28]. Serebrennikov et al. [29] demonstrated that MoB2/B4C multilayer systems outperform conventional ma- terials (Mo, W, Pt) in terms of energy resolution and reflec- tivity, making them ideal for precision X-ray optics and syn- chrotron applications. Orlovskaya et al. [30] demonstrated that diboride ceramics, including zirconium diboride (ZrB2), hafnium diboride (HfB2), osmium diboride (OsB2), and iridium diboride (IrB2), exhibit exceptional mechanical proper- ties, particularly in terms of hardness and Young' s modulus.

Several studies have been conducted to quantitatively in- vestigate the neutron-shielding properties of boron com- pounds or boron-containing materials. Li et al. [31] in- vestigated the shielding properties of composites made with boron ores from China for fast neutrons from a 252Cf source.

This study combined experimental measurements and Monte Carlo simulations to evaluate the total macroscopic removal cross sections, deposited energies, and absorbed doses. The results suggested that a higher boron content improved the neutron shielding capabilities of these materials. Korkut et al. conducted a comprehensive investigation into the fast neu- tron shielding behavior (FNSB) of various boron compounds, including magnesium diboride (MgB2), sodium borohydride (NaBH4), and potassium borohydride (KBH4) [32]. The re- sults demonstrate that MgB2 outperforms NaBH4 and KBH4 in terms of shielding efficiency, primarily because of its sig- nificantly higher boron content. In a follow-up study, Korkut et al. [33] investigated the effect of boron number density on neutron shielding in three boron ores by combining ex- periments with FLUKA simulations [34]. Their results con- firmed that a higher boron density directly increases the Σ, thereby improving the shielding efficiency owing to enhanced neutron-boron interactions. Sarıyer et al. [35] studied neu- tron shielding in concrete composites with B4C and FeB ad- ditives. Their results showed that both materials enhanced neutron attenuation; however, FeB outperformed B4C owing to the combined benefits of boron neutron absorption and iron density,

which improved energy dissipation. Ozdogan et al. [36] investigated the FNSB of composites containing B4C, polyester resin, and titanium oxide in various proportions.

The composites with higher boron contents exhibited larger ΣR and Σ and lower neutron transmission ratios. Using exper- iments and simulations, Soltani et al. [37] studied the thermal neutron shielding behavior (TNSB) in B4C-reinforced HDPE composites. They found that smaller boron particle sizes in- creased the neutron interaction probability, whereas higher boron content improved the shielding performance through enhanced neutron absorption.

In summary, incorporating an optimal amount of boron compounds into composite materials significantly enhances their neutron-shielding capabilities. The choice of boron compounds for shielding applications is governed by two primary factors: neutron absorption efficiency and cost- processability balance. Compounds with a higher boron num- ber density and boron content exhibit superior neutron shield- ing performance [31]. Although rare-earth borides such as GdB6 show exceptional neutron shielding efficiency, their high cost is prohibitive; thus, some lightweight borides such as B4C offer viable trade-offs between performance and af- fordability [24]. The effectiveness of these boron-based com- posites is primarily influenced by factors such as the boron content, boron number density, and particle size. These pa- rameters collectively determine the ability of a material to at- tenuate neutrons, making them critical considerations in the design and optimization of advanced shielding solutions for applications in nuclear technology, medical radiation protec- tion, and space exploration.

Owing to boron' s high affinity for both light and heavy el- ements, it can form a wide range of compounds with differ- ent chemical compositions. It is important to systematically investigate the neutron shielding properties of boron com- pounds to screen suitable shielding materials. In this study, the thermal and fast neutron shielding properties of various boron-containing compounds were analyzed. The key factors that may affect the including boron content (weight percent of boron), boron number density (number of boron atoms per unit), and mass density were studied. In Sect. II, the theoret- ical basis is introduced; in Sect. III, detailed information on the selected boron-containing compounds is introduced; and in Sect. IV, the neutron shielding performance of the boron- containing compounds is discussed.

II. THEORETICAL BASIS A. Fast neutron effective removal cross-section Neutrons interact with matter via three primary mecha- nisms: elastic scattering, inelastic scattering, and neutron capture reactions. The likelihood of a fast or fission-energy neutron undergoing its first collision is quantified by the removal cross-section [38]. This parameter represents the probability of removing neutrons from an uncollided beam, thereby reducing the flux of penetrating neutrons. The ef- fective removal cross-section remains relatively constant for neutron energies ranging from 2–12 MeV, making it a reli- able metric for evaluating shielding materials

within this en- ergy range. For compounds or mixtures, the effective removal cross-section can be calculated using the following equation: ΣR = (cid:80) iρi(ΣR/ρ)i.

In this context, ρi represents the partial density of the ith con- stituent element in the material. Here, ρi is defined as the density of the specific element, ΣR/ρi denotes the mass re- moval cross-section of the ith element. These parameters are essential for calculating the overall removal cross-section of the composite material, as they quantify the contribution of each element to the neutron shielding performance.

The partial density ρi can be calculated as the product of the weight fraction ωi of the ith element and the overall den- sity of the sample, as expressed by the following equation: ρi = ωi × ρs In recent years, several user-friendly computational tools have been developed to facilitate the analysis and design of radiation-shielding materials. Notable examples include Phy- X [39], MERCSF-N [40], MRCsC [41], NXcom [42] and ParShied [43]. These programs leverage extensive databases of elemental removal cross-sections and incorporate empirical models to predict the shielding performance of various materials. By providing accurate and efficient calculations, these tools have become indispensable for researchers and en- gineers in fields such as nuclear energy, medical physics, and space exploration. The integration of such software into the design process not only enhances the precision of the shield- ing material selection but also accelerates the development of innovative solutions tailored to specific radiation environ- ments. thermal neutron transmission ratios and macroscopic cross-section The thermal neutron shielding properties of selected boron- based composite materials can be evaluated by analyzing their neutron transmission ratios and macroscopic cross-sections (Σ). Although the Σ is expressed in units of cm−1, which may cause confusion as it resembles a linear attenuation coefficient rather than the traditional cross-section units of cm2, it is widely used in the literature to describe neutron shield- ing performance. The value of Σ can be derived from neutron transmission measurements, providing a quantitative measure of a material' s ability to attenuate thermal neutrons.

However, the experimental determination of these prop- erties can be challenging, especially for boron-containing compounds such as TiB2, MgB2, and SiB6, which typi- cally exist as solid powders at room temperature. Handling powdered boron compounds under neutron irradiation neces- sitates specialized facilities and stringent safety protocols, which were inaccessible for this computational study. Several high-performance boron compounds (e.g., ZrB12 and GdB6) are challenging to synthesize in the bulk quantities required for experimental neutron irradiation tests. To address these limitations, the Monte Carlo method has emerged as a pow- erful computational tool for simulating neutron interactions and predicting the shielding performance. For instance, Qian et al. [44] highlighted the effectiveness of Monte Carlo simu- lations in overcoming the experimental constraints.

In this study, the Monte Carlo N-Particle Transport Code, version 5 (MCNP5)

[45] was employed to simulate the ther- mal neutron shielding behavior of boron composites. The simulation geometry is illustrated in Fig. 1 [Figure 1: see original paper], was carefully designed to replicate real-world conditions, ensuring accurate and reliable results. The use of MCNP5 circumvents the prac- tical difficulties associated with handling powdered materials and provides a cost-effective and efficient alternative to exper- imental testing. By leveraging this computational approach, researchers can gain deeper insights into the shielding mech- anisms of boron composites, optimize material compositions, and accelerate the development of advanced shielding solu- tions for applications in nuclear science and technology.

Fig. 1. (Color online) MCNP5 simulation geometry. In the simulation setup, the thermal neutron source was positioned at the center of the shielding structure. The boron composite samples under investigation were modeled as spherical shells, with a neutron detector placed on the outer surface to measure the transmitted neutron flux. This detec- tor utilizes the F2 tally function in MCNP5 to record neutron and secondary γ-ray flux data. To ensure the reliability of the simulation results, the MCNP5 code utilized the ENDF/B-VI Table 1 . The parameter details of MCNP5 input card MCNP input Thickness of shield Detector Parameter details 0.001 (cm) pos=0 0 0 par=1 erg=2.53 $\times$ 10−8 F2:n and F2:p neutron cross-section database and set the total number of in- cident neutrons (nps) to 108 to reduce the statistical errors to less than 1%. During the simulation, the convergence of the geometric model was verified by adjusting the spherical shell thickness (1–10 µm), and the results showed that the relative deviation of the Σ value due to thickness variation was less than 2%. More details of the MCNP5 input are presented in Table 1. Based on the Beer-Lambert law [46], the macro- scopic cross-section (Σ) of a material can be determined us- ing the following formula: $\Sigma(E) = -$ (cid:19) (cid:18) I where I is the transmitted neutron flux, I0 is the incident neutron flux, and x is the thickness of the shielding mate- rial. This relationship provides a direct method for calculat- ing the macroscopic cross-section, which quantifies the abil- ity of a material to attenuate thermal neutrons. By combining this theoretical framework with MCNP5 simulation results, researchers can accurately assess the shielding performance of boron composites, even in scenarios where experimental measurements are impractical.

In addition, the macroscopic cross-section (Σ) can be cal- culated manually using the following equation [47]: $\Sigma =$ (cid:80) iWi(Σj/ρ).

Here, Wi represents the partial density of the ith constituent element, while (Σj/ρ)i is the neutron mass attenuation coef- ficient of the ith constituent for a specific interaction type (j), as defined in Eq. 5. Σj/ρ = Additionally, NA stands for Avogadro' s constant, A is the atomic weight of the ith element, and σt is the micro- scopic cross-section of the ith element. These microscopic cross-section values can be retrieved from the comprehensive database available at the International Atomic Energy Agency (IAEA) website [48]. This resource provides essential nu- clear data for accurate calculations and analyses in neutron-

shielding studies.

III. MATERIALS AND METHODS In this study, a comprehensive series of boron-containing compounds with exceptional neutron absorption properties were systematically selected and investigated for their poten- tial applications in nuclear shielding and radiation protection.

Table 2 . The chemical compositions, density, boron concentration and boron number density of the investigated samples.

Composition NaBH4 ZrB12 Mo2B5 BPE-5 Density (g/cm3) Boron concentration 16.22% 8.82% 20.04% 28.58% 31.11% 47.07% 61.81% 69.78% 78.26% 43.55% 19.16% 58.71% 5.33% 21.97% 10.52% 12.82% 18.88% 15.50% 15.55% 29.37% 10.68% 10.80% 10.40% 11.00% 30.19% 31.05% 29.20% Boron number density (atoms/nm3) The selected compounds, which exhibit a wide range of boron concentrations (ranging from 5.33% to 78.26%), mass den- sities (varying between 1.07 g/cm3 and 14.15 g/cm3), and boron number densities (spanning from 12.39 atoms/cm3 to 118.03 atoms/nm3), include both well-established and emerg- ing materials: FeB, Fe2B, KBH4, NaBH4, TiB2, MgB2, CaB6, SiB6, B4C, ZrB2, ZrB12, Mo2B, Mo2B5, WB2, W2B5, NbB2, CoB, NiB, CrB2, TaB2, VB2, HfB2, ReB2, LuB2, SmB6, B2O3, and GdB6. Furthermore, the TNSB of commer- cially available polyethylene-boron composites (BPE-5) [28] was evaluated alongside these boron compounds for compar- ative analysis. These materials were chosen based on their unique combination of neutron absorption capabilities, ther- mal stability, and mechanical properties, making them suit- able for nuclear applications. The mass density values were obtained from reliable literature sources, including the com- prehensive work by Knoch et al. on borides [24], recent stud- ies by Orlovskaya et al. [30], and Serebrennikov et al. [29], as well as verified data from the reputable material database, MatWeb [49]. The comprehensive dataset, including detailed compositions, precise boron concentrations, and calculated boron number densities, is system- atically presented in Table 2, providing a valuable reference for researchers in the field of nuclear-materials science.

IV. RESULT AND DISCUSSION A. Fast neutron shielding performance The recently developed Phy-X software [39], which incor- porates an updated database and a refined empirical model, was employed to calculate the macroscopic removal cross- sections (ΣR) for fast neutrons in various boron compounds.

These results were compared with those obtained using the NXcom program [42], a well-established tool for radiation shielding analysis. The calculated ΣR values for the inves- tigated boron compounds are presented in Table 3 . Notably, the results generated by the Phy-X software showed excel- lent agreement with those derived from the NXcom program, demonstrating the reliability and accuracy of both computa- tional tools.

The influence of mass density on the fast neutron shielding properties of various boron compounds is shown in Fig. 2 [Figure 2: see original paper].

Among the studied materials, tungsten diboride (WB2) ex- hibits the highest values, attributed to its significantly higher mass density of 14.15 g/cm3. In contrast, potassium borohy- dride (KBH4), with the lowest mass density of 1.11 g/cm3, demonstrates the lowest ΣR values. This trend highlights a strong positive correlation between mass density and neutron shielding efficiency, as materials with greater densities tend to provide more effective neutron attenuation owing to in- creased atomic interactions. As shown in the figure, most of the data points align closely with the fitting curve, indi- cating a consistent relationship between the mass density and shielding performance. However, a few compounds, such as boron nitride (BN), iron boride (FeB), and potassium borohy- dride (KBH4), deviated slightly from the curve. These devia- tions may arise from differences in the material composition, crystalline structure, or other factors influencing the neutron interaction probabilities. Despite these minor discrepancies, the overall trend confirms that boron compounds with higher mass densities generally exhibit superior fast-neutron shield- ing capabilities.

The relationship between the ΣR values of boron com- pounds and their boron concentration, as well as boron num- ber density, is illustrated in Figs. 3 and 4. As depicted in Fig. 3 [Figure 3: see original paper], tungsten diboride (WB2) exhibits the highest ΣR val- ues despite having a relatively moderate boron concentration of 10.52%. This observation challenges the conventional as- sumption that materials with higher boron concentrations in- herently possess superior neutron-shielding properties. For instance, boron carbide (B4C), which has the highest boron concentration at 78.26%, demonstrates only average fast neu- tron shielding behavior compared to other boron compounds under study. This suggests that boron concentration alone is not the sole determinant of the shielding performance. Fig- ure 3 further reveals that the FNSB of boron compounds does not exhibit a direct correlation with boron concentration. In- stead, other factors, such as material density, atomic struc- ture, and the presence of additional elements, may play sig- nificant roles in influencing the neutron attenuation efficiency.

For example, the high density and unique atomic arrangement of WB2 likely contribute to its exceptional shielding perfor- Table 3. Effective removal cross-section (cm−1) calculated by Phy-X and NXcom program for different the boron compounds Composition Phy-X NXcom Composition Phy-X NXcom Composition Phy-X NXcom ZrB12 Mo2B5 NaBH4 (Color online) Effective removal cross-section with mass Fig. 2. density for different the boron compounds.

Fig. 3. (Color online) Effective removal cross-section with boron concentration for different the boron compounds. mance, even with a lower boron concentration. These find- ings underscore the complexity of neutron shielding mechanisms and highlight the need to consider multiple material properties when designing effective shielding solutions for neutron radiation.

The boron number density, which varies across boron com- pounds, is another critical factor that may influence the FNSB of these materials. Figure 4 [Figure 4: see original paper] illustrates the relationship be- tween the values and the

boron number density for vari- ous boron compounds. As shown in the figure, only a sub- set of compounds, including potassium borohydride (KBH4), sodium borohydride (NaBH4), boron trioxide (B2O), mag- nesium diboride (MgB2), calcium hexaboride (CaB), silicon hexaboride (SiB6), chromium diboride (CrB2), gadolinium hexaboride (GdB6), boron carbide (B4C), and zirconium do- decaboride (ZrB12), follow the expected trend where higher boron number density corresponds to larger ΣR values. How- ever, this trend did not hold for all compounds. For instance, tungsten diboride (WB2) and calcium hexaboride (CaB6) ex- hibit nearly identical boron number densities; however, their FNSB properties differ significantly. This discrepancy sug- gests that the boron number density alone cannot fully ac- Fig. 4. (Color online) Effective removal cross-section with boron number density for different the boron compounds. count for the variations in the neutron shielding performance.

The non-proportional distribution of values with the number density of boron compounds may indicate that the number density is not the only key factor in the FNSB for boron com- pounds.

To determine whether the density and boron number den- sity are the dominant factors influencing the FNSB of boron compounds, the variations in ΣR values were analyzed as a function of the product of the density and boron number density, as illustrated in Fig. 5 [Figure 5: see original paper]. An exponential fitting curve was also included to model this relationship. In contrast to the scattered distribution observed in Figs. 3 and 4, the data points in Fig. 5 exhibit a much closer alignment with the fitting curve, indicating a strong correlation. Only a few com- pounds, such as iron boride (Fe2B), boron nitride (BN), and calcium hexaboride (CaB6), deviated slightly from this trend.

The exponential increase in ΣR values with the product of the density and boron number density suggests that these two pa- rameters collectively play a significant role in determining the FNSB of boron compounds. This relationship highlights the synergistic effect of density and boron number density on the neutron shielding performance, as higher values of both pa- rameters enhance the probability of neutron interactions and energy absorption. The close fit of most data points to the exponential curve further supports the idea that these factors are the primary drivers of the shielding efficiency. dride (KBH4, ΣR=0.082 cm−1) and sodium borohydride (NaBH4, ΣR=0.108 cm−1) exhibit slightly lower ΣR values than water and graphite, the majority of boron compounds demonstrate superior ΣR values. This enhanced performance highlights their exceptional fast neutron shielding capabilities and suggests their promising potential for advanced radiation- shielding applications. Although this study shows that tung- sten diboride (WB2) exhibits the best performance in fast neutron shielding (ΣR=0.225 cm−1), its high cost and com- plex manufacturing process limit its industrial application. In contrast, boron carbide (B4C), with its lightweight properties (density of 2.50 g/cm3) and high boron content (78.26%), has become the material of choice for reducing the weight and space of neutron shielding [3]. However, the low density of B4C may lead to multiple

scattering of fast neutrons, re- quiring the enhancement of the overall shielding efficiency through composite material design (e.g., mixing with high- density tungsten particles). Additionally, the brittleness of boron carbide may affect its stability under dynamic loading conditions, which could be improved in the future through nano-reinforcement or fiber composite technology.

B. Thermal neutron shielding performance The thermal neutron transmission ratios (I/I0) of various boron compounds are presented in Fig. 6 [Figure 6: see original paper]. The results indi- cated that the transmission ratios of the selected boron com- posites ranged from 0.017 to 0.98. The lowest transmission ratio, observed for gadolinium hexaboride (GdB6), signifies its exceptional TNSB.

Fig. 5. (Color online) Effective removal cross-section with the prod- uct of density and boron number density for different boron com- pounds.

Furthermore, the ΣR values of commonly used neutron moderators demonstrate significant variation: water (H2O) exhibits a ΣR of 0.103 cm−1, polyethylene ((C2H4)n) shows 0.122 cm−1, and graphite possesses 0.113 cm−1. These materials have been extensively employed as fast neu- tron moderators in radiation-shielding applications owing to their effective moderation properties. Notably, among boron-containing compounds, although potassium borohy- Fig. 6. Thermal neutron transmission ratios of boron compounds.

The macroscopic cross-section (Σ) values for the boron compounds studied at a neutron energy of 0.025 eV are pre- sented in Table 4 . Notably, the Σ values derived from the MCNP5 simulations show excellent agreement with those calculated manually using Eq. (4). To quantify the consis- Table 4. Σ values and secondary γ-rays fluence of boron compounds for thermal neutron Composition NaBH4 ZrB12 Mo2B5 Σ (cm−1) Manual calculated 0.56% 0.45% 3.77% 1.35% 2.14% 4.15% 4.80% 5.47% 6.77% 2.96% 1.42% 4.59% 0.11% 1.56% Secondary γ-rays fluence (cm−2) Composition BPE-5 Σ (cm−1) Manual calculated 0.80% 0.93% 1.20% 0.82% 2.37% 2.17% 0.53% 1.39% 0.50% 0.55% 2.13% 1.91% 4070.34 3985.34 2.13% 2.91% Secondary γ-rays fluence (cm−2) Fig. 7 [Figure 7: see original paper]. (Color online) Macroscopic cross-section of thermal neutrons with mass density and boron concentration for different the boron compounds. tency between the simulated and calculated results, the per- centage relative deviation (RD) was determined using Eq. 6 [50]. The RD values fell within a narrow range of 0.11% to 6.77%, demonstrating a high level of accuracy in the simula- tion outcomes. This close alignment between the simulated and manually calculated values underscores the reliability of the MCNP5 code in predicting neutron shielding properties and validates the robustness of the computational approach employed in this study. Furthermore, the secondary γ-ray fluences (cm−2) are also presented in Table 4. As we known, 10B can absorb the thermal neutrons and release secondary γ-rays, the reaction formula is given as eq. 7. (cid:12) (cid:12) (cid:12) (cid:12) (cid:12) (cid:12) (cid:12) (cid:12) ΣMCNP − ΣCalculation ΣMCNP 10B + n(0.025 eV) $→$4 He +7 Li + γ(0.48 MeV) To gain deeper insights into the factors influencing the TNSB

of the selected boron compounds, the Σ for thermal neutrons was analyzed in relation to the mass density, boron concentration, and boron number density, as illustrated in Figs. 7 and 8. These figures provide a comprehensive visualization of how these parameters collectively affect the shield- ing performance of boron-containing compounds. The distri- bution shown in Fig. 7 (a) and (b) are similar, indicating that the Σ of thermal neutrons is not proportional to density and boron concentration.

As shown in Fig. 8 [Figure 8: see original paper], most data points closely align with the fitting curve, except for gadolinium hexaboride (GdB6).

This trend indicates that boron compounds with higher boron number densities generally exhibit larger Σ values, reflecting their enhanced thermal neutron-shielding capabilities. No- tably, GdB6 exhibits a significantly higher Σ value than other boron compounds, attributable to the extraordinarily high thermal neutron cross-section of 157Gd (253909.786 cm−1) at 0.025 eV, which far exceeds that of 10B (3844.16 cm−1), far exceeding the Σ value of 10B. Owing to its relatively low boron number density, the TNSB of commercially available C. Future Research Directions This study primarily focused on the influence of the boron number density, mass density, and boron content on the neu- tron shielding performance. However, it is important to ac- knowledge that the structural morphology, such as porosity, grain boundaries, and nanoscale material design, can also play a significant role in neutron attenuation. These mi- crostructural characteristics may affect the real-world perfor- mance of shielding materials by altering the neutron interac- tion probabilities, scattering mechanisms, and overall mate- rial integrity. To address these gaps, further investigations (1) microstruc- are recommended in the following areas: tural optimization: systematic studies on how porosity, grain size, and phase distribution influence neutron shielding in boron composites [57, 58]. (2) Advanced fabrication techniques: methods such as spark plasma sintering or additive manufacturing to control the morphology and minimize de- fects [59, 60].

WB2 is a refractory ceramic characterized by exceptional hardness (20 GPa) and high thermal stability (melting point 2800 ◦C) [24], making it ideal for use in extreme en- vironments.

Its dense atomic structure and tungsten con- tent enhance radiation shielding performance; however, its high brittleness and poor processability necessitate compos- ite designs (e.g., metal matrix bonding) for practical applica- tions [16]. GdB6 offers outstanding neutron absorption ow- ing to gadolinium' s high cross-section, coupled with mod- erate mechanical strength (15 GPa) and thermal stability (melting point 2500 ◦C) [51, 52]; however, its mechan- ical properties often require reinforcement (e.g., polyethy- lene matrix integration). ZrB12 stands out for its excep- tional thermal resilience (melting point > 3000 ◦C) and high boron number density (118.03 atoms/nm3), providing an op- timal balance of neutron attenuation and structural integrity for high-temperature nuclear components [23, 61]. Future efforts should focus on optimizing the material composition and structural design to balance the shielding efficiency,

cost, and processability, thereby promoting the practical applica- tion of boron-based composite materials in the nuclear en- ergy, aerospace, and medical fields.

Fabrication techniques play a pivotal role in optimizing the neutron-shielding performance of boron-containing compos- ites and alloys. Advanced methods such as spark plasma sin- tering and powder metallurgy have been employed to fab- ricate dense, homogeneous composites such as B4C/Al and WB/Al, en- suring uniform boron dispersion and enhanced mechanical integrity [62]. For polymer-based shields (e.g., HDPE/B4C), melt blending and hot pressing are widely used to achieve optimal particle-matrix adhesion, whereas cold spraying has emerged for creating layered structures with minimal porosity [63]. In alloy systems (e.g., borated steels), arc melting and mechanical alloying are critical for achieving high boron solubility and structural stability under irradiation [24]. Future efforts should focus on scalable techniques, such as additive manufactur- ing, to address challenges in complex geometries and industrial adoption.

Future research could also explore the development of Fig. 8. (Color online) Macroscopic cross-section of thermal neutrons with boron number density for different the boron compounds. polyethylene-boron composites (BPE-5) demon- strates infe- rior performance compared to other boron compounds. In ad- dition to GdB6, B4C (Σ=447.37 cm−1) and ZrB12 (Σ=474.67 cm−1) also demon- strate outstanding TNSB.

Among the various factors examined, the boron number density emerged as the most significant determinant of TNSB in boron compounds. However, further research is essential to fully understand the generation of secondary particles re- sulting from neutron capture in these materials. As is widely recognized, neutron capture reactions, such as the (n, α) re- action in 10B and similar reactions in elements such as 149Sm and 157Gd, produce secondary gamma rays [51]. The energy of the secondary gamma rays produced by 10B, 149Sm, and 157Gd was 0.48 MeV, 7.89 MeV, and 7.88 MeV, respectively.

Furthermore, as TNSB increased, a corresponding increase in secondary gamma- ray production was observed, as shown in Table 4. These secondary emissions must be carefully con- sidered in the design of radiation-shielding systems, as they can compromise the overall shielding effectiveness. To ad- dress this, the de- sign of multilayer shielding structures com- bining an outer layer of high-density materials (e.g., tungsten or lead) with an inner layer of high boron number den- sity ma- terials (e.g., B4C or GdB6) could optimize the overall perfor- mance by simultaneously attenuating neutrons and minimiz- ing secondary radiation [16, 52–56]. This approach not only improves neutron attenuation but also reduces the secondary radiation burden, making boron-based materials more versa- tile and effective for radiation shielding applications. Con- tinued explo- ration of these compositional adjustments is vital for advancing the development of next-generation shielding materials that meet the stringent demands of mod- ern radia- tion protection. multi-component boron-based composite materials, such as combining GdB6 with polyethylene, to leverage the syner- gistic effects of hydrogen moderation and boron capture for enhanced shielding efficiency.

The synergistic use of ZrB12 and GdB6 in nuclear reactor control rods is worth exploring.

The high-temperature stability of ZrB12 and its high boron number density render it suitable for fast neutron absorption, whereas GdB6 can efficiently capture thermal neutrons. Such combinations can optimize the neutron absorption dynamics of control rods while enhancing their durability in extreme environments.

V. SUMMARY In this study, the fast neutron shielding properties of se- lected boron compounds were evaluated using the Phy-X and NXcom programs to analyze their ΣR. The analysis of ΣR in relation to mass density, boron content, boron number den- sity, and the product of mass density and boron number den- sity revealed that mass density and boron number density are the primary factors influencing fast neutron shielding per- formance. Specifically, the ΣR values of boron compounds ranged from 0.082 cm−1 (KBH4) to 0.225 cm−1 (WB2), with mass density and boron number density identified as dom- inant factors. An exponential correlation was observed be- tween ΣR and the product of these two parameters, with WB2 (ρ=14.15 g/cm3, boron number density of 82.94 atoms/nm3) exhibiting the highest ΣR.

To assess the thermal neutron shielding behavior, the Σ val- ues were determined using both the MCNP5 simulation code and manual calculations. The results from these two methods show excellent agreement, with Σ varying from 23.98 cm−1 (BPE-5) to 4070.34 cm−1 (GdB6). GdB6 achieving excep- tional performance owing to the high absorption cross-section of 157Gd. In addition, the key factors affecting thermal neu- tron shielding, such as mass density, boron content, and boron number density, were systematically evaluated. The findings indicate that a higher boron number density correlates with superior Σ values, highlighting its critical role in enhanc- ing thermal neutron attenuation. The results also revealed that boron compounds with higher boron number densities, such as B4C (Σ=447.37 cm−1) and ZrB12 (Σ=474.67 cm−1), [1] M. Almatari, H.M.H. Zakaly, H.O. Tekin et al., Synthesis and characterization of B2O3-Bi2O3-SrO glasses for radiation shielding applications. Inorg. Chem. Commun. 164, 113993 (2025). doi:10.1016/j.inoche.2025.113993 [2] S.A. Tijani, K.A. Mahmoud, M.I. Sayyed et al., Radia- tion shielding properties of zinc borate glasses doped with heavy metal oxides. Mater. Chem. Phys. 307, 128672 (2023). doi:10.1016/j.matchemphys.2023.128672 [3] Y. Chen, L. Wang, X. Liu et al., Microstructure and radiation shielding properties of Gd2O3-doped boron Int. 50, 12345-12352 (2024). carbide ceramics. Ceram. demonstrated outstanding thermal neutron shielding perfor- mances, making them promising candidates for use as addi- tives in the development of advanced radiation-shielding materials.

Although Monte Carlo simulations provide a robust the- oretical framework for evaluating neutron shielding proper- ties, this study acknowledges the absence of experimental validation. To mitigate these limitations, the MCNP5 results were cross-validated with manual calculations, achieving ex- cellent agreement.

Therefore, future studies should prioritize experimental validation to improve accuracy, particularly for industrial-grade shielding composites.

In conclusion, this study systematically reveals the key factors affecting the neutron shielding performance of boron compounds and provides theoretical support for the engineer- ing applications of materials such as WB2, GdB6, B4C, and ZrB12. These findings can provide valuable guidance for fu- ture researchers in designing next-generation neutron shield- ing materials, such as composites, glasses, and ceramics. Fu- ture efforts should focus on optimizing the generation of sec- ondary particles resulting from neutron capture in these ma- terials and optimizing the elemental composition to minimize secondary gamma radiation. By addressing these challenges, boron-based materials can be further developed to meet the stringent demands of modern radiation protection, paving the way for the next generation of advanced shielding solutions.

VI. AUTHORS CONTRIBUTION Zhi-Cheng Qian was responsible for the writing, editing, and revising of the manuscript.

Jun Cai and Jin-Sen Xie contributed to the critical review and revision of the paper.

Chang-Yuan Li and Jian-Hua Wang conducted the method- ology design and investigation. Hui-Quan Li and De-Feng Chen performed data validation and analysis. Zhi-Hong Zhang and Xian-Wei Guo handled the software development and computational work.

VII. DECLARATIONS Conflict of interest The authors declare that they have no confict of interest. doi:10.1016/j.ceramint.2024.09.088 [4] R. Kumar, S.P. Singh, A. Kumar al., Neutron shielding performance of boron nitride reinforced alu- minum composites. J. Nucl. Mater. 568, 153619 (2022). doi:10.1016/j.jnucmat.2022.153619 [5] M.I. Sayyed, K.A. Mahmoud, S.A.M. Issa et al., Evaluation of gamma-ray and neutron shielding properties of B2O3-PbO2- Bi2O3 glasses. Radiat. Phys. Chem. 155, 281-286 (2018). doi:10.1016/j.radphyschem.2018.11.012 [6] H.O. Tekin, E. Kavaz, M.I. Sayyed, The investiga- tion of gamma-ray and neutron shielding parameters of Na2O-CaO-P2O5 glasses with varying boron con- tent. Radiat. Eff. Defects Solids 174, 951-964 (2019). doi:10.1080/10420150.2019.1674301 [7] M.G. Dong, X.X. Xue, V.P. Singh et al., Shielding effective- ness of boron-containing ores in Liaoning province of China against gamma rays and thermal neutrons. Nucl. Sci. Tech. 29, 58 (2018).doi:10.1007/s41365-018-0397-x [8] M. G. Dong, X.X. Xue, Y. Elmahroug et al., Investigation of shielding parameters of some boron containing resources for gamma ray and fast neutron. Results Phys. 13, 102129 (2019). doi:10.1016/j.rinp.2019.02.065 [9] E. Zorla, C. Ipbüker, A. Biland et al., Radiation shielding properties of high performance concrete reinforced with basalt fibers infused with natural and enriched boron. Nucl. Eng. Des. 313, 306-318 (2017). doi: 10.1016/j.nucengdes.2016.12.029 [10] H.L. Zhang, X.B. Zuo, Q. Q. Sun

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Note: Figure translations are in progress. See original paper for figures.