

THE ANALYSIS OF X/GAMMA-RAYS AND THERMAL NEUTRONS SHIELDING AND ELASTIC MODULI PROPERTIES OF BARIUM VANADIUM ZINC BORATE GLASS SERIES

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Abstract

The barium vanadium zinc borate glass series in compositions $x\text{BaO} : 30\text{V}_2\text{O}_3 : 10\text{ZnO} : (60-x)\text{B}_2\text{O}_3$ (where $x = 0, 10, 20, 30, 40$ and 50 mol%) have been simulated and analyzed on their X/gamma-rays shielding and elastic moduli properties. The X/gamma-rays and thermal neutrons shielding properties were simulated using the FLUKA Monte Carlo code. The results of gamma-rays shielding were compared with the results from WinXCom. The Makishima-Makinzie model was used to determine the elastic moduli properties of the glass series. The results found that the increasing BaO concentration by replacing B_2O_3 which causes the density to increase and improved X/gamma-rays shielding properties. Whereas the result for thermal neutrons shielding and elastic moduli properties decreased with increasing BaO content. The results of this study are useful in enhancing the efficiency of materials for shielding X/gamma-rays.

Keywords: X/gamma-Rays; Thermal Neutrons; Elastic Moduli

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Introduction

The use of ionizing radiation has grown dramatically in sectors such as geology, agriculture, space exploration, medicine, archaeology, and so on (Benson, 2002; Singh *et al.*, 2014; Tijani *et al.*, 2018; Power *et al.*, 2022; Tamal *et al.*, 2022). Ionizing radiation, such as X/gamma rays, and neutrons, can cause cancer, genetic damage, and tissue destruction in humans (Cucinotta *et al.*, 2001; Al-Buriahi *et al.*, 2022). As a result, during the last decade, glass, one of the materials used to protect radiation, has become the most essential alternative for the safety of persons and ecosystems exposed to harmful rays. Glass, as one of the inorganic materials studied and developed for cutting-edge material science, is therefore widely used in advanced technology in our daily life (Hrabovsky *et al.*, 2022). Borate glasses have various applications when compared to other forms of glass, and they are particularly excellent as radiation shielding materials (Sallam *et al.*, 2020; Sayyed, 2022; Sayyed *et al.*, 2023). This is owing to the unique features of boron oxide when hosted in a glass matrix, which results in a glass system with improved optical, mechanical, chemical, and physical capabilities (Elkelany *et al.*, 2021; Sayyed, 2022). When BaO is mixed with B₂O₃, barium borate glass is created, this will result in improved properties of this glass system, especially in optical and radiation shielding (Sayyed *et al.*, 2019; Sayyed *et al.*, 2020). When V₂O₅ is mixed with B₂O₃, borovanadate glass is generated, which is a mixed network of the former. The role of vanadium, on the other hand, is proportional to its concentration (Mohamed and Yahya, 2018). Adding the appropriate quantity of vanadium to a glass system improves its structural and physical qualities (Kosuge, 1967; Guo *et al.*, 2020). ZnO can act as a modifier or network former in the glass structure. ZnO is well-known for its low cost, non-toxicity, and environmental acceptability (Du and Ilegbusi, 2004; Klink and Crouch, 2009; Sumalatha *et al.*, 2013).

FLUKA is a Monte Carlo code that was created to investigate the radiation shielding capabilities of various materials used in radiation applications (Pires and Medhat, 2016; Canel *et al.*, 2019). Although the scientific results obtained from these experiments are valuable and reliable, the expense of the equipment, the difficulty in getting the radiation source, and numerous constraints are important in examining the radiation shielding properties. Monte Carlo simulations can help to reduce the aforementioned constraints and issues, as well as the time and radiation exposure of those

participating (Pires and Medhat, 2016). The key advantage of the simulation approach is that it generates theoretical data for the experiment's variable geometry and a number of primary radiations to test the feasibility of certain experimental observations.

The xBaO: 30V₂O₅: 10ZnO: (60-x)B₂O₃ glass series will be examined for its X/gamma-rays shielding properties by FLUKA simulation. Gamma rays with energy ranging from 59.54-662 keV and X-rays with energy ranging from 60-120 kVp were studied. The major characteristics to be investigated are the mass attenuation coefficient, half value layer, mean free path, and percent radiation transmittance. Furthermore, the glass samples' radiation shielding properties are compared to standard radiation shielding materials. Also, elastic moduli for glass series are discussed.

Theory and Determination

The density (ρ ; g/cm³) of glass series is a parameter used to explained the structural changes of glass and can be determined in Equation (1) (Samdani *et al.*, 2022; Ravangvong *et al.*, 2023):

$$\rho = (0.53) \frac{(\sum M_i x_i)}{(\sum V_i x_i)} \quad (1)$$

here M_i , V_i and x_i are molecular weight, packing density factor, and molar fraction of i^{th} component, respectively.

The mass attenuation coefficients (MAC) express the probability of interaction of X/gamma-rays with the interacting medium. The MAC of the glass series was derived from WinXCom software for X/gamma-rays energy range 59.54-662 keV using the following Equation (2) (Ravangvong *et al.*, 2023):

$$MAC = \sum_i w_i (\mu_m)_i \quad (2)$$

here $(\mu_m)_i$ and w_i are the mass attenuation coefficient and weight fraction of the i^{th} element in the mixture.

Half value layer (HVL) means as the thickness of the sample that reduces the intensity of X/gamma-rays (I) to 50% of its initial intensity (I_0) and can be calculated from equation the linear attenuation coefficient (μ) by using in Equation (3) (Sayyed *et al.*, 2020; Ravangvong *et al.*, 2023):

$$HVL = \frac{0.693}{\mu} \quad (3)$$

Mean free path (MFP) is average distance between two successive interactions of X/gamma-rays in medium and simulated from Equation (4) (Samdani *et al.*, 2022; Ravangvong *et al.*, 2023):

$$MFP = \frac{1}{\mu} \quad (4)$$

The transmission factor (TF) is a value using estimates the coefficient of X-rays transport through a specific thickness of materials as can be calculated using the Equation (5) (Hanfi *et al.*, 2023):

$$TF = \frac{I}{I_0} \times 100 = e^{-\mu x} \quad (5)$$

Maskishima and Mackenzie have been calculated elastic moduli (EM) such as Young's modulus (E), Bulk (K), Shear modulus (G) and Longitudinal modulus (L) of oxide glasses by theoretically model (M-M model) base on chemical component, packing density (V_t) and dissociation energy per unit volume (G_t) of glasses as following (Ravangvong *et al.*, 2023):

$$E = 8.36V_tG_t \quad (6)$$

$$K = 10V_t^2G_t \quad (7)$$

$$G = \frac{30V_t^2G_t}{(10.2V_t-1)} \quad (8)$$

$$L = K + \left(\frac{4}{3}\right)G \quad (9)$$

Simulation Determination

The theoretical glass series for this work, the BaO based on V_2O_5 : ZnO: B_2O_3 in formula $x\text{BaO}$: $30V_2O_5$: 10ZnO : $(60-x)\text{B}_2\text{O}_3$ (x increased from 0-50 mol% in 10 mol% increments) has been illustrated in Table 1.

FLUKA Monte Carlo is a coding using for high energy simulation in particle-nuclear sciences and engineering shielding. In this work, the FLUKA version 2011.2x-4 with schematic set up for simulate X/gamma-rays and thermal neutrons are exhibited in Figure 1 and Figure 2. The simulation for μ and MAC of material samples with thickness (x) can be estimated using Equation (10) and Equation (11), respectively (Kumar, 2017; Alzahrani *et al.*, 2023; Sriwongsa *et al.*, 2023):

$$I = I_0 e^{-\mu x} \quad (10)$$

$$MAC = \frac{\ln(I_0/I)}{\rho x} \quad (11)$$

Table 1. The chemical composition, density and molar volume for glass series (mol%)

Elements	Glass code (mol%)					
	BVZ1	BVZ2	BVZ3	BVZ4	BVZ5	BVZ6
BaO	0	10	20	30	40	50
V_2O_5	30	30	30	30	30	30
ZnO	10	10	10	10	10	10
B_2O_3	60	50	40	30	20	10
Density (ρ , g/cm ³)	3.0343	3.3155	3.6032	3.8978	4.1995	4.5086

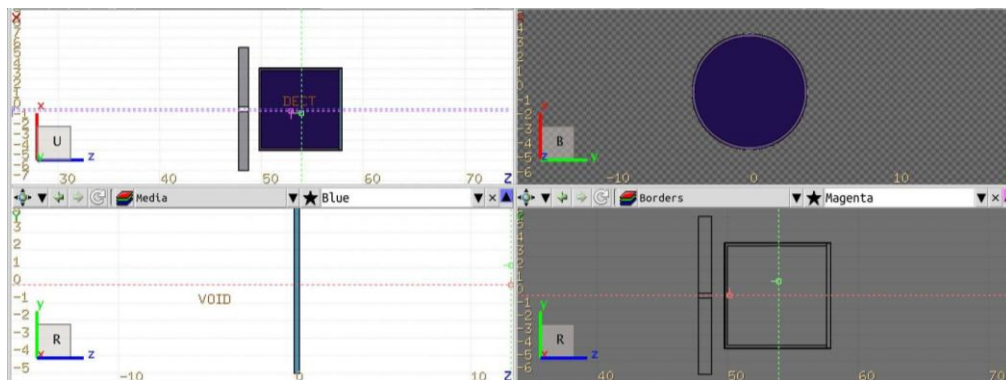


Figure 1. The schematic set up to simulate X/gamma-rays

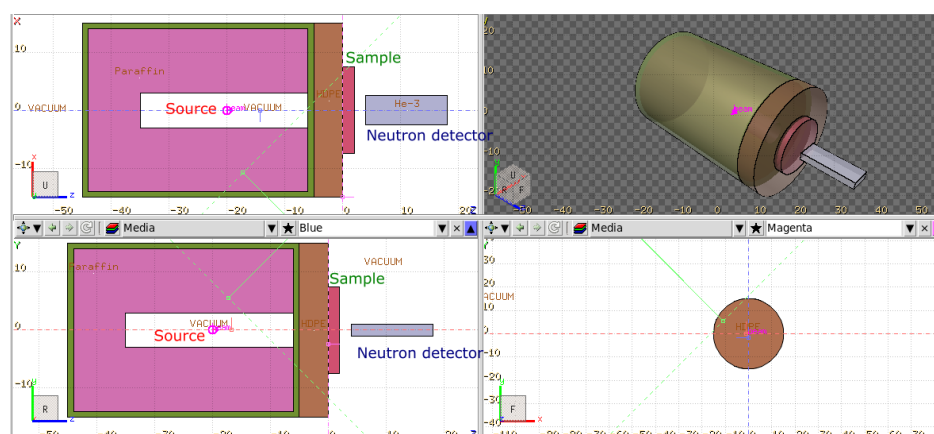


Figure 2. The schematic set up to simulate thermal neutrons

Results and Discussions

The densities and molar volume of glass series were illustrated in Figure 3. It was found that the densities of glass series were increased with increasing BaO content due to the replacement of BaO with higher density and molecular weight than B_2O_3 . That indicated the presence of Ba^{2+} ions were changed borate glass network by converting more $[BO_3]^{-3}$ triangles to BO_4 tetrahedral (Limkitjaroenporn *et al.*, 2011; Elkhoshkhany *et al.*, 2018; Glumglomchit *et al.*, 2018; Sriwongsa *et al.*, 2023).

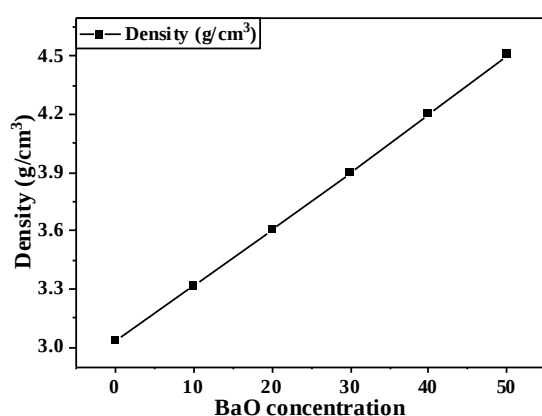


Figure 3. The density for glass series

X/gamma-rays shielding

The mass attenuation coefficient (MAC) for glass series have been simulated X and gamma-rays at energy range 60-120 kVp and 59.6-662 keV, respective. The ^{241}Am (59.6 keV), ^{133}Ba (81, 356, 161 and 384 keV), ^{152}Eu (122 and 245 keV), ^{22}Na (511 keV), and ^{137}Cs (662 keV) were used for

gamma-rays energy sources. The MAC for gamma-rays with both of the FLUKA simulation and WinXCom program for theoretical. The MAC values for X and gamma-rays were enlisted in Figure 4 and Figure 5, respectively. The results found that the MAC for X and gamma-rays were increased with increasing BaO content and BVZ6 had the highest MAC value due to this sample had the largest BaO content and the highest density. While the MAC values for both rays decreased with increasing energy because the photoelectric effect (PE) is the main process which they cross section varies with $E^{-3.5}$ and $Z^{4.5}$. This reflected that at low X and gamma-rays energy, both-rays were attenuated higher than at high energy and the probability of X and gamma-rays attenuation increased with increasing BaO content. In addition, the simulation values of MAC are in good agreement with the theoretical values (Agar *et al.*, 2019; Sayyed *et al.*, 2019).

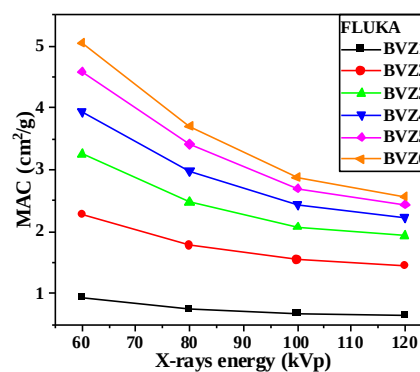


Figure 4 MAC with X-rays energy

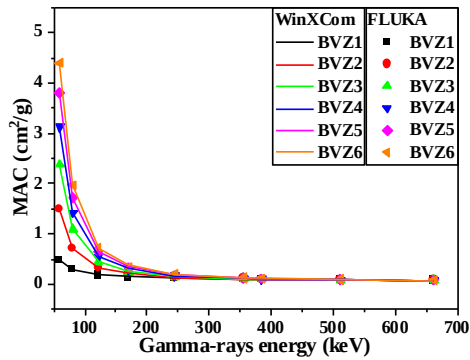


Figure 5 MAC with gamma-rays energy

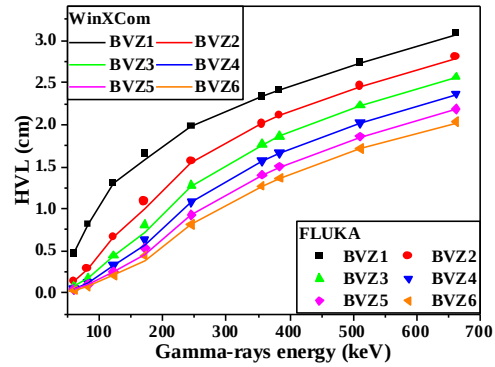


Figure 7 HVL with gamma-rays energy

Half value layers (HVL) evaluate the length of the substance necessary to reduce X/gamma-rays energy to half tenth of their initial levels. While the MFP parameter is the distance traveled by the incident X/gamma-rays energy intrant the material of the samples before the collision. For the HVL and MFP with X and gamma-rays energy for glass series as shown in Figure 6 - Figure 9. It found that the HVL and MFP for BVZ6 glass sample increased with increasing energy. It means that at high X and gamma-rays energy, both-rays can more penetrating as reflected the material need more thickness to attenuated them. And the HVL and MFP for BVZ6 glass sample is the lowest value due to this sample had the highest density. It indicated that BVZ6 glass samples had excellent X and gamma-rays shielding (Agar *et al.*, 2019; Sayyed *et al.*, 2019; Sriwongsa *et al.*, 2023).

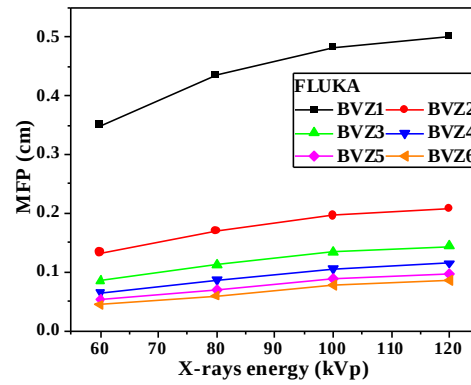


Figure 8 MFP with X-rays energy

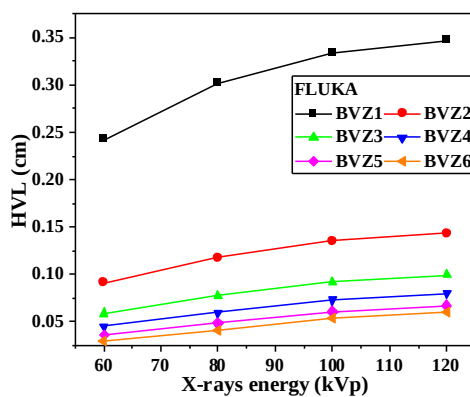


Figure 6 HVL with X-rays energy

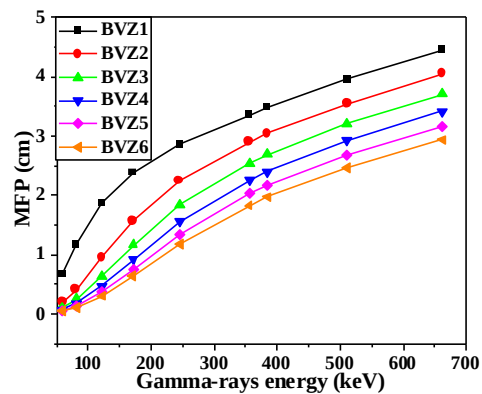


Figure 9 MFP with gamma-rays energy

HVL has been compared between glass series and some standard shielding materials for X and gamma-rays at 120 kVp and 662 keV as exhibited in Figure 10 and Figure 11, respectively. They were found that BVZ glass series had X-rays shielding property better than commercial glass, red brick, concrete and X-ray window at starting 10 mol% of BaO content. While gamma-rays shielding property, the BVZ glass series has been found to have better shielding properties than commercial window glass, ordinary concrete and hematite-serpentine (Kumar, 2017; Kaewjaeng *et al.*, 2021(a); Sriwongsa *et al.*, 2023).

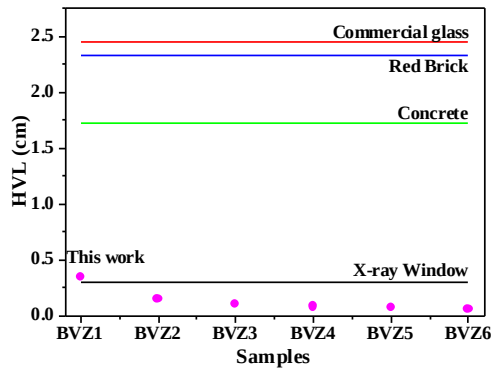


Figure 10 HVL with some standard materials for X-rays

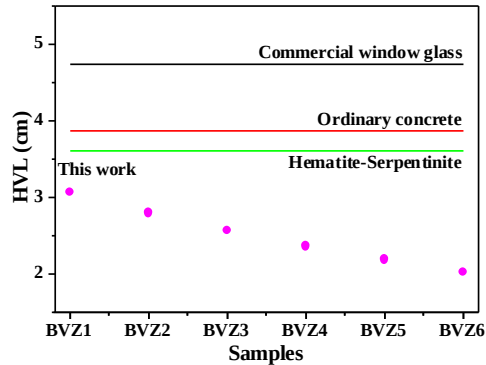


Figure 11 HVL with some standard materials for gamma-rays

The transmission factor (TF) is parameter related to the X and gamma-rays penetration which evaluated based on the glass thickness and the MAC of glass series. Figure 12 and Figure 13 clarifies the change in TF with the X and gamma-rays energy

for BVZ glass series. It found that the TF increased with increasing for both-rays energy and decreased with increasing BaO content. This event due to PE is main process and involved the loss of X and gamma-rays energy which had enough energy to escaped from glass thickness. In addition, BVZ6 glass sample had the lowest TF value. It reflected that BVZ6 glass sample was superb X and gamma-rays shielding (Al-Saeedi *et al.*, 2022).

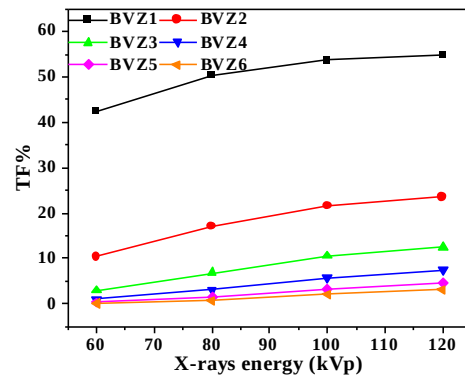


Figure 12 TF% with X-rays energy

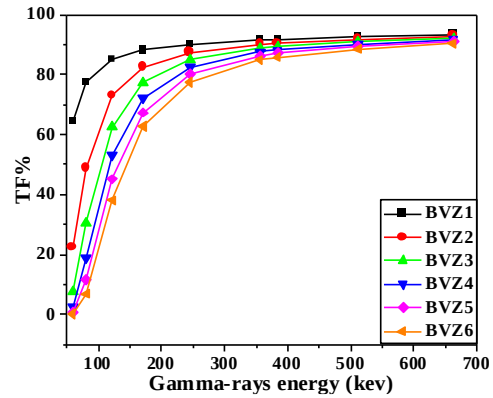


Figure 13 TF% gamma-rays energy

Thermal neutrons shielding

The thermal neutrons simulation has been estimated the numbers 10^8 of thermal neutrons which is a large enough value for studying trend values and the simulation for μ and MAC of material samples with thickness (x) can be estimated using equation (10) and equation (11), respectively (Kumar, 2017; Sriwongsa *et al.*, 2023; Alzahrani *et al.*, 2023; Battistoni, *et al.*, 2016). The relationship between the MAC for thermal neutrons

and BaO content as exhibited in Figure 14. The trend of MAC value decreased with increasing BaO content. It indicated that thermal neutrons shielding property is being decreased at high BaO content (Kaewjaeng *et al.*, 2021(b)). This event because of absorption cross-section (σ_{abs}) for B (767 barn) higher than Ba (1.1 barn) (Sears, 1992; Tiamduangtawan *et al.*, 2020).

Elastic Moduli

The EM for BVZ glass series has been exhibited in Figure 15. These EM (E, K, G and L) values for glass series decreased with increasing of BaO content. The obtained results can be linked to having lower dissociation energy (G_i) and packing density (V_i) of BaO (39.5×10^9 J/m³ and 13.3×10^{-6} m³/mol) than B₂O₃ (82.8×10^9 J/m³ and 20.8×10^{-6} m³/mol). These results lead to the strength of BVZ glass series is being attenuated at high BaO content (Inaba *et al.*, 2003; El-bashir *et al.*, 2017).

The comparison EM for BVZ glass series with 80NaPO₃-20MoO₃ and 80NaPO₃-20WO₃ as exhibited in Figure 16. It was found that E and G values for BVZ1-5 glass samples were higher than 80NaPO₃-20MoO₃ and 80NaPO₃-20WO₃. While K and L values for all glass samples were higher than 80NaPO₃-20MoO₃ and 80NaPO₃-20WO₃. These results indicated that BVZ glass series had EM properties better than 80NaPO₃-20MoO₃ and 80NaPO₃-20WO₃ (Afaneh *et al.*, 2022).

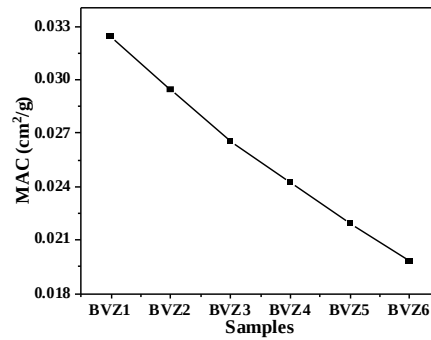


Figure 14 MAC of thermal neutrons for BVZ glass series

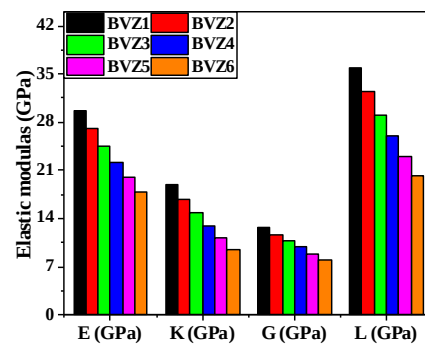


Figure 15 The elastic moduli for BVZ glass series

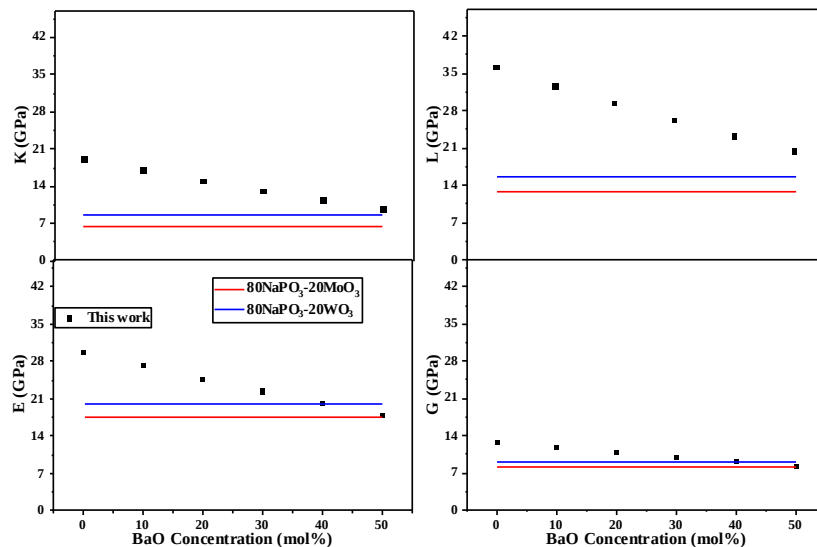


Figure 6 HVL with X-rays energy

Conclusions

The X/gamma-rays, thermal neutrons shielding and elastic moduli properties of the V_2O_3 : ZnO: B_2O_3 glass series have been simulated and analyzed the effect of BaO addition in the borate glass structure in formula $x\text{BaO} : 30V_2O_3 : 10ZnO : (60-x)B_2O_3$ (where $x = 0, 10, 20, 30, 40$ and 50 mol%). The densities calculation shows increased trend with an increasing of BaO content due to BaO had higher density and molecular weight than B_2O_3 . Besides, the X/gamma-rays and thermal neutrons shielding properties of the BVZ glass series have been simulated using FLUKA Monte Carlo code. The results of X and gamma-rays shielding were compared with the results from WinXCom. The addition of BaO content causes an increase in mass attenuation coefficient, while the half value layer, mean free path and transmission factor were decreased. In addition, the HVL has been compared between glass series and some standard shielding materials for X and gamma-rays. They were found that BVZ glass series had X and gamma-rays shielding property better than with some standard shielding materials. It indicated that BVZ6 glass samples had excellent X and gamma-rays shielding. Whereas the thermal neutrons shielding, the opposite was true. And the increasing BaO content were results in the EM (E, K, G and L) which led to the strength of BVZ glass series is being attenuated at high BaO content.

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