ARTICLE IN PRESS

Journal of Non-Crystalline Solids xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Journal of Non-Crystalline Solids

journal homepage: www.elsevier.com/locate/jnoncrysol

Investigation of gamma radiation shielding properties of lithium zinc bismuth borate glasses using XCOM program and MCNP5 code

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ARTICLE INFO

Keywords:
Bi_2O_3-B_2O_3-ZnO-Li_2O glasses
XCOM
MCNP5
Radiation shielding
Mass attenuation coefficient
Mean free path

ABSTRACT

In this work, we examined the usefulness of the lithium zinc bismuth borate glass systems for various radiation shielding applications and for this purpose, the mass attenuation coefficients for the glasses in the composition 50 Bi_2O_3–15 B_2O_3–(35-x) ZnO–(x) Li_2O (x = 0, 5, 10, 15, 20 mol%) were calculated by both XCOM software and MCNP5 simulation code, respectively, within the energy range 0.015 MeV–10 MeV. The obtained results indicated good agreement between mass attenuation coefficient values derived from XCOM program and MCNP5 code. The obtained mass attenuation coefficients are then used to calculate the effective atomic number (Z_{eff}), half value layer (HVL) and mean free path (MFP) for the glasses. Among the selected glasses, the glass with 35 mol% ZnO was found to possess superior gamma-ray shielding effectiveness due to its higher values of both mass attenuation coefficient and effective atomic number and lower values of both HVL and MFP. The MFP values of the present glasses were compared with different glass systems and ordinary concrete. In addition, the macroscopic effective removal cross-section for fast neutron (Σ_R) values was also evaluated. It is found that the Σ_R values for the studied glasses lie within the range 0.1286–0.1587 cm^{-1}.

1. Introduction

Optically transparent glasses have recently gained tremendous interest among researchers because of their potential applications in neutron and γ-ray radiation-shielding materials instead of concrete that is currently in use as a traditional radiation shielding material [1–5]. Though concrete (opaque to visible light) is effective for shielding γ-radiations due to its dense, complex, and heterogeneous microstructure when it is exposed to the γ-radiations for longer periods of time its mechanical strength can be reduced. On the contrary, glasses with adjustable physical, thermal and chemical properties allow visibility while absorbing harmful radiations like gamma-rays and neutrons, thereby ensuring the protection of workers [1–7].

Heavy metal oxide (HMO) such as lead oxide (PbO) glasses have been restricted in various practical applications as they have some harmful effects on human health and surrounding environment [8]. Thus, very recently, there has been an increasing interest regarding the synthesis of HMO glasses like bismuth oxide (Bi_2O_3) containing glasses instead of PbO, for radiation shielding applications because of their unique properties, such as non-toxicity, high density, high refractive index, long infrared cut-off wavelengths, high third-order nonlinear optical susceptibility, high radioactive resistance and moisture resistance etc. [4,6,9]. Bi^{3+} ion has high density and high effective atomic number Z_{eff}, but possesses small field strength, so it cannot form a glass, by itself. However, Bi_2O_3 can occupy both network-forming and network modifying positions depending on its concentration in the glass composition. Therefore, Bi_2O_3-based glasses are excellent candidates for radiation detection in high energy and nuclear physics, medical imaging and homeland security [4,6,7,9–11].

Compared to various oxide glasses such as silicates, phosphates etc., borate glasses can be synthesized at lower melting temperatures with near-ultraviolet to the near-infrared optical transparency (∼300 nm to ∼2.5 μm) and show higher bond strength and high thermal stability [12,13]. Also, in borate glasses, various complex structural units like diborate, triborate, tetraborate and pentaborate exist due to the formation of BO_4 tetrahedral units (non-bridging oxygens) and BO_3 triangular units. It is also well known that the structure of vitreous B_2O_3 consists of a random network of boroxyl rings and BO_3 triangles

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http://dx.doi.org/10.1016/j.jnoncrysol.2017.04.018
Received 16 March 2017; Received in revised form 15 April 2017; Accepted 18 April 2017

connected by B–O–B linkages [12,13]. It was evident that the addition of ZnO in glasses causes low rates of crystallization, lower melting temperature and enhances the glass forming region [14]. Li_2O, an alkali metal oxide, acts as a modifier in glasses and changes the glass network structure by creating nonbridging oxygens (NBOs). Furthermore, increasing amount of Li_2O creates more NBOs in the glass structure [15,16].

Usually, the mass attenuation coefficient (μ/ρ), mean free path (MFP), half value layer (HVL), effective atomic number (Z_{eff}) and electron density (N_e) are the important parameters in order to evaluate the interaction of γ-rays with shielding materials. In this work, for Bi_2O_3-B_2O_3-ZnO-Li_2O glasses, by using XCOM program we report the γ-ray shielding parameters such as μ/ρ, Z_{eff}, HVL, MFP, and macroscopic effective removal cross-section values for fast neutrons for their potential application in γ-ray and neutron detectors. In addition, the μ/ρ values of the present glasses were calculated using MCNP5 code and compared with XCOM results. The density values of the glasses with the chemical composition of 50 Bi_2O_3–15 B_2O_3–(35-x) ZnO–(x) Li_2O (x = 0, 5, 10, 15, 20 mol%) were adopted from Ref. [17].

2. Radiation shielding parameters-theoretical basis and method of computation

The glasses were synthesized by the conventional melt-quenching method at 1100–1200 °C. The density (ρ) of the glasses was calculated using Archimedes principle, by using xylene (ρ = 0.86 g/cm^3) as the immersion liquid and compared with the theoretical values. Table 1 presents the nominal composition of the glasses along with their calculated and theoretical density values [17].

2.1. Mass attenuation coefficient

The mass attenuation coefficient (μ/ρ) values of the Bi_2O_3-B_2O_3-ZnO-Li_2O glasses were calculated by applying mixture rule ($(\mu/\rho)_{glass} = \sum_i^n w_i (\mu/\rho)_i$) where w_i is the proportion by weight and $(\mu/\rho)_i$ is mass attenuation coefficient of the ith element obtained by using XCOM software [18]. The μ/ρ values of the glasses were evaluated by the transmission method according to Lambert-Beer's law ($I = I_0 e^{-\mu t}$), where I_0 is incident photon intensity and 'I' is the attenuated photon intensity, μ (cm^{-1}) is the linear attenuation coefficient and 't' is the mass thickness of the slab. Depending on the application of radiation shielding materials, the study of the photon energy range will be varied. For the studied glasses possible application in gamma ray-shielding, up to 10 MeV photon energy ranges sufficient to evaluate, so we did calculations in the range, 0.015 MeV–10 MeV.

2.2. Effective atomic number (Z_{eff})

The effective atomic number (Z_{eff}) indicates that the gamma-ray attenuation in the material is related to the interaction of radiations with matter. The effective atomic number is the ratio between the total atomic effective cross-section and the total electronic effective cross-section as given below [19]:

Table 1
Nominal composition of the studied glasses (mol%) and their density values [17].

Sample code	B_2O_3	Bi_2O_3	ZnO	Li_2O	Density (g/cm^3) theoretical	Density (g/cm^3) calculated
A	15	50	35	0	6.79	5.98
B	15	50	30	5	6.61	5.83
C	15	50	25	10	6.44	5.66
D	15	50	20	15	6.26	5.56
E	15	50	15	20	6.08	5.45

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad (1)$$

The mass attenuation coefficient can be used to evaluate the total atomic cross-section (σ_a) using the following equation [19]:

$$\sigma_a = \frac{\mu/\rho}{N_A \sum_i \frac{w_i}{A_i}} \quad (2)$$

where A_i is the atomic weight of element i, and N_A is the Avogadro constant.

In addition, the total electronic cross-section, (σ_e), is expressed by the following equation [19]:

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} \left(\frac{\mu}{\rho}\right)_i \quad (3)$$

where f_i denotes the fractional abundance of the element i and Z_i the atomic number of the ith element.

2.3. Half-value layer

It is useful to express the attenuation of gamma-ray in terms of another quantity which is the half-value layer (HVL). The HVL is the thickness, at which the transmitted intensity is 50% of the initial intensity. The HVL reflects the fact that energetic photons have a capability to penetrate the material as photon energy increases. The HVL for the present glasses can be calculated using the following relation [20]:

$$HVL = \frac{In(2)}{\mu} \quad (4)$$

where μ is the linear attenuation coefficient (which is equal to the multiplication of μ/ρ and density of the glass).

2.4. Mean free path

In addition, the mean free path (MFP) of the present glasses can be calculated according to the equation [21]:

$$MFP = \frac{1}{\mu} \quad (5)$$

2.5. Macroscopic effective removal cross sections for fast neutrons (Σ_R)

On the other hand, the macroscopic effective removal cross section for fast neutrons (Σ_R) is the probability of a neutron undergoing specific reaction per unit length of moving through the shielding material [22]. Σ_R values in the present glasses can be evaluated by utilizing the following equation [23]:

$$\sum_R = \sum_i W_i (\sum_R / \rho)_i \quad (6)$$

where $\Sigma_{R/\rho}$ (cm^2/g) and W_i represent the mass removal cross-section of the ith constituent and the partial density (g/cm^3) respectively.

In this work, MCNP5 code created by the Los Alamos National Laboratory, USA was utilized for the simulation of (μ/ρ) of the present glasses as targeted materials. It is well known that MCNP5 is a general-purpose Monte Carlo N-Particle code and can be used for modeling the radiation transport for the interaction of gamma ray, X-ray, electrons or neutron radiation with the matter.

3. Results and discussion

To study the shielding properties of glasses in the composition 50 Bi_2O_3–15 B_2O_3–(35-x) ZnO–(x) Li_2O (x = 0 (glass A), 5 (glass B), 10 (glass C), 15 (glass D), 20 (glass E) mol%), the mass attenuation coefficients (μ/ρ) in the energy range 0.015 MeV to 10 MeV were