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Calculations on Linear Attenuation Coefficient and Fast Neutron Removal Cross-section for B_2O_3-TeO_2 Glass System via Phy-X/PSD

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Abstract

With the increase of irradiation emitted from high-technology applications, the scientific community has intensively concentrated to develop radiation protection materials, recently. In this study, we aimed at investigating the borotellurite (BT) system as a potential radiation shielding glass in X-rays applications. For this, xB_2O_3 - $(100\text{-}x)TeO_2$ system (x: 5 to 25 mol% with a step of 5) was designed to understand the variations in radiation shielding characteristics (Ba-133) using Phy-X/PSD software. Further, some physical property calculations such as average molecular weight ($M_{average}$) and glass density (ρ_{glass}) were carried out. The radiation shielding computations clearly showed that the linear attenuation coefficient (*LAC*) decreased against the increasing photon energy for all glass series. In detail, the *LAC* was found to be in a decreasing trend as B_2O_3 replaced TeO_2 in the glass network. On the other hand, fast neutron removal cross-section (FNRCS) results demonstrated that the insertion of B_2O_3 led to an improvement in neutron attenuation. That is, FNRCS for BT5 to BT25 samples were equal to 0.1071, 0.1074, 0.1077, 0.1080, and 0.1083 1/cm in the respective order. Lastly, the addition of B_2O_3 from 5 to 25 mol% caused $M_{average}$ and ρ_{glass} to decrease from 155.1 to 137.1 g.mol^{-1} and from 5.5095 to 4.8675 g.cm^{-3}, respectively. In summary, this study signified that adding B_2O_3 in replacement for TeO_2 could diminish photon shielding competencies, but enhanced neutron attenuation characteristics.

Phy-X/PSD ile B_2O_3-TeO_2 Cam Sistemi için Lineer Zayıflama Katsayısı ve Hızlı Nötron Giderme Kesiti Hesaplamaları

Özet

Yüksek teknoloji uygulamalarından yayılan radyasyonun artmasıyla birlikte, bilim camiası son zamanlarda radyasyondan korunma malzemeleri geliştirmeye yoğun bir şekilde odaklanmıştır. Bu çalışmada, X-ışınları uygulamalarında potansiyel bir radyasyon koruyucu cam olarak borotellürit (BT) sistemini araştırmayı amaçladık. Bunun için xB_2O_3 - $(100\text{-}x)TeO_2$ sistemi (x: 5'lik bir adımla % 5 ila 25 mol) Phy-X/PSD yazılımı kullanılarak radyasyon kalkanı özelliklerindeki (Ba-133) varyasyonları anlamak için tasarlanmıştır. Ayrıca ortalama moleküler ağırlık (M_{Ort}) ve cam yoğunluğu (ρ_{cam}) gibi bazı fiziksel özellik hesaplamaları yapılmıştır. Radyasyon kalkanı hesaplamaları, tüm cam serileri için artan foton enerjisine karşı lineer zayıflama katsayısının (*LAC*) azaldığını açıkça göstermiştir. Ayrıntılı olarak, cam ağda B_2O_3 içeriğinin TeO2'nin yerini aldığından *LAC* parametresinin azalma eğiliminde olduğu bulundu. Öte yandan, hızlı nötron giderme kesiti (FNRCS) sonuçları, B_2O_3'ün eklenmesinin nötron zayıflamasında bir iyileşmeye yol açtığını göstermiştir. Yani BT5 ila BT25 numuneleri için FNRCS, ilgili sırayla 0.1071, 0.1074, 0.1077, 0.180 ve 0.1083 1/cm'ye eşittir. Son olarak, B_2O_3 içeriğinin molce %5'ten %25'e eklenmesi, M_{Ort} ve ρ_{cam} parametrelerinin sırasıyla 155.1'den 137.1 g.mol^{-1}'e ve 5.5095'ten 4.8675 g.cm^{-3}'e düşmesine neden oldu. Özetle, bu çalışma TeO_2'nin yerine B_2O_3 eklenmesinin foton koruma yeterliliklerini azaltabileceğini, ancak nötron zayıflama özelliklerini artırabileceğini gösterdi.

1. INTRODUCTION

In parallel to the developments in medical applications, many benefits have been brought to humankind. The progression in diagnosis, monitoring, and treatment activities, though, offer better life quality.[1,2] Despite great advancements, people have been at risk in subjection to the equipment and/or devices used. Namely, irradiations emitted from high-energy-capable devices such as X-rays, mammography, or bone densitometry have a strong probability to damage surrounding people.[3,4] This damage may vary with respect to dose, time, or distance, nevertheless, skin burns, eye-driage, or harming on living tissues can be regarded as possible health problems.[5,6] To cope with negative consequences, the presence of a radiation protection material has strongly been recommended by the scientific community. Such a protection material can be placed around the surrounding area so that the photon energy can effectively be attenuated to some extent. Therefore, the utilization of a radiation shielding material in these applications has become a must, and thus definite standards have been put forward.

Although alternative materials such as metallic lead[7], concretes[8], or polymers[9] have prevalently been preferred in accordance with standards, they become insufficient if a transparent appearance is of interest. In medical applications, the rooms where those devices are placed must have an observation window in order to follow patients outside.[10] Hence, glass materials having a transparent feature have become an indispensable choice, in this regard. In addition to the transparency, glass materials have a chance of recycling/reusing, diverse compositional ranges, superior optical and thermal properties, and different production techniques.[11,12] For the mentioned reasons, using glass materials in radiation shielding applications seems to be very suitable for gaining more performance.

In very recent times, researchers have extensively centered on different glass systems for medical diagnostic energy levels (eg. 100 keV). The literature studies have mainly investigated silicates, borates, phosphates, and chalcogenides to find out high-performance attenuation characteristics against incoming photon energies.[13,14] In these studies, experimental (eg. narrow-beam setup), theoretical (eg. XCOM), and simulation (eg. MCNP) attempts have been performed on the intended glass systems to reveal the variations in photon and/or neutron attenuation properties.[15,16] In comparison to the given glass types, tellurite (TeO_2)-based glass systems attract many researchers owing to their opportunity for high ion solubility, great linear and non-linear optical features, and high-density properties.[17,18] Yet more, ensuring high-density is an essential concept, this is because the increasing glass density leads to the obtainment of higher attenuation competencies. In the case of inserting boron oxide (B_2O_3), which enables the enhancement of physical, mechanical, and thermal properties, borotellurite (BT) glass system, has become usable against both photon and neutron shielding purposes.[19] Most especially, the impact of adding boron atoms within a glass network attenuates more neutrons in comparison to high-radii elements. To the best of our knowledge, borotellurite glass system has been tried to be understood in different aspects such as thermal and structure, however, the gap in literature in terms of borotellurite glass system's behaviour against high photon and neutron energies has still require valuable attempts for better understanding.[20-22] With the given reasons, the authors strongly believes that the BT glass system can be understood so as to achieve better performance in radiation protection applications.

Within the present theoretical work, we explored the borotellurite glass system by designing the following glass composition: $xB_2O_3 + (100-x)TeO_2$ where x equals 5 to 25 mol% with a step of 5. To the best of our knowledge, these ratios have not been studied nor reported in the literature within the scope of radiation shielding applications. The designed glass series, BT5 to BT25, was then defined to the user-friendly software, Phy-X/PSD, to compute photon and neutron shielding properties at Ba-133 radioactive source energies. As a result of calculations, the significant parameters as linear attenuation coefficient (*LAC*) and fast neutrons removal cross-section (FNRCS) were evaluated. The influence of inserting B_2O_3 into the borotellurite glass system was discussed and reported in the upcoming titles.

The behavior of borotellurite glass system against high photon and neutron energies was theoretically investigated in this study using Phy-X/PSD software. The effect of insertion of B_2O_3 into the borotellurite glass system on the linear attenuation coefficient (*LAC*) and fast neutrons removal cross-section (FNRCS) were specifically evaluated in detail.

2. MATERIALS & METHODS

The present study mainly focused on the impact of B_2O_3 on borotellurite (BT) glass systems in terms of theoretical radiation shielding properties and physical features. For this purpose, Table 1 lists the batch designs and the corresponding codes for the samples. After that, we performed theoretical computations on photon and neutron shielding characteristics with the use of newly-developed user-friendly Phy-X/PSD software.[23] In this software, glass compositions in mol% are simply defined and their theoretical glass density values are inserted. Once these are completed, the intended photon energies are selected followed by providing computations begin. Here, the most important parameter, linear attenuation coefficient (*LAC*), is calculated by using Equation 1.

$$\frac{I}{I_o} = \exp(-\mu x) \tag{1}$$

where I, I_0, μ, and x signify transmitted photon energy, incoming photon energy, linear attenuation coefficient (*LAC*), and thickness, respectively.

Table 1. Batch designs and the corresponding sample codes.

Code	B_2O_3 (mol%)	TeO_2 (mol%)
BT5	5	95
BT10	10	90
BT15	15	85
BT20	20	80
BT25	25	75

Equation 2 is applied to calculate the fast neutrons removal cross-section (*FNRCS*).

$$FNRCS = \sum_i \rho_i \, (FNRCS/\rho)_i \tag{2}$$

where ρ_i and $(FNRCS/\rho)_i$ define partial density and mass removal cross section.

Lastly, we used Equation 3 and Equation 4 for calculating average molecular weight ($M_{average}$) and glass density (ρ_{glass}), respectively.

$$M_{average} = \sum M_i . x_i \quad (3)$$

where M_i is the molecular weight of the i^{th} constituent and x_i is the molar fraction of the i^{th} constituent.

$$\rho_{glass} = \frac{1}{\sum v_i . f_i} \quad (4)$$

where v_i is the specific volume of 1 g of the i^{th} constituent and f_i is the weight fraction of the i^{th} constituent.

3. RESULTS AND DISCUSSION

In radiation shielding applications, it is critical to figure out the glass density values. This is because the increasing glass density paved the way for the enhanced radiation attenuation characteristics. With this in mind, Figure 1 plots the variations in average molecular weight ($M_{average}$) and glass density (ρ_{glass}) as a function of increasing B_2O_3 content. It is clear that both parameters show a decreasing behavior with the insertion of higher B_2O_3 amount. $M_{average}$ decreases from 155.1 to 137.1 g.mol^{-1} while ρ_{glass} reduces from 5.5095 to 4.8675 g.cm^{-3}. The reason behind these decrements can be associated with the lower molecular weight of B_2O_3 (69.63 g.mol^{-1}) when compared to TeO_2 (159.6 g.mol^{-1}). Such a decreasing trend can be found in the recent literature studies, as well.[24,25] Therefore, we can conclude that B_2O_3 causes a diminishment in overall ρglass in the BT glass systems.

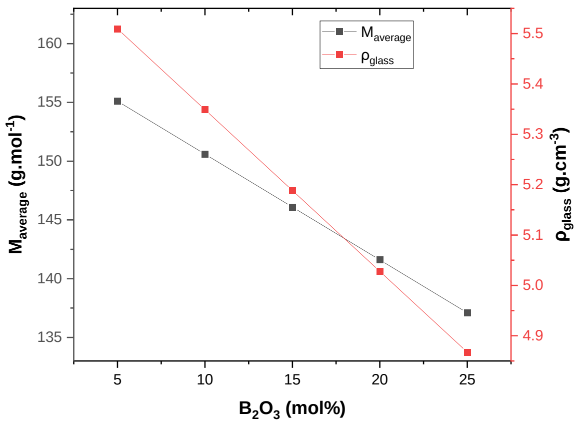

Figure 1. Variations in $M_{average}$ and ρ_{glass} as a function of B_2O_3 content.

The radiation shielding computations via Phy-X/PSD software were successfully carried out for the BT glass series. One of the most essential parameters, linear attenuation coefficient (LAC), was calculated against irradiations emitted from Ba-133 isotope. The findings for LAC values versus photon energies are revealed in Figure 2 on the basis of the increasing B_2O_3 doping rate. The photon energies can be given as follows: 0.03082, 0.035, 0.0354, 0.0358, 0.0496, 0.0532, 0.081, 0.161, 0.2234, 0.2764, 0.3029, 0.356, and 0.384 MeV. In the lower photon energies (*eg.* 0.03082 MeV), the *LAC* values are relatively high, however, these values show a sharp decrease through intermediate (*eg.* 0.081 MeV) and high (*eg.* 0.0384 MeV) photon energies. These behaviors may be attributed to the three mechanisms: photoelectric effect, Compton scattering, and pair production process at low, intermediate, and high energy levels, respectively.[26] When the influence of B_2O_3 on the *LAC* parameter is evaluated we observe that the increasing B_2O_3 contribution leads to the decreasing *LAC* values at lower and intermediate photon energies. For example, at 0.0358 MeV, LAC for BT5 is equal to 118.77 cm^{-1} whereas BT10 to BT25 is found to be 112.53, 106.3, 100.07, and 93.85 cm^{-1} in the respective order. In the high photon energy levels, the difference among BT samples in terms of *LAC* values becomes lower. From the findings, it is evident that B_2O_3 in replacement for TeO_2 results in diminishing photon shielding abilities.

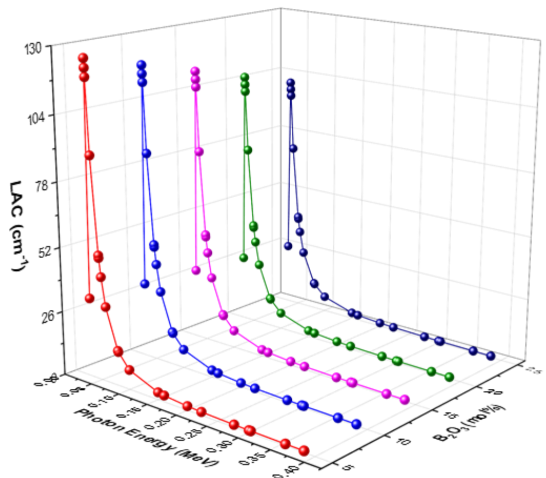

Figure 2. The findings for LAC values versus photon energies on the basis of the increasing B_2O_3 doping rate.

For better understanding of the LAC values, the authors certainly consider that a comparison should be made. For this, Figure 3 plots the LAC values for the alternative radiation shielding materials, as well as our glass samples at two different photon energies, namely 0.0801 an 0.3029 MeV. As it is well-known that the higher the LAC value the better the radiation protection abilities, one should understand the figure in this way. At 0.0801 MeV, our glass samples have higher LAC values that that of concrete materials (barite, hematite, limonite, magnetite, and bauxite-40).[27] Further, BT5 and BT10 samples show higher LAC than ZTT3 glass sample.[28] On the one hand, at 0.3029 MeV, ZTT3 dominates over the remaining in terms of LAC value. Nevertheless, BT5 have great possibility to compete with it. From the findings, we can conclude that BT5 and BT10 can be used as an alternative radiation shielding material.

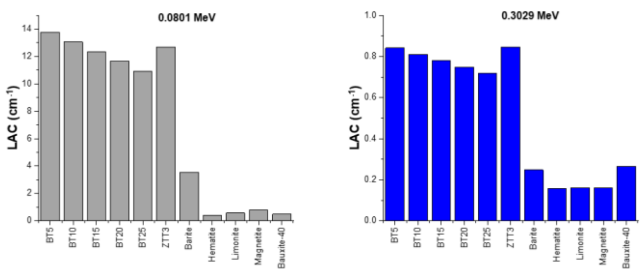

Figure 3. Comparison of the LAC values among alternative radiation shielding materials.

Fast neutrons removal cross-section (*FNRCS*) is an important parameter to assess the neutron attenuation capabilities of the intended material systems. In Figure 4, we display the findings of *FNRCS* for the BT5 to BT25 glass series. The increasing B_2O_3 content ensures *FNRCS* parameter to increase, which in turn enhances neutron attenuation. The values of *FNRCS* for the BT series equal to 0.1071, 0.1074, 0.1077, 0.1080, and 0.1083 1/cm in the respective order. Such an increase in the values may be linked to the lower atomic radius of the boron element. This is because a lower atomic radius is favorable for attenuating neutron particles. In our study, lower atomic radius, boron element (0.85 A°), replaces higher atomic radius tellurium element (2.1 A°). The recent literature investigations confirm the impact of B_2O_3 on the FNRCS increase.[29] For these reasons, one can use a high B_2O_3 amount for gaining more neutrons attenuated in the BT glass system.

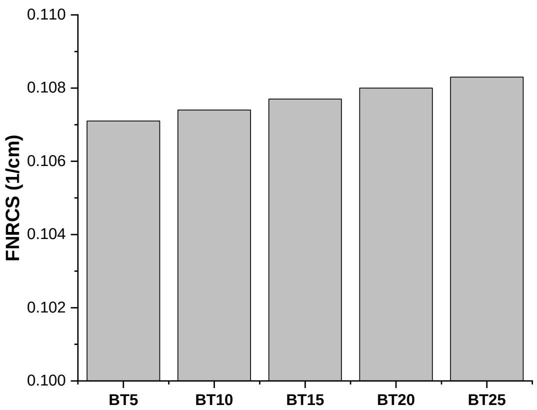

Figure 3. The findings of *FNRCS* for the BT5 to BT25 glass series.

4. CONCLUSIONS

The present investigation addressed the theoretical radiation shielding competencies and physical properties of borotellurite (BT) glass system. The intended BT glass systems had the following batch design: xB_2O_3 - $(100-x)TeO_2$ system (x: 5 to 25 mol% with a step of 5). Afterward, newly-developed user-friendly Phy-X/PSD software was utilized for determining linear attenuation coefficient (*LAC*) and fast neutrons removal cross-section (*FNRCS*) parameters at Ba-133 radioactive source energies. Furthermore, theoretical calculations for average molecular weight ($M_{average}$) and glass density (ρ_{glass}) were carried out to understand the influence of B_2O_3 on the BT glass network. According to the physical calculations, the insertion of B_2O_3 from 5 to 25 mol% caused $M_{average}$ and ρ_{glass} to decrease from 155.1 to 137.1 g.mol^{-1} and from 5.5095 to 4.8675 g.cm^{-3}, respectively. On the other hand, radiation shielding computations revealed that the linear attenuation coefficient (*LAC*) decreased against the increasing photon energy for all glass series. Besides that, the *LAC* decreased at all photon energies as B_2O_3 replaced TeO_2 in the glass network. Lastly, *FNRCS* for BT5 to BT25 samples were found to be 0.1071, 0.1074, 0.1077, 0.1080, and 0.1083 1/cm in the respective order. In conclusion, the authors reported that the increasing B_2O_3 doping rate in the BT glass system is beneficial for attenuating more neutrons, but may not be preferable for photon shielding.

- The insertion of B_2O_3 from 5 to 25 mol% caused $M_{average}$ and ρ_{glass} to decrease from 155.1 to 137.1 g.mol^{-1} and from 5.5095 to 4.8675 g.cm^{-3}, respectively.
- The linear attenuation coefficient (*LAC*) decreased against the increasing photon energy for all glass series.
- The *LAC* decreased at all photon energies as B_2O_3 replaced TeO_2 in the glass network.
- *FNRCS* for BT5 to BT25 samples were found to be 0.1071, 0.1074, 0.1077, 0.1080, and 0.1083 1/cm in the respective order.

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