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Determination of Radiation Characteristics of Samarium and Boron Doped Indium Oxide Thin Film by Simulation Method

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Abstract

In this study, the addition of samarium (Sm) and boron (B) to indium oxide (In_2O_3) thin films at rates of 5%, 10%, and 20% was investigated, and radiation properties were determined using the Monte Carlo N-Particle (MCNP6.2) simulation program. The reason for choosing In_2O_3 in the study is that In_2O_3 has high chemical stability, optical transparency, excellent electrical properties, and semiconductor properties. It is also widely used in various applications, including displays, solar cells, and sensors. Since In_2O_3 is used in sensors, it is aimed to be investigated for integration into radiation detector systems. At this point, it will provide a new idea. The simulation results obtained were compared with the values in the National Institute of Standards and Technology (NIST-XCOM) database, and it was observed that the simulation gave efficient results. According to the simulation analyses, it was observed that Sm provided better radiation shielding properties than B.

Keywords: Boron; Thin film; Indium oxide; MCNP; Radiation; Samarium.

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Samaryum ve Bor Katkılı İndiyum Oksit İnce Filmin Radyasyon Karakteristiklerinin Simülasyon Yöntemiyle Belirlenmesi

Öz

Bu çalışmada, indiyum oksit (In_2O_3) ince filmine %5, %10 ve %20 oranlarında samaryum (Sm) ve bor (B) katkılanarak radyasyon özellikleri Monte Carlo N-Particle (MCNP6.2) simülasyon programıyla belirlenmeye çalışılmıştır. Çalışmada In_2O_3'ün seçilmesinin sebebi; In_2O_3'ün yüksek kimyasal kararlılığa, optik şeffaflığa, mükemmel elektriksel özelliklere ve yarı iletken özelliklere sahip olmasıdır. Aynı zamanda ekran, güneş pilleri ve sensörler gibi birçok alanda yaygın olarak kullanılmaktadır. In_2O_3'ün sensörlerde kullanıldığı için radyasyon dedektör sistemlerine entegrasyonu amacıyla araştırılması amaçlanmaktadır. Bu noktada yeni bir fikir sunmuş olacaktır. Elde edilen simülasyon sonuçları Ulusal Standartlar ve Teknoloji Enstitüsü (NIST-XCOM) veri tabanındaki değerlerle karşılaştırılarak yapılan simülasyonun verimli sonuçlar verdiği gözlenmiştir. Simülasyon analizlerine göre Sm'nin B'den daha iyi radyasyon zırhlama özelliği kazandırdığı gözlenmiştir.

Anahtar Kelimeler: Bor; İnce film; İndiyum oksit; MCNP; Radyasyon; Samaryum.

1. Introduction

Today, it is important to minimize the effects of radiation in environments where radiation is used. For this purpose, there are intensive studies on technological developments in various sectors, such as medicine, materials science, and energy, in order to protect against radiation or to utilize radiation more efficiently. One of these is the design and improvement of thin films. In some studies, different elemental additives can be used to improve the physical properties of thin films. Radiation and particles, including electromagnetic waves and transmissions from nuclear inter-level transitions, are a pervasive and fundamental aspect of our time. These radiation and particles are emitted from a variety of sources, both natural and artificial, and play a crucial role in people's lives, particularly in scientific, industrial, and medical practices. The need for protection has necessitated extensive research into materials that can reduce the harmful effects of radiation. Ionizing radiation, with its ability to remove tightly bound electrons from atoms, can also cause unwanted damage to the cell structures of living organisms. The necessity to protect against these potential hazards has led to the research and development of materials that function as shielding [1–4].

Natural sources of ionizing radiation include external cosmic rays. In addition, terrestrial radiation from the Earth's crust, radioactive isotopes in the environment, and artificial sources used for diagnostic purposes in medicine are also in this category [5]. On the other hand, industrial processes and nuclear energy production also involve the use of ionizing radiation. Of course, in energy production, concrete and lead are used for shielding structures. However, transparent materials with high MAC (mass attenuation coefficient) (non-toxic like lead) are of interest to researchers [6–9]. Glass compositions play a very important role in various industrial applications, especially in the field of radiation protection due to specific properties of the materials [10]. One of them is the MAC values for glass compositions, which are crucial for optimizing glass in radiation protection applications [11]. On the other hand, numerous questions remain unanswered regarding the use of transparent materials for this purpose, and further studies are needed in these areas. This study aims to utilize glass as an alternative and environmentally friendly material for gamma radiation shielding applications.

Indium oxide (In_2O_3), studied as a thin film, is an n-type semiconductor with a bandgap of 3.5-3.7 eV [12]. It also has high electrical conductivity and outstanding optical transparency [13]. In_2O_3 thin films can be synthesized using various techniques, including sol-gel dip coating, RF and DC sputtering, chemical vapor deposition, and spray pyrolysis [14]. Of these, the spray pyrolysis method is easy, low-cost, and suitable for industry as large areas can be coated with this method. In addition, the phase, size, and morphology of the thin film can be controlled [15]. It is crucial to obtain ultrafine powders with high purity, high porosity, and a large surface area through spray pyrolysis [16]. The electrical resistance and optical transmission of this film have been studied [17]. The physical properties of In_2O_3 thin film have been reported to be extensively improved by iron doping [18]. In_2O_3 is widely preferred in thin film designs due to its high semiconductor properties. At the same time, some physical properties can be created by doping various elements to In_2O_3. In thin film designs, it is also important for it to be transparent for use in sensors and detectors. For example, molybdenum element is doped into In_2O_3 to increase its conductivity and transparency properties [19].

Various elements are being tested to increase the physical properties of devices used in nuclear technologies. One of these is Sm. Since Sm is a high-purity element, it is the focus of the studies [20]. Stainless steels are also used for radiation protection in nuclear applications. According to the researches, Sm doping has also been tried to strengthen the shielding properties of stainless steel used in radiation shielding processes. The results indicate that Sm has positive contributions to radiation shielding [21]. There are also studies on the radiation properties of Sm-doped compounds. In one of these studies, radiation permeability coefficients were investigated Sm doped zinc bismuth silicate. The change in radiation shielding properties under the influence of silica at low photon energies was investigated [22].

Another element widely used in research on the radiation properties of compounds is B. Boron has a positive effect in slowing down radiation types such as thermal neutrons. Therefore, when examining studies on B-containing compounds, it is evident that high performance is achieved in terms of radiation shielding [23]. When we examine the studies investigating the radiation properties of alloys composed of iron and B, it has been observed that there is a positive correlation between the photon shielding property and the amount of B. This shows that B-containing samples can be used for radiation shielding [24].

The main objective of this study is to determine the radiation protection properties of In_2O_3 thin films by obtaining other parameters, such as MAC, LAC, and HVL for different types of glasses produced by doping In_2O_3 thin films with different proportions of Sm and B at 5%, 10% and 20%. The reason for choosing In_2O_3 is that it has high chemical stability, optical transparency, excellent electrical properties, and semiconductor properties. Due to these properties, it offers the opportunity to be used in nuclear applications. Sm, one of the elements doped in In_2O_3, provides a high density to In_2O_3. At the same time, it increases its high-purity feature. The other element doped in In_2O_3, B, contributes to the increase in radiation shielding feature.

2. Materials and Methods

In this study, Indium oxide doped with different ratios of Sm and B was investigated as a radiation shielding material. The individual doping rates of Sm and B materials were decided as 5%, 10%, and 20%. The values of the related shielding materials are given in Table-1.

Table 1: Percentage ratios and densities of the samples.

Sample Name	Doped Material	Main Material	Density (g/cm^3)
	Sm (%)	**In_2O_3 (%)**	**(g/cm^3)**
sm1	0	100	7.13
sm2	5	95	7.12
sm3	10	90	7.09
sm4	20	80	7.00
Sample Name	**Doped Material**	**Main Material**	**Density (g/cm^3)**
	B (%)	**In_2O_3 (%)**	**(g/cm^3)**
b1	0	100	7.13
b2	5	95	6.92
b3	10	90	6.70
b4	20	80	6.30

The Monte Carlo N-Particle (MCNP6.2) simulation program, a Monte Carlo-based tool, was utilized in this study. MCNP is a radiation transport program that is frequently used and preferred in radiation modeling in the scientific world. Input files were prepared, and calculations were performed using the experimental setup shown in Fig. 1. The experimental setup consists of a source emitting radiation at various energy levels (0.284 MeV, 0.347 MeV, 0.511 MeV, 0.662 MeV, 0.826 MeV, 1.17 MeV, 1.33 MeV, and 2 MeV), 0.0002 cm-thick thin film samples, and a detector system that detects gamma rays passing through the samples. f4 (Average photon flux n/cm2) was used for the detector tally card. The simulation was performed with 10 million stories for each sample and each energy value.

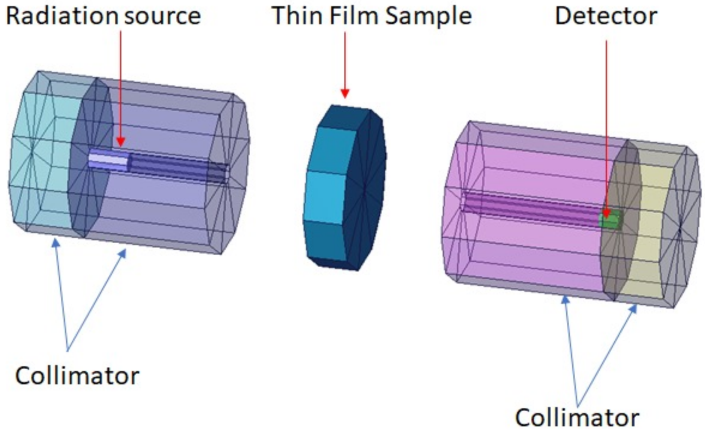

Figure 1: MCNP experimental setup.

The Linear Attenuation Coefficient (LAC) (Eqn. (2)), Mass Attenuation Coefficient (MAC) (Eqn. (3)), Mean Free Path (MFP) (Eqn. (4)), Half Value Layer (HVL) (Eqn. (5)) and Tenth Value Layer (TVL) (Eqn. (6)) values of each sample were calculated according to the Beer-Lambert Law stated in Eqn. (1) using the data in the outputs obtained from the simulation [25]. These equations represent the radiation characteristics of the respective samples [26].

$$I = I_0 e^{-\mu x} \tag{1}$$

Where I_0 is the intensity from the radiation source, I is the intensity detected by the detector, x is the sample thickness and μ is the LAC.

$$LAC = \mu\ (1/cm) \tag{2}$$

$$MAC = {}^{\mu}/_{\rho} \left(\frac{cm^2}{g}\right) \tag{3}$$

Here ρ is the density of the sample.

$$MFP = \frac{1}{LAC} = \frac{1}{\mu}(cm) \tag{4}$$

$$HVL = \frac{\ln(2)}{LAC} = \frac{\ln(2)}{\mu}(cm) \tag{5}$$

$$TVL = \frac{\ln(10)}{LAC} = \frac{\ln(10)}{\mu}(cm) \tag{6}$$

The LAC, MAC, MFP, HVL, and TVL values were compared with the NIST-XCOM data using the data from the simulation outputs [27]. This study is simulation-based and experimental results are not available. Therefore, to verify the accuracy of the simulations, the results obtained were compared with NIST-XCOM values. The NIST-XCOM program is utilized for calculating mass attenuation coefficients and cross sections of interaction for different elements, compounds, and mixtures in the energy range 1 keV–100 GeV [28,29]. According to the comparison results, the simulation was found to be efficient.

3. Results and Discussion

3.1. Results for Sm Doped In_2O_3 Samples

The LAC, MAC, MFP, HVL and TVL results obtained using MCNP6.2 simulation program for Sm doped In_2O_3 thin film are given in Figs. 2–6, respectively.

LAC (1/cm)				
Energy (MeV)	sm1	sm2	sm3	sm4
0.284	1.17824	1.17824	1.21751	1.25679
0.347	0.94257	0.94257	0.94257	0.98184
0.511	0.66763	0.66763	0.66763	0.66763
0.662	0.54981	0.54981	0.54981	0.54981
0.826	0.47126	0.47126	0.47126	0.47126
1.17	0.39271	0.39271	0.39271	0.39271
1.33	0.35344	0.35344	0.35344	0.35344
2	0.31417	0.31417	0.2749	0.2749

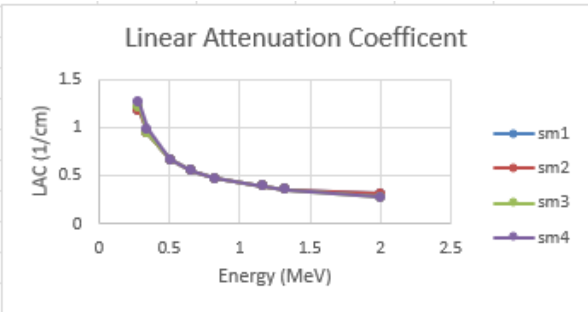

Figure 2: LAC values of Sm doped In_2O_3 samples.

MAC (cm^2/g)				
Energy (MeV)	sm1	sm2	sm3	sm4
0.284	0.16525	0.16548	0.17172	0.17726
0.347	0.1322	0.13238	0.13294	0.13848
0.511	0.09364	0.09377	0.09417	0.09417
0.662	0.07711	0.07722	0.07755	0.07755
0.826	0.0661	0.06619	0.06647	0.06647
1.17	0.05508	0.05516	0.05539	0.05539
1.33	0.04957	0.04964	0.04985	0.04985
2	0.04406	0.04412	0.03877	0.03877

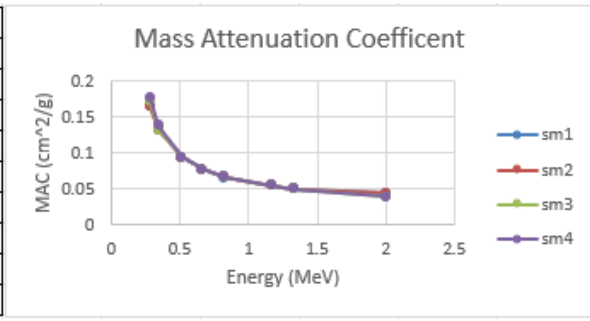

Figure 3: MAC of Sm doped In_2O_3 samples.

MFP (cm)				
Energy (MeV)	sm1	sm2	sm3	sm4
0.284	0.84873	0.84873	0.82135	0.79567
0.347	1.06093	1.06093	1.06093	1.01849
0.511	1.49783	1.49783	1.49783	1.49783
0.662	1.81881	1.81881	1.81881	1.81881
0.826	2.12197	2.12197	2.12197	2.12197
1.17	2.54638	2.54638	2.54638	2.54638
1.33	2.82932	2.82932	2.82932	2.82932
2	3.183	3.183	3.63773	3.63773

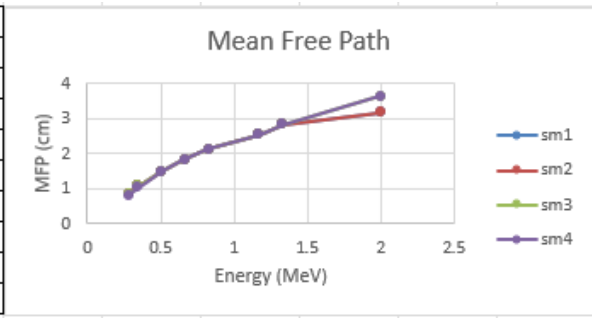

Figure 4: MFP of Sm doped In_2O_3 samples.

HVL (cm)				
Energy (MeV)	sm1	sm2	sm3	sm4
0.284	0.58829	0.58829	0.56931	0.55152
0.347	0.73538	0.73538	0.73538	0.70596
0.511	1.03822	1.03822	1.03822	1.03822
0.662	1.26071	1.26071	1.26071	1.26071
0.826	1.47084	1.47084	1.47084	1.47084
1.17	1.76502	1.76502	1.76502	1.76502
1.33	1.96114	1.96114	1.96114	1.96114
2	2.20629	2.20629	2.52148	2.52148

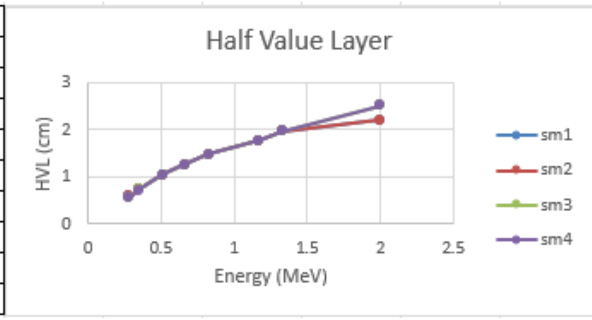

Figure 5: HVL of Sm doped In_2O_3 samples.

TVL (cm)				
Energy (MeV)	sm1	sm2	sm3	sm4
0.284	1.95427	1.95427	1.89122	1.83211
0.347	2.44289	2.44289	2.44289	2.34516
0.511	3.44888	3.44888	3.44888	3.44888
0.662	4.18797	4.18797	4.18797	4.18797
0.826	4.88601	4.88601	4.88601	4.88601
1.17	5.86326	5.86326	5.86326	5.86326
1.33	6.51476	6.51476	6.51476	6.51476
2	7.32913	7.32913	8.37618	8.37618

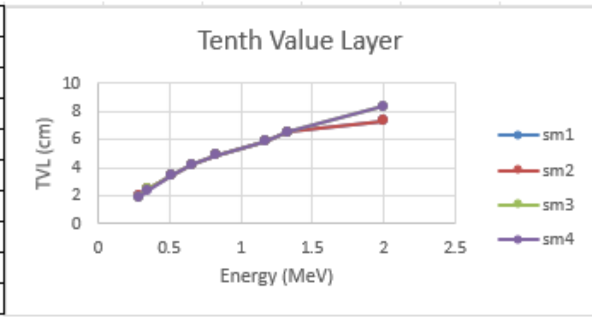

Figure 6: TVL of Sm doped In_2O_3 samples.

When the LAC values of the Sm-doped In_2O_3 samples were examined, it was observed that the LAC values increased as the doping ratio increased. Only at an energy of 2 MeV, a deviation was observed in the LAC values of the sm3 and sm4 coded samples. For this reason, Sm-doped In_2O_3 thin films do not give the desired results at very high energies. When the obtained results are compared with XCOM, the fact that the error rates are higher than the others support this situation. When the MFP values are examined, it is seen that the values deviate as the doping ratio increases at high energies. Since the MFP values of the samples express the amount of radiation passing through the substance without interacting, these results show that Sm-doped In_2O_3 thin films are not efficient at high energies.

3.2. Results for B Doped In_2O_3 Samples

LAC, MAC, MFP, HVL and TVL results obtained using MCNP6.2 simulation program for B doped In_2O_3 thin film are given in Figs. 7–11, respectively.

LAC (1/cm)				
Energy (MeV)	b1	b2	b3	b4
0.284	1.17824	1.09968	1.0604	0.94257
0.347	0.94257	0.90329	0.82474	0.78546
0.511	0.66763	0.62836	0.62836	0.54981
0.662	0.54981	0.51053	0.51053	0.47126
0.826	0.47126	0.47126	0.43199	0.43199
1.17	0.39271	0.39271	0.35344	0.35344
1.33	0.35344	0.35344	0.35344	0.31417
2	0.31417	0.2749	0.2749	0.2749

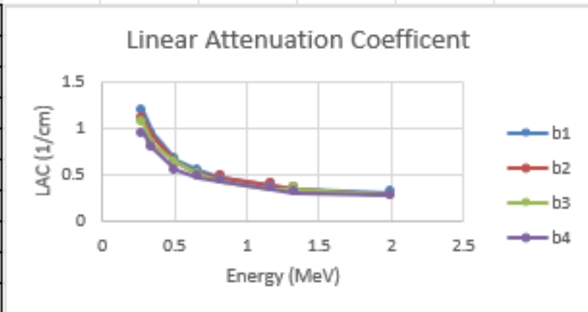

Figure 7: LAC of B doped In_2O_3 samples.

MAC (cm^2/g)				
Energy (MeV)	b1	b2	b3	b4
0.284	0.16525	0.15891	0.15827	0.14961
0.347	0.1322	0.13053	0.12309	0.12468
0.511	0.09364	0.0908	0.09378	0.08727
0.662	0.07711	0.07378	0.0762	0.0748
0.826	0.0661	0.0681	0.06448	0.06857
1.17	0.05508	0.05675	0.05275	0.0561
1.33	0.04957	0.05108	0.05275	0.04987
2	0.04406	0.03972	0.04103	0.04363

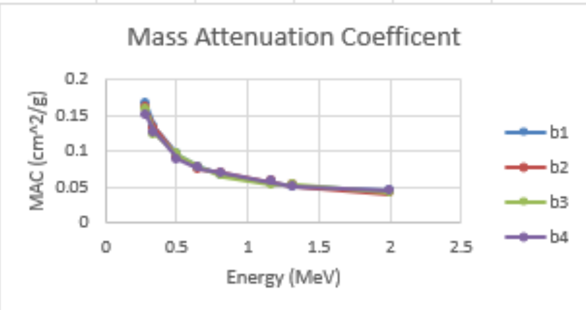

Figure 8: MAC of B doped In_2O_3 samples.

MFP (cm)				
Energy (MeV)	b1	b2	b3	b4
0.284	0.84873	0.90936	0.94304	1.06093
0.347	1.06093	1.10707	1.21251	1.27314
0.511	1.49783	1.59145	1.59145	1.81881
0.662	1.81881	1.95873	1.95873	2.12197
0.826	2.12197	2.12197	2.31488	2.31488
1.17	2.54638	2.54638	2.82932	2.82932
1.33	2.82932	2.82932	2.82932	3.183
2	3.183	3.63773	3.63773	3.63773

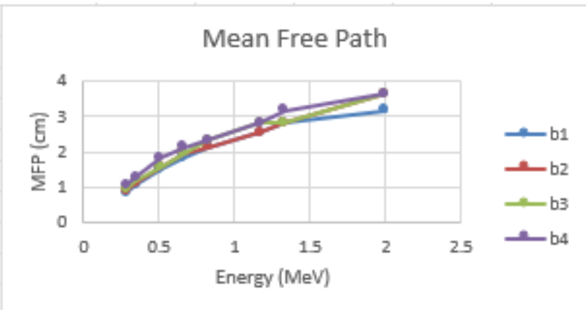

Figure 9: MFP of B doped In_2O_3 samples.

HVL (cm)				
Energy (MeV)	b1	b2	b3	b4
0.284	0.58829	0.63032	0.65367	0.73538
0.347	0.73538	0.76736	0.84045	0.88247
0.511	1.03822	1.10311	1.10311	1.26071
0.662	1.26071	1.35769	1.35769	1.47084
0.826	1.47084	1.47084	1.60455	1.60455
1.17	1.76502	1.76502	1.96114	1.96114
1.33	1.96114	1.96114	1.96114	2.20629
2	2.20629	2.52148	2.52148	2.52148

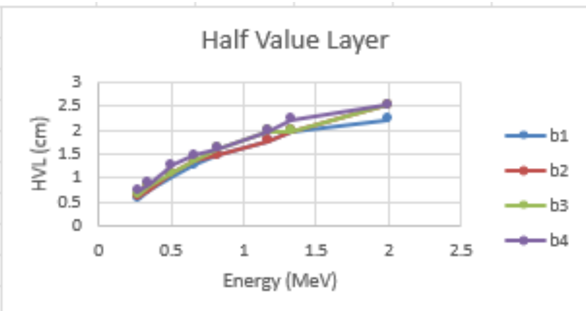

Figure 10: HVL of B doped In_2O_3 samples.

TVL (cm)				
Energy (MeV)	b1	b2	b3	b4
0.284	1.95427	2.09387	2.17143	2.44289
0.347	2.44289	2.54911	2.79191	2.93151
0.511	3.44888	3.66445	3.66445	4.18797
0.662	4.18797	4.51014	4.51014	4.88601
0.826	4.88601	4.88601	5.33021	5.33021
1.17	5.86326	5.86326	6.51476	6.51476
1.33	6.51476	6.51476	6.51476	7.32913
2	7.32913	8.37618	8.37618	8.37618

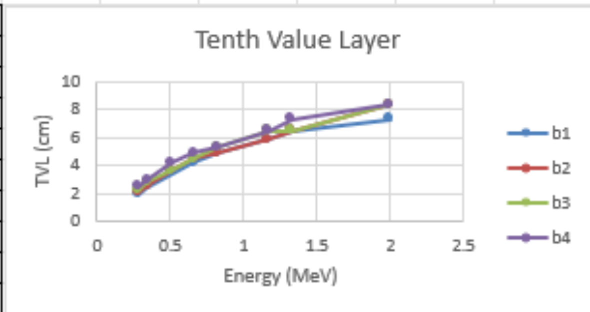

Figure 11: TVL of B doped In_2O_3 samples.

When the LAC values of the B-doped In_2O_3 samples were examined, it was observed that the LAC values decreased as the B ratio increased. This situation demonstrates that doping with B did not have a positive effect on the radiation properties. When compared with the XCOM values, it was seen that the error rates were below 5%. This situation demonstrates that the simulation outputs were not erroneous and that doping B into In_2O_3 did not contribute to the radiation shielding properties. Similarly, when the MFP values were examined, it was seen that the values for each sample at each energy increased.

According to the results obtained in this study, if a comparison is desired between Sm and B, it can be said that Sm is more efficient in radiation shielding due to its higher density than B.

4. Conclusion

In this simulation-based study, an attempt was made to obtain data for the most frequently used energy values in nuclear applications. It can be considered a study that is recommended for glass forms suitable for use in nuclear applications. When the MAC values obtained in the study are compared with the NIST-XCOM data, the difference rates do not exceed 5%. These difference rates indicate that the simulation is efficient (available upon request). In this study, Sm has a higherdensity when compared with B. Therefore, it is seen that Sm is more efficient in terms of radiation shielding. Additionally, Sm can be preferred for glass components worldwide due to its abundant presence. Upon examining the literature, it becomes apparent that numerous studies have been conducted on samples in glass form. The study conducted is simulation-based only and cannot be compared with experimental data. At this point, experimental studies can be recommended for Sm-doped In_2O_3 glass samples. In addition, experimental studies of other elements with high densities, electrical and optical properties, such as Sm, are also recommended.

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