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The Effect of TiO_2 on Optical and Radiation Shielding Properties of BaO B_2O_3 Glasses

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Abstract: The optical properties of a new family of $xTiO_2$ (65-x) $B_2O_3$35BaO glasses are investigated. The optical parameters such as average single bond strength, optical electronegativity, optical energy gap, refractive index, optical basicity and third order nonlinear susceptibility are discussed with respect to titanium concentration. Gamma ray transmission and the parameters which affect these processes; attenuation coefficients and half value layer, were studied using the mixture rule of the XCOM program, in the energy range (1 keV-100 GeV). The results obtained probably provide good biased for prediction of new nonlinear materials and can be used as an environmentally friendly substitute for lead for industries besides their radiation-shielding property.

Keywords: Borate Glass, Optical Property, Radiation Shields

1. Introduction

Radiation shielding has become a subject of increasing interest among many applications in which radiation is being used, such as, the use of atomic energy and radioactive isotopes. Since glass is a solid and transparent material, there is a great effort being put into creating types that can protect users against small amounts of radiation without loss of transparency. These types of glasses have been developed to accomplish double tasks by allowing visibility while absorbing gamma radiation.

Nonlinear optical materials have long been studied due to their practical and potential usages in optical information processing technology [1]. The optical energy gap and the refractive index are the most interesting and fundamental properties of glass materials. The refractive index is used to determine the suitability of glassy materials to be optical devices [2]. Optical nonlinearity is caused by the electronic polarization of the material upon exposure to intense light beams. Polarizability is one of the most important properties which govern the nonlinerarity response of the material [1]. The optical basicity is a useful parameter for correlating and predicting properties of oxide systems covering a broad range of application [3]. Also, the optical electronegativity is one of the most important parameters in understanding the nature of chemical bonding [4]. Recently, glasses containing boron oxide have attained great attention, since they are used in the wide area of applications [5]. The structure, electrical and optical properties of these glasses have been studied [6-9]. Transition metal ions doped borate glasses have many applications in microelectronics, optical glasses and solid state laser [10].

Glasses with high TiO_2 content are of great interest in basic research and technological applications because of their optical properties and good chemical resistance [11, 12]. The purpose of the present paper to study the physical properties of 35 BaO $xTiO_2$ (65-x) B_2O_3 (where x=30, 40, 50, 55) glasses and also the transmission factors mass attenuation coefficients and half value layer (HVL) are studied.

2. Theoretical Background

The density of all the glasses under study can be calculated from the following expression:

$$d= X_{CeO2}\, d_{CeO2} + X_{BaO}\, d_{BaO} + X_{B2O3} d_{B2O3} \qquad (1)$$

Where X is the molar fraction and d is the values of theoretical density respectively [9].

Molar volume = (total molecular weight) /(density of the sample). The total molecular weight can be calculated as follows:

Total molecular weight $=X_{CeO2}\ Z_{CeO2} + X_{BaO}\ Z_{BaO} + X_{B2O3}\ Z_{B2O3}$

Where Z is the molar weights of constituent oxides [9].

The optical electronegativity can be calculated as follows,

$$\Delta\chi^{*}= X_{CeO2}\Delta\chi^{*}_{CeO2} X_{BaO}\ \Delta\chi^{*}_{BaO} + X_{B2O3}\Delta\chi^{*}_{B2O3} \qquad (2)$$

Where $\Delta\chi^{*}$ is the values of the optical electronegativity of CeO_2, BaO and B_2O_3, respectively [10].

The optical energy gap can be calculated by [11]

$$E_{opt}=0.2688\Delta\chi^{*} \qquad (3)$$

The optical basicity can be calculated [11]

$$\text{Optical basicity} = -0.5\Delta\chi^{*}+1.7 \qquad (4)$$

The electronic polarizability [11] of oxide ions can be calculated

$$= 0.9\Delta\chi^{*}+3.59 \qquad (5)$$

The linear refractive index, n_0, can be calculated [4]

$$n_0=-0.73 \ln (0.102\Delta\chi^{*})+0.5511 \qquad (6)$$

The third order nonlinear susceptibility in esu units is given by the following relation [5],

$$\chi^{(3)}=(1.4\text{x}10^{-11})/((E_{opt}-1.96)(E_{opt}-1.31)(E_{opt}-0.65)) \qquad (7)$$

The nonlinear refractive index n_2 can be expressed as [2, 12],

$$n_2= ((12\text{x}3.14) /n_0)\ (\chi^{(3)}) \qquad (8)$$

For a simple oxide A_pO_q, the molar polarizability α_m can be calculated as follows [13, 14] $\alpha_m = (p\ \alpha_i + q\ \alpha_0^{-2})$ where α_i is the polarizability of cation and α_o^{-2} is the polarizability of oxide ion. The molar refraction R_m can be calculated by [13] $R_m=2.52\alpha_m$.

As a photon makes its path through a matter, there is a probability that it makes an interaction with the material such as absorption (photoelectric effect), scattering (Rayleigh or Compton scattering) or splitting (pair production). Therefore, part of the incident beam of intensity (I_o) will be partially or completely removed from the beam as a result of interaction within the absorber of thickness *t*.

This reduces the transmitted intensity that reaches the to (I), where, introducing μ, the linear attenuation coefficient, μ_m is a mass attenuation coefficient measure of how strongly a chemical species or substance absorbs or scattering radiation at a given wavelength, per unit mass is given by;

$$I_{(t)} = I_0 e^{-(\mu m)\,\rho\, t} \qquad (9)$$

Where ρ is the density, μ_m is the mass attenuation coefficient ($cm^2 g^{-1}$).

HVL signifies the thickness of a material required to reduce the intensity of the emergent radiation to half its incidents magnitude.

$$\text{HVL} = \text{Ln } 2/\mu \qquad (10)$$

3. Discussion and Results

3.1. Density and Molar Volume

The density of all the glasses under study calculated from the equation (1). The values of theoretical, experimental [12] density and molar volume for all the studied glasses are listed in table 1. It is clear that, the values of density increase, and the values of molar volume decrease for all the studied samples by increasing TiO_2 content. It was found that the values of theoretical density are greater than the experimental one [12] due to chemical and topological defects of the prepared samples.

Table 1. *Molecular weight, molar volume, theoretical and experimental density of all the studied samples.*

Sample	Molecular weight (g/cm^3)	Density (g/cm^3) (Theoretical)	Density (g/cm3) (Experimental)	Molar volume (V_m) (g/cm^3)
35BaO 30 TiO_2 35 B_2O_3	101.997	4.141	4.004	24.63
35 BaO 40TiO_2 25B_2O_3	103.02	4.321	4.232	23.84
35 BaO 50TiO_2 15B_2O_3	104.05	4.501	4.348	23.12
35 BaO 55TiO_2 10 B_2O_3	104.56	4.591	4.397	22.77

3.2. The Theoretical Optical Electronegativity ($\Delta\chi^{*}$) and Optical Energy

The values of optical electronegativity decrease and average single bond strength decrease with increasing TiO_2 content so the samples are considered to be ionic in nature, and are listed in table 2.

The value of theoretical optical band gap energy decreases with increasing TiO_2 content. The decrease in the values of average single bond is responsible for the decrease of optical band gap energy. Also, the theoretical values of E_{op} are larger than the experimental values [12], this due to the amorphous nature of prepared samples.

Table 2. *Optical electronegativity, theoretical and experimental optical energy gap, average single bond strength.*

Sample	**Optical electronegativity**	**Theo. optical energy gap (eV)**	**Exp. optical energy gap (eV)**	**Average single bond strength (KJ/mol)**
35BaO 30 TiO_2 35 B_2O_3	1.444	5.37	3.62	295.20
35 BaO 40TiO_2 25B_2O_3	1.272	4.73	3.59	275.90
35 BaO 50TiO_2 15B_2O_3	1.100	4.09	3.57	256.6
35 BaO 55TiO_2 10 B_2O_3	1.014	3.77	3.56	246.95

3.3. The Optical Basicity and the Electronic Polarizability of Oxide Ions

The optical basicity, addresses the ability of oxide glass in contributing the negative charges in the glass matrix. In other words, it defines the electron donating power of the oxygen in the oxide glass.

The values of optical basicity and the electronic polarizability of oxide ions for all the studied samples are listed in table 3. The increased optical basicity of the glasses with TiO_2 content indicates that the glass system is basic in nature. The electronic polarizability of oxide ion increases with increasing the optical basicity. The values of molar polarizability and The molar refraction R_m [13] are shown in table 3 illustrate that the glasses under investigation become more polarized by increasing TiO_2 content.

Table 3. *Optical basicity, oxide ion polorazibility, refractive index, molar refractivity and third order nonlinear susceptibility.*

Sample	**Optical basicity (A_{th})**	**Oxide ion polarizability (α^{02-}) $(A^0)^3$**	**Molar polorazability α_m $(A^0)^3$**	**Molar refractivity (cm^3/mol)**	**Refractive index**	**Third order nonlinear susceptibility χ^3x10^{-13}esu.**
35BaO 30 TiO_2 35 B_2O_3	0.978	2.2004	5.02	12.65	1.949	2.46
35 BaO 40TiO_2 25B_2O_3	1.064	2.042	5.11	12.88	2.042	4.06
35 BaO 50TiO_2 15B_2O_3	1.15	2.510	5.17	13.03	2.148	6.85
35 BaO 55TiO_2 10 B_2O_3	1.014	2.587	5.19	13.09	2.207	9.02

3.4. The Linear Refractive Index and Third Order Nonlinear Susceptibility

The values of the refractive index in table 3 increase by increasing TiO_2 content. The refractive index depends on the polorazibility of glass material [2] so the values of refractive index increase as well as the values of molar polorazibility increase.

Figure 1 shows that the correlation between refractive index and density where both of them have the same trend and that high density and refractive index of these samples gave rise to attenuation.

The value of experimental third order nonlinear susceptibility values [4] were found to be in the range (1.49-3.04) x10^{-13} esu, but the values of theoretical third order nonlinear optical susceptibility for all the studied sample, were found to be in the range (2.46-9.02) x 10^{-13} esu, this means that all the studied samples are probably good candidates for nonlinear optical applications [15]. Also, we found that third order nonlinear susceptibility increases with decreasing the optical energy gap and increasing the refractive index as is evident in figure 2 and figure 3.

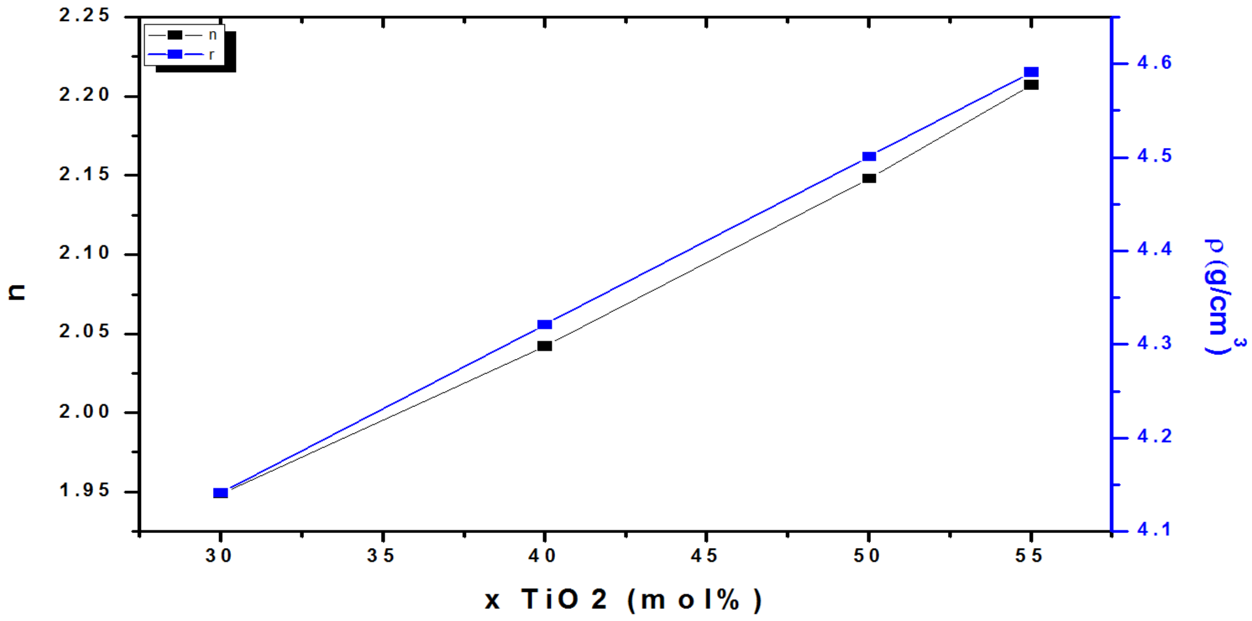

Figure 1. *Concentration of TiO2 vs. refractive index and density of glass samples.*

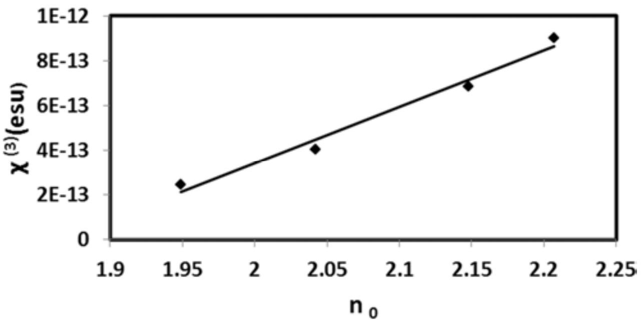

Figure 2. *Third order non linear susceptibility as a function of linear refractive index.*

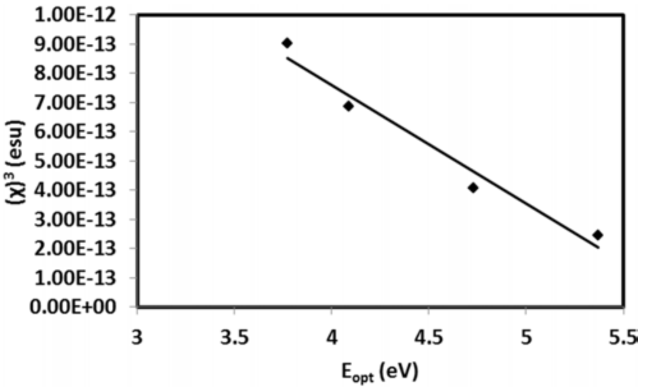

Figure 3. *Third order nonlinear susceptibility as a function of the optical energy gap.*

3.5. Total Mass Attenuation Coefficient (μ_m) and Shielding Properties

The mass attenuation coefficient In the case of a compound of various elements, it is assumed that the contribution of each element of the compound to the total photon interaction is additive, obeying the mixture rule of the XCOM computer program, for calculating mass attenuation coefficients or photon interaction cross-sections for any element, compound or mixture, at energies from1 keV to 100 GeV [16]. The values of μ_m for gamma-ray at different energies ranged from [(1-911 keV), (1–100 MeV) and (150 MeV-100 GeV)] low, medium and high energies, respectively.

From the figures 4, 5 and 6, it is clear that the mass attenuation coefficient is inversely proportional to energy, and that's related to the dependency of the μ_m on the interaction between photons and matter, when the photon energy increases, the transmitted photons increase and the absorbed photons decrease, as a result the μ_m decreases. Also, as the density increases the mass attenuation coefficient decreases; this confirms the contribution of the absorption process (photoelectric effect), scattering process (Compton, coherent) and pair production [17].

Another definition which is associated with μ_m is the half value layer (HVL), it represents the quantity of gamma radiation to half. The direct relation between it and energy is found as is evident in figure 7, 8 and 9, and it explains why the number of interactions becomes higher when the distance between the interactions gets smaller.

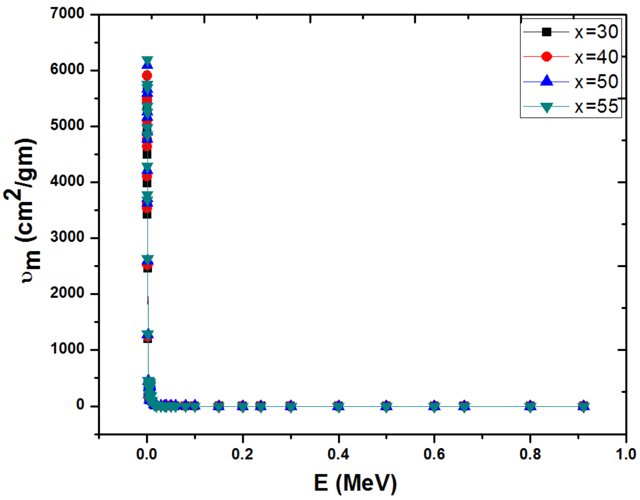

Figure 4. *The mass attenuation coefficients of the samples at low energies (1- 911 keV).*

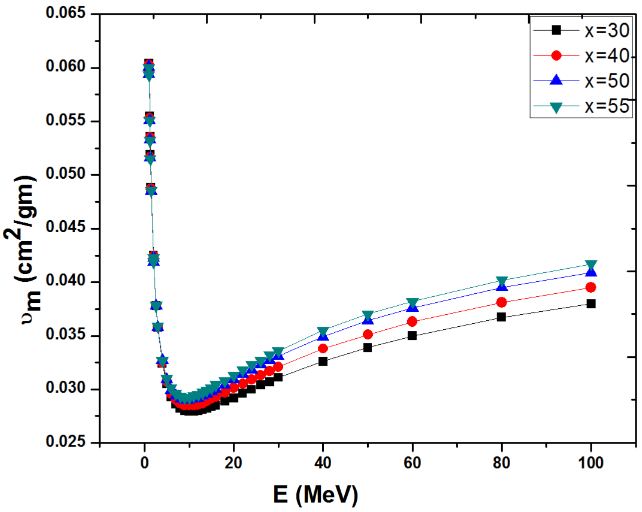

Figure 5. *The mass attenuation coefficients of the samples at medium energies (1–100 MeV).*

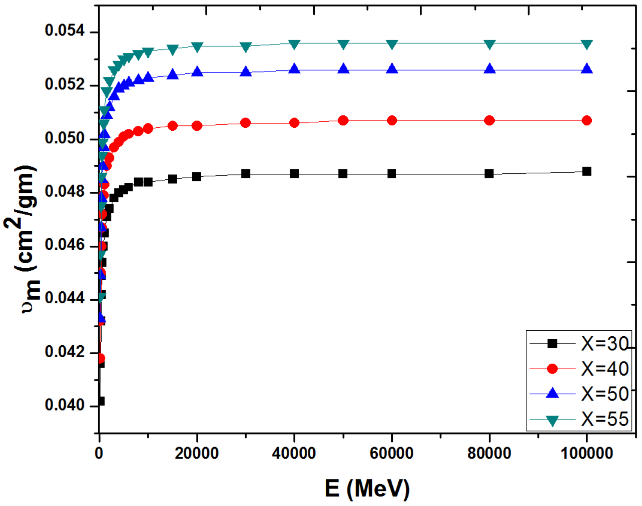

Figure 6. *The mass attenuation coefficients of the samples at high energies (150 MeV–100 GeV).*

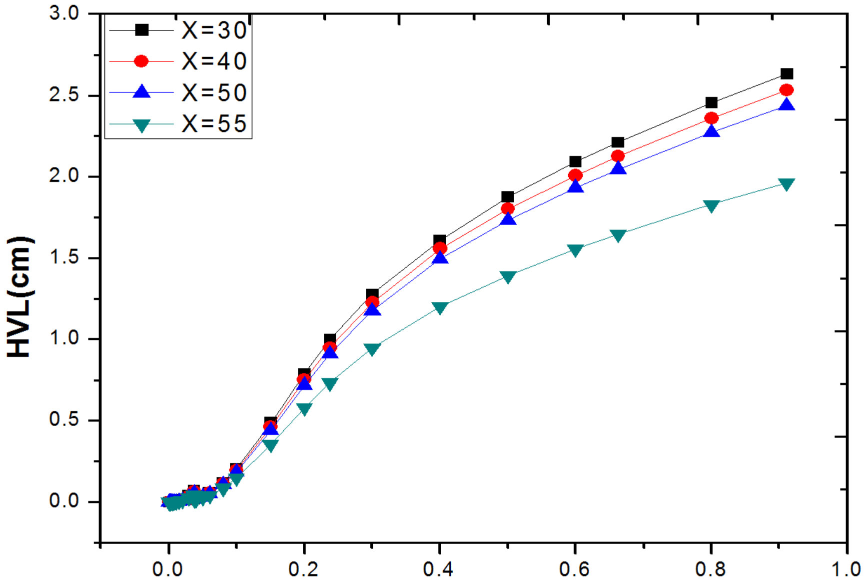

Figure 7. *The HVL of the samples at low energies (1–911 KeV).*

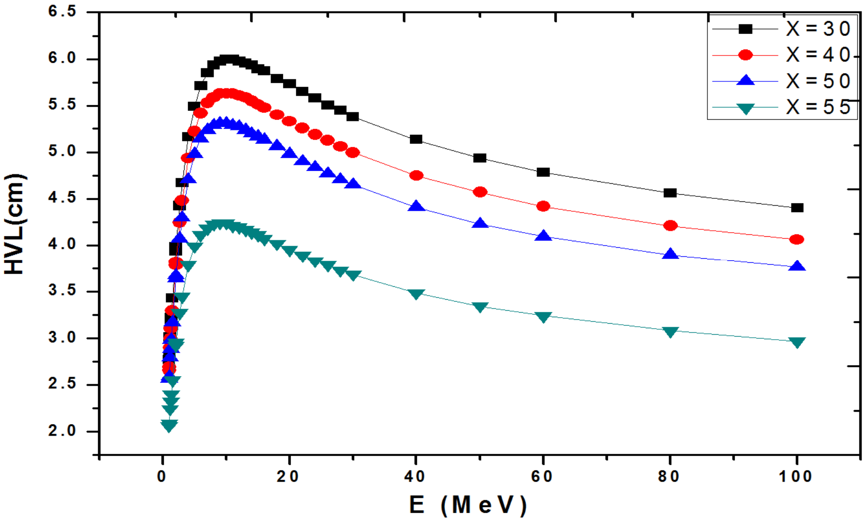

Figure 8. *The HVL of the samples at medium energies (1–100 MeV).*

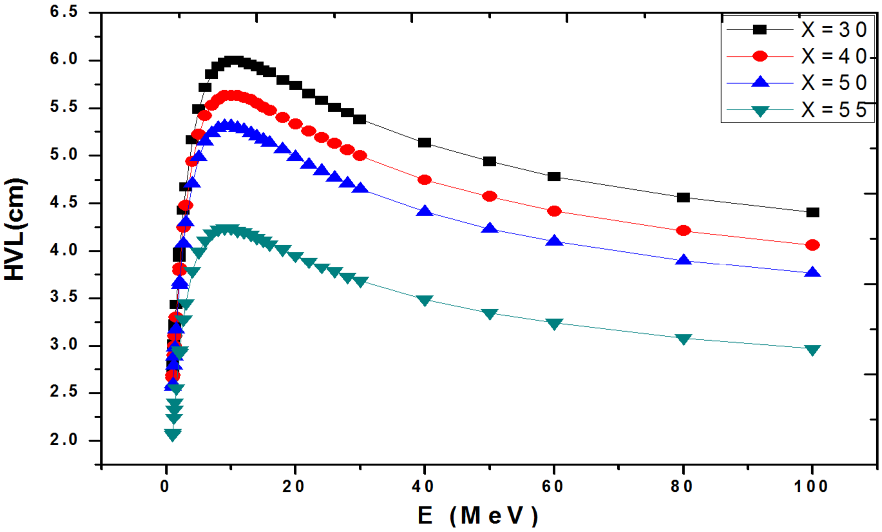

Figure 9. *The HVL of the samples at high energies (150 MeV–100 GeV).*

4. Conclusion

The electronic polarizability and oxide ion polarizability increase with increasing refractive index and decreasing optical band gap energy. The optical basicity of the glass materials increase by increasing number of oxide ion polarizability. The optical basicity shows that the glass materials are more basic. It is suggested that the ability of oxide ionized to donate electrons to surrounding cations increases.

The previous relations represent is a good basis for predicting new nonlinear optical materials and glasses could be produced both in terms of transparency and radiation shielding.

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