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Physical and Optical Properties of CeO_2 BaO B_2O_3 Glasses

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Abstract: The influence of compositional variations on the physical properties such as density, molar volume, optical electronegativity, optical energy gap, refractive index, optical basicity, oxide ion polarizability, molar refraction, third order nonlinear susceptibility, non linear refractive index and metallization with the variation in CeO_2 content has been studied theoretically for x CeO_2 (20-x) BaO 80 B_2O_3, where (x = 0, 2, 4, 6, 8 and 10) and analyzed the physical parameters related to these compositions with theoretical predictions.

Keywords: Susceptibility, Polarizability, Optical Basicity, Metallization

1. Introduction

Nonlinear optics is the study of phenomena that occur as a consequence of the modification of the optical properties of a material system in the presence of light. Dimitrov and Sakka [1], found that the most important factors which govern the nonlinear response of simple oxide are the linear refractive index and the optical energy gap which are related with oxide metallicity. It is suggested that oxides with a high nonlinear refractive index are found to possess a high linear refractive index and a small optical energy gap which has been attributed to the increase of oxide metallicity. The estimation of electronic polarazibility of ions is the subject of the so called polarizability approach in material science. The plorizability approach has shown renewed interest because of the need to design optical functional materials and to search for novel glasses with higher optical performance, such as oxide glasses with high third order nonlinearities [2]. It is suggested that oxides with a high nonlinear refractive index are found to possess high values of optical basicity and high values of oxide ion polorizability [3-6]. Cerium doped glasses show potential applications in the field of laser windows optics and communication [7]. The optical properties of CeO_2 doped BaO B_2O_3 glasses have been studied [8]. It was found that, the value of the optical energy gap decrease due to formation of BO_4 groups with an additional of cerium oxide content. Also, the presence of boron oxide helps for conversion of Ce^{3+} to Ce^{4+} ions. The purpose of the present paper to study the physical properties of x CeO_2 (20-x) BaO 80 B_2O_3 where (x = 0, 2, 4, 6, 8 and 10).

2. Theoretical Calculations

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

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

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:

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

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

The optical electronegativity can be calculated as follows,

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

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

The optical energy gap can be calculated [11]

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

The optical basicity can be calculated [11]

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

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

$$= 0.9\Delta\chi^*+3.59 \quad (5)$$

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

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

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

$$\chi^{(3)}=(1.4x10^{-11})/((E_{opt}-1.96)(E_{opt}-1.31)(E_{opt}-0.65)) \quad (7)$$

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

$$n_2 = ((12x3.14) / n_0) (\chi^{(3)}) \quad (8)$$

3. Discussion and Results

3.1. Density and Molar Volume

The values of theoretical density for all the studied glasses are listed in table 1. It is clear that, the values of density increase by increasing CeO_2 content. This due to the replacement of the oxide (BaO) by oxide (CeO_2). So the addition of CeO_2 to network causes some type of structural re-arrangement of the atoms. There is a possibility for the alteration of the geometrical configuration upon substitution of CeO_2 into the glass network. Molar volume is an important physical property, it is noted that, the density increases, congruent with a decrease in the molar volume as the CeO_2 content as shown in table 1.

Table 1. *Composition, molecular weight, theoretical density, experimental density, molar volume, for all the Studied samples.*

Sample	Molecular weight (g/mole)	Density (g/cm^3)	Molar volume V_m (cm^3)
20BaO 80 B_2O_3	86.362	3.112	27.751
2CeO_2 18 BaO 80 B_2O_3	86.738	3.140	27.624
4CeO_2 16 BaO 80 B_2O_3	87.114	3.168	27.498
6CeO_2 14 BaO 80 B_2O_3	87.489	3.197	27.366
8CeO_2 12 BaO 80 B_2O_3	87.865	3.225	27.245
10$CeO_2$10 BaO 80 B_2O_3	88.241	3.253	27.126

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

The values of optical electronegativity for all the studied samples are listed in table 2. It is clear that $\Delta\chi^*$ decreases with increasing CeO_2 content so the samples are considered to be covalent in nature.

The value of theoretical optical band gap energy decreases by increasing CeO_2 content. This decreasing due to formation of BO_4 groups with an additional of cerium oxide content [8]. Also, the presence of boron oxide helps for conversion of Ce^{3+} to Ce^{4+} ions, these two factors, are responsible for the decrease of the values of optical energy gap [8]. Also, it is clear that the theoretical values of E_{op} are larger than the experimental values, this due to the amorphous nature of prepared samples.

Table 2. *Composition, optical electronegativity, theoretical and experimental optical energy gap, for all the Studied samples.*

Sample	Optical electronegativity	Theoretical optical energy gap (eV)	Experimental optical energy gap (eV)
20BaO 80 B_2O_3	2.0898	7.77	2.80
2CeO_2 18 BaO 80 B_2O_3	2.0799	7.74	2.18
4CeO_2 16 BaO 80 B_2O_3	2.0700	7.70	2.00
6CeO_2 14 BaO 80 B_2O_3	2.0600	7.66	1.63
8CeO_2 12 BaO 80 B_2O_3	2.0504	7.63	1.54
10CeO_2 10 BaO 80 B_2O_3	2.0405	7.59	1.47

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

The theoretical 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 for all the studied samples are listed in table 3. The increased optical basicity of the glasses with CeO_2 content indicates that the glass system is basic in nature.

Also the electronic polarizability of oxide ion increase with increasing the optical basicity. The values of the electronic polarizability of oxide ions are listed in Table 3.

Table 3. *Composition, optical basicity, oxide ion polorazibility, refractive index, molar refractivity, for all the Studied samples.*

Sample	Optical basicity (A_{th})	Oxide ion polarizability (α^{02-}) (A^0) ^{3}	Molar refractivity (cm^3/ mol)	Refractive index
20BaO 80 B_2O_3	0.655	1.619	10.454	1.679
2CeO_2 18 BaO 80 B_2O_3	0.660	1.628	10.439	1.683
4CeO_2 16 BaO 80 B_2O_3	0.665	1.637	10.436	1.686
6CeO_2 14 BaO 80 B_2O_3	0.670	1.646	10.430	1.690
8CeO_2 12 BaO 80 B_2O_3	0.675	1.655	10.417	1.693
10CeO_2 10 BaO 80 B_2O_3	0.680	1.664	10.415	1.697

3.4. The Linear Refractive Index

Table 3 shows that the values of the refractive index increase by increasing CeO_2 content. The refractive index depends on the oxide ion polorazibility of glass material [12 - 15]. The values of refractive index increase as well as the values of the oxide ion polorazibility increase due to the creation of non oxygen bridging atoms.

3.5. The Molar Refraction

The molar refraction can be calculated [2, 16] with respect to the optical band gap. The molar refraction = the molar volume (1-(optical energy gap/20)$^{0.5}$). The values of molar refraction are listed in table 3. It is clear, that the values of the molar refraction increase by increasing CeO_2 content.

3.6. The Metallization Criterion

The metallization criterion (the nature of metallic and non metallic of oxide glasses) can be calculated and explained [2, 13] on predicting the nature of solids which is metallic or non metallic based on the condition of (molar refraction /molar volume) <1 (insulator) and >1 (metal), by using the following equation (2),

Metallization criterion = 1- (molar refraction/molar volume). The metallization criterion values are listed in table 4. It is clear that the metallization criterion values are found to be less than one and thus all the studied samples exhibit insulating behavior [17 -20].

Table 4. *Composition, metallization criterion, third order nonlinear susceptibility, nonlinear refractive index, for all the Studied samples.*

Sample	The metallization criterion	(Third order nonlinear susceptibility) χ^3x10^{-13}esu.	(Nonlinear refractive index)*10^{-12}
20BaO 80 B_2O_3	0.623	5.24	1.176
2CeO_2 18 BaO 80 B_2O_3	0.622	5.31	1.189
4CeO_2 16 BaO 80 B_2O_3	0.620	5.41	1.209
6CeO_2 14 BaO 80 B_2O_3	0.619	5.52	1.231
8CeO_2 12 BaO 80 B_2O_3	0.618	5.60	1.246
10CeO_2 10 BaO 80 B_2O_3	0.616	5.71	1.268

3.7. The Third Order Nonlinear Susceptibility and Nonlinear Refractive Index

The values of third order nonlinear susceptibility are listed in table 4. It was found that the values of third order nonlinear optical susceptibility for all the studied samples increase by increasing CeO_2 content. Also from table 3 and table 4, it can be noticed that the third order nonlinear susceptibility increases with decreasing the optical energy gap and increasing the refractive index for all the studied samples.

It can be noticed that from table 4 by increasing CeO_2 content, the values of nonlinear refractive index increase. Figure 1 and 2 seen that nonlinear refractive index increases with decreasing the optical energy gap and increasing the refractive index for all the studied samples.

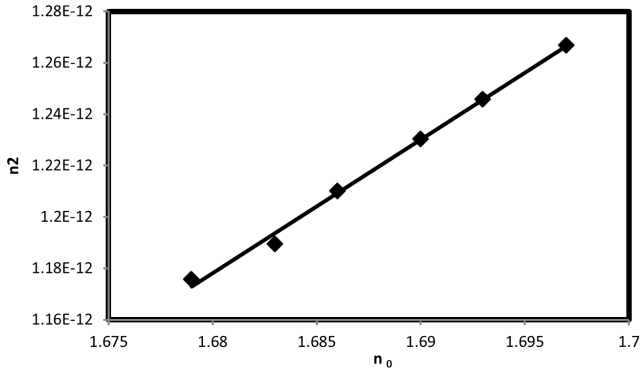

Figure 1. *The nonlinear refractive index as a function of refractive index.*

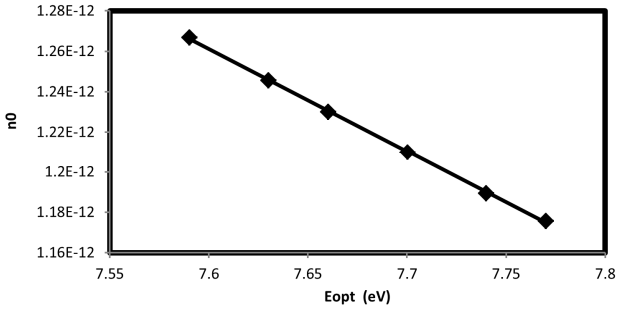

Figure 2. *Nonlinear refractive index as a function of the optical energy gap.*

4. Conclusion

From all the above discussion, it was found that, the optical basicity of the glass materials increase by increasing number of oxide ion polarizability. The value of 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. Also, both of the values of third order nonlinear susceptibility and the values of nonlinear refractive index increase with decreasing the optical energy gap and increasing the refractive index for all the studied samples. Finally, all the above values are a good basis for predicting new nonlinear optical materials.

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