Research/Technical Note

A New Empirical Method for Estimating the Refractive Index of Oxide Glasses Using Internal Structure Information

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Abstract: This paper is a simple idea aims to how to get an imagination about the variation of glass refractive index with its internal structure. In the present work an empirical equation for the refractive index of a glass sample has been achieved as function of both the glass molar Volume and the glass electronegativity. Like this equation, may be used to determine and estimate the refractive index value of an inorganic oxide glass sample, if its density measured with high accuracy.

Keywords: Oxides Glasses, Amorphous Materials, Refractive Index, Density, Molar Volume

1. Introduction

Many years ago a lot of scientific research papers especially in the field of the glass technology, had concerned and focused on the study of the inorganic oxide glass structure and the glass optical properties. These glasses have a lot of potential applications, For example; Borate glasses containing alkali or alkaline earth cations, are good candidates for ion conduction and suitable for the fabrication of solid state batteries [1]. While Borate glasses with heavy metal ions such as Bi, Pb, Zn etc. exhibit good nonlinear optical properties [2], [3]. Borate glasses containing lead oxide have several applications including radiation shields, optical, and thermal properties [3], [4]. Similarly bismuth containing oxide glasses have advantages such as host materials for lasers, long IR cut-off, glass ceramics, memory, and switching devices [5], [6], [7]. Therefore, this work has been performed and aims to investigate an empirical relation correlate the glass structure directly to its optical properties especially the refractive index.

Table 1. Glass System [13]: 60% B₂O₃ – 30% PbO – 10% Bi₂O₃ – x% Nd₂O₃.

x	0	0.1	0.2	0.5	01
n _{exp}	1.65	1.63	1.65	1.63	1.64
n _{gomaa}	1.52	1.52	1.52	1.52	15.2
Δn	± 0.13	± 0.11	± 0.13	± 0.11	± 0.12

Table 2. Glass System [14]: 60% B₂O₃ – 20% ZnO – 8% Al₂O₃ – (12-x)% Bi₂O₃ – x% Dy₂O₃.

x	0.5	01	1.5	02	2.5
n _{exp}	1.80	1.80	1.80	1.80	1.80
n _{gomaa}	1.74	1.74	1.74	1.74	1.74
Δn	± 0.06	± 0.06	± 0.06	± 0.06	± 0.06

Table 3. Glass System [15]: (63-x)% B₂O₃ – 15% ZnO – 20% Bi₂O₃ – 2% EuO – xLi₂O.

x	0	5	10	15
n _{exp}	2.44	2.44	2.44	2.44
n _{gomaa}	2.10	2.27	2.45	2.65
Δn	± 0.34	± 0.17	± 0.01	± 0.015

Table 4. Glass System [16]: 20% B₂O₃ – (80-x)% TeO – x% Al₂O₃.

X	0	5	10
n _{exp}	2.28	2.26	2.25
n _{gomaa}	1.98	1.97	1.96
Δn	± 0.3	± 0.29	± 0.29

Table 5. Glass System [17]: (75-x)% B₂O₃ - x% WO₃ - 25% GeO₃.

X	25	30	35	470	45	50	55	60	65
n _{exp}	1.82	1.83	1.85	1.86	1.88	1.90	1.91	1.93	1.94
n _{goma}	1.78	1.81	1.83	1.85	1.87	1.89	1.91	1.94	1.96
Δn	0.02	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.01

2. Theoretical Background

2.1. Density and Molar Volume

The density of solid material is a good tool to recognize any changes occur in its internal structure. So the density measurement is common feature in most glass research papers. Both the density and the molecular weight are used to calculate the volume occupied by one mole of atoms in the glass matrix, like this volume is called glass molar volume. The values of the glass molar volume are useful for getting a good imagine about the glass homogeneity, stability, transition temperature as well as the variation of the refractive index. The molar volume V_m of a glass sample may described mathematically by the following relation, where M_w and ρ are the Molecular weight and density of a glass sample [8], [9].

$$V_m = \frac{M_w}{\rho}$$

Where, M_w and ρ are the molecular weight and density of the glass sample.

2.2. Electronegativity

The electronegativity of an atom is known as the relative ability of this atom to attract the chemical bond electrons toward itself. For a group of atoms the average electronegativity was introduced by both of Asokamani (1989) [10] and Marquez (2006) [11], [12] as seen in the following formula; Where χ_i refers to Pauling electronegativity, n_i is the number of atoms of i^{th} elements while N is the total atoms in the chemical compound.

$$\chi_{av} = \frac{\sum_{i=1}^N n_i \chi_i}{N}$$

This relation has been reformulation [12], as following, to be suitable to calculate electronegativity for the oxide glasses; where r_j is molar fraction of the oxide j^{th} in the glass matrix

$$\chi_{glass} = \frac{\sum_{i=1}^N n_i \chi_i}{N} r_j$$

By inspecting a lot of related papers the author tried to get empirical mathematical formula correlate both the molar volume and the electronegativity of the oxide glasses to their refractive index values. Finally, after many erroneous attempts the following formula has been achieved; where n_{goma} is the glass refractive index, A and B are the numbers of cations and all atoms in the glass chemical formula, respectively.

$$n_{goma} = 3.44 \frac{A}{B} \left(\frac{1}{V_m} \right)^{-\chi_{glass}}$$

For testing this relation, it was be used to calculate the values of refractive index that already measured and investigated throughout many published papers for many glass systems. The following tables 1, 2, 3, 4 and 5 exhibit comparison processes between the measured and calculated n values, for many glass systems, as examples of the validity of the suggested formula.

3. Results & Discussion

By inspecting the pervious tables carefully it can be observed that the behavior of the calculated refractive index is mostly the same of the measured one. Like result may use to expect and get primary logic imagination about the change of refractive index with the change in the glass structure without any optical measurements. Also, all the previous tables show that the calculated value of the refractive index is increasing or decreasing from the measured values by an amount differ from a glass system to another. This difference between the calculated and measured Value of the refractive index was found to depend on the accuracy in the density measurements in addition to the molar volume and electronegativity calculations. Generally, Data in the previous tables refer to the possibility of expectation of the refractive behavior depending on the structure parameters. In other word, the new empirical relation can be used to check the glass density if its refractive index had measured in an accurate method.

According to the estimated relation, by plotting $\ln n$, the measured refractive index, versus the reciprocal of the glass molar volume the glass electronegativity can be obtained as seen in figure 1.

Figure 1. Ln of the refractive index verses rescipocal of molar volume.

4. Conclusion

An empirical relation was investigated to calculate the glass refractive index using the glass molar volume and glass electronegativity.

$$n_{goma} = 3.44 \frac{A}{B} \left(\frac{1}{V_m} \right)^{-\chi_{glass}}$$

This empirical relation success in relate/correlate the glass refractive index, and hence, the glass optical properties to the internal changes in its structure.

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