ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Computational Spectroscopic Analysis By Using Clausius–Mossotti Method For Sodium Borate Glass Doped Neodymium Oxide.

Elbashar YH[a]*, and Aly Saeed[b]

[a]Department of Physics, Faculty of science, Aswan University, Aswan, Egypt.
[b]Basic Science Department, Faculty of Engineering, Egyptian-Russian University-Cairo, Egypt.

ABSTRACT

The present work study the refractive index by using Clausius–Mossotti method, which deals with the ion refraction of the atoms for glass system with chemical composition as (x-42) B_2O_3. (100-x) Na_2CO_3.40ZnO.2Nd_2O_3 (where x=100, 95, 90, 85,80and75), density was measured, and the molar mass, refractive index, molar refraction, reflectance, phase velocity, Brewster angle, polarizability, electric susceptibility and elasto optic coefficient were estimated.

Keywords: spectroscopic analysis, Clausius–Mossotti, glass science

Corresponding author

INTRODUCTION

Photonic glass has developed in many applications [1-6]. Zinc borate glass is very attractive to the glass fabricators and scientists because of the melting point of this type of glass low, and that can be easy to be shaped and mold. This type of glass have some peculiar properties like low thermal expansion coefficient, good electrical resistance and chemical stability [7]. The significance of its optical properties leads to the scientist for doping this type of glass by rare earth elements [8-11]. Clausius–Mossotti method was very successive for calculating the refractive index from ion refraction which is standard for every element in the period table [12, 13]. The estimating of elasto optic coefficient from refractive index by using Clausius–Mossotti can be calculated for non-cubic crystal and glass [14-16]. The laser designer focus on this type of study for high power solid state laser, because of the changing of the refractive index due to the stresses due to pumping and thermal effect, the study done in both modeling and measurements for various type of laser mediums and optical fibers[17-22]. The present article deals with the effect of Na_2O addition of elasto optic coefficient mathematically by using Clausius–Mossotti model.

EXPERIMENTAL

Sample preparation

Neodymium doped Borate glass system with a chemical composition (x-42) B_2O_3. (100-x) Na_2CO_3.40ZnO.2Nd_2O_3 (where x=100, 95, 90, 85,80and75), was prepared by conventional melting method in a porcelain crucible by heating up to 1150 ^{0}C. The well mixed powders were preheated at 600 ^{0}C for 1.5 hours to release gases, and then heated up to 1150 ^{0}C for 1 hour with clockwise shaking to ensure high homogeneity. The casting glass were quenched and annealing in at 410, 405, 400, 370, 350 and 350 ^{0}C respectively for 1h holding time, and the furnace was switched off to reach the room temperature.

XRD analysis

The X-ray powder diffraction (XRD) technique was used for glass samples. The measurement was obtained by using Bruker AXS D8 Advance XRD diffractometer. The results observed no peaks were indicating crystalline nature of the prepared samples.

Density measurements

The densities of glass samples were determined at room temperature by the conventional method Archimedes using a liquid toluene as immersing liquid [23]. The molar volume V was calculated using the relation below [24]:

$$V = \frac{M_{glass}}{\rho_{glass}} \text{ cm}^3 \quad (1)$$

RESULT AND DISCUSSION

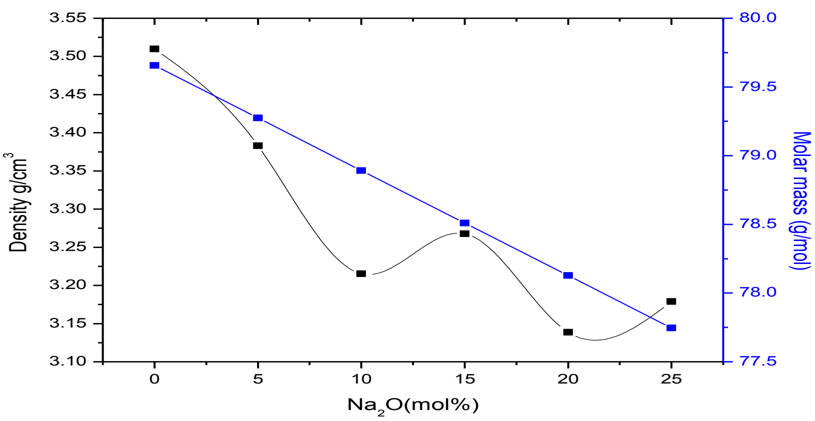

Figure 1: Molar mass, density as a function of Na_2O mol. % for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

Neodymium doped zinc borate sodium glass with chemical composition as (X-42) B_2O_3. (100-x) Na_2CO_3.40ZnO.2Nd_2O_3 (where x=100, 95, 90, 85,80and75) were evaluated and achieved with the variation of the Na_2O concentration and densities with molar mass as shown in Fig.1

The calculation of molar refraction as shown in Fig.2 can be calculating by using Clausius–Mossotti as the following equation [25, 26]:

$$R = \sum_i A_i R_i \qquad (2)$$

Table 1: The ion refraction for the elements that used in the glass system.

Ion	Ionic refraction
B^{+3}	0.006
Na^{+}	0.47
Zn^{+2}	0.71
Nd^{+3}	1.41
O^{-2}	6.95

Where A_i Atomic fractions and R_i Ionic refraction

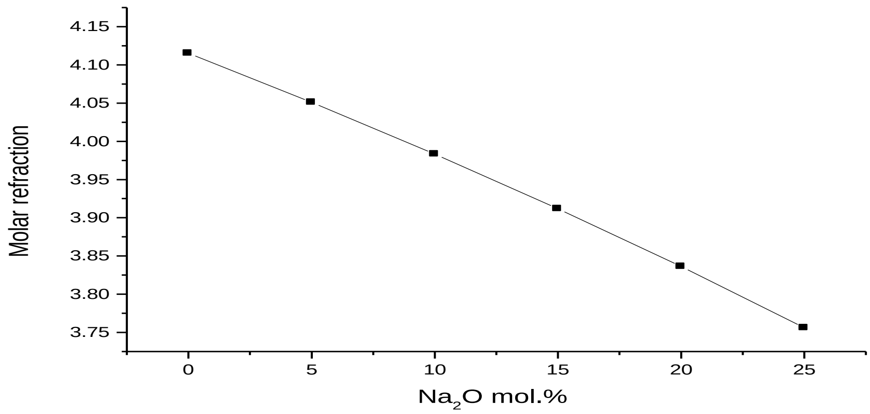

Figure 2: Molar refractivity vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

The refractive index as shown in Fig.3 can be calculating by the following equation [25]:

$$R = \frac{M}{\rho}\frac{n^2-1}{n^2+2} \qquad (3)$$

where M is the molecular weight , ρ is the density and n refractive index

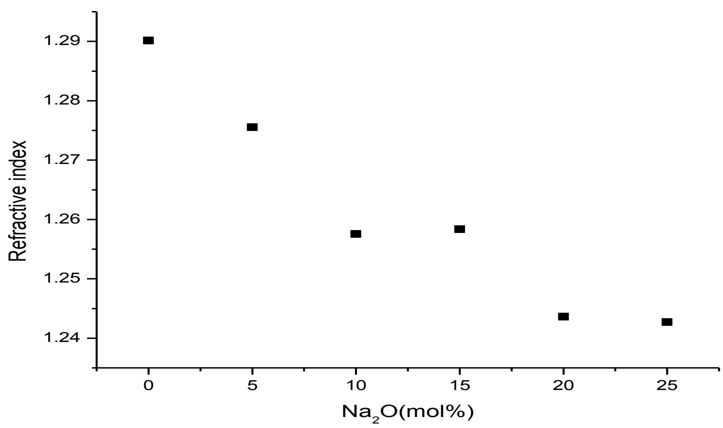

Figure 3: Refractive index vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

The reflectance as shown in Fig.4 can be calculated by the using the following equation [27]:

$$R = \frac{(n-1)^2}{(n+1)^2} \quad (3)$$

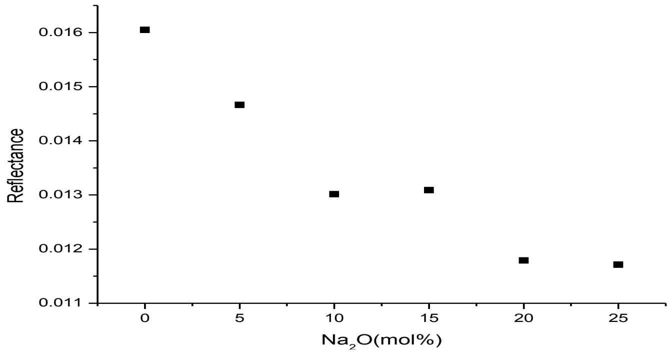

Figure 4: reflectance vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

The permittivity, polarizability[28] and elasto optic coefficient as shown in Figs.5,6,7 were calculated by the following equations[29]:

$$\varepsilon = n^2 \quad (4)$$

$$\gamma = \frac{3}{4\pi N}\frac{\varepsilon-1}{\varepsilon+2} \quad (5)$$

$$p \approx \frac{(1-B)(1+2B)}{3} \quad \textbf{(6)}$$

$$B = \frac{1}{\varepsilon} \quad \textbf{(7)}$$

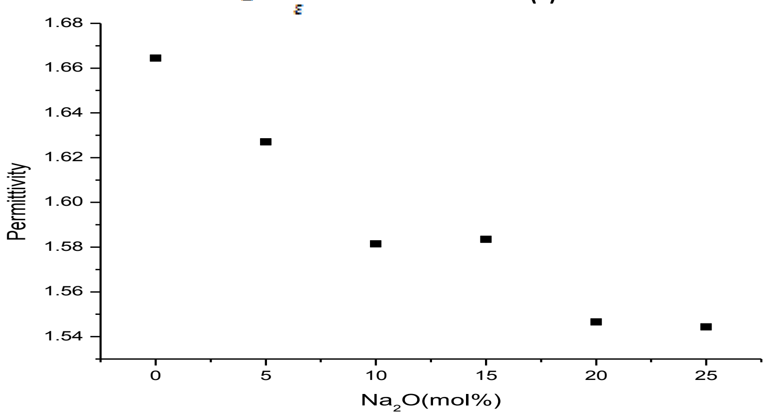

Figure 5: Permittivity vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

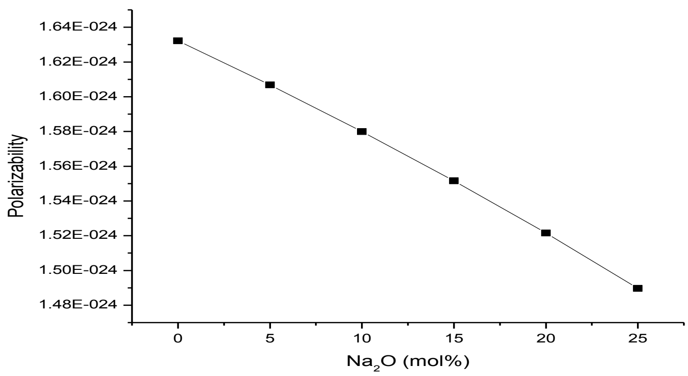

Figure 6: Polarizability vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

ISSN: 0975-8585

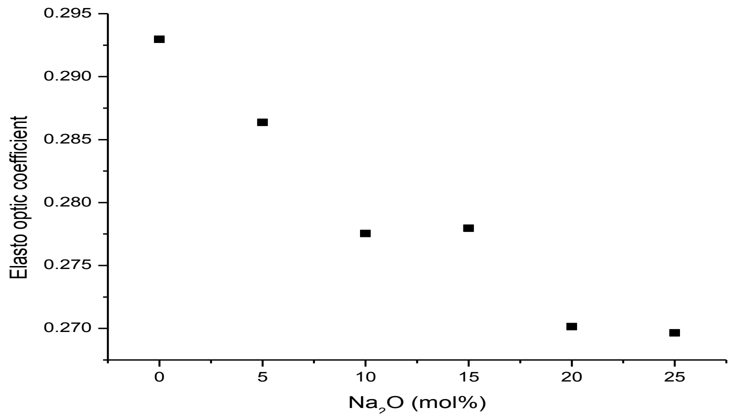

Figure 7: Elasto optic coefficient vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

The Electric susceptibility as shown in Figs.8 was calculated by the following equation [28]:

$$\chi = \frac{(\varepsilon-1)}{4\pi} \qquad (8)$$

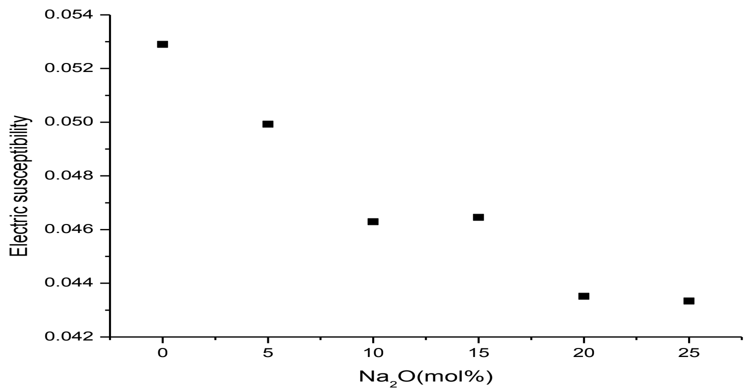

Figure 8 Electric susceptibility vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

The Brewster's angle as shown in Figs.9 was calculated by the following equation [30]:

$$\text{Brewster's angle} = \arctan\left(\frac{n_2}{n_1}\right) \qquad (9)$$

n_1= 1 for air

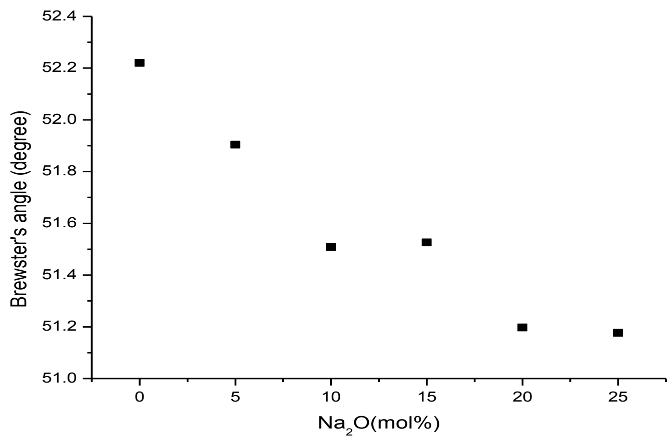

Figure 9: The Brewster's angle vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

The speed of light of the medium as shown in Figs.10 was calculated by the following equation [31]:

$$v = \frac{c}{n} \quad (11)$$

Where c the speed of light in the vacuum 3 x 10^8, v is the speed of light in the medium and n the refractive index

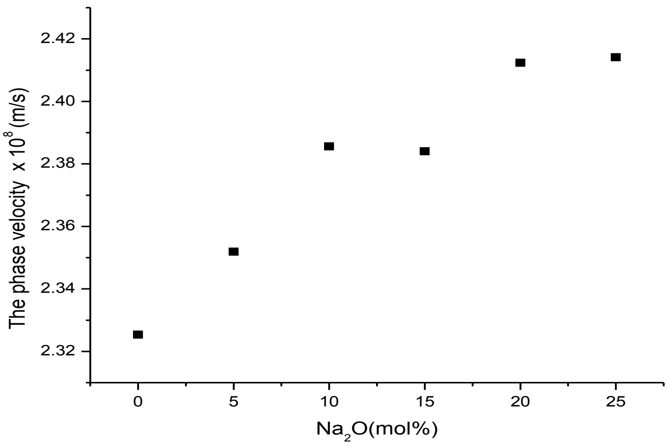

Figure 10: The speed of light of the medium vs. Na_2O mol.% for B_2O_3-Na_2O-ZnO- Nd_2O_3 glasses

CONCLUSION

We investigated some optical properties by using Clausius–Mossotti method like refractive index, molar refraction, reflectance, phase velocity, Brewster angle, polarizability, electric susceptibility and elasto optic coefficient. The method is successive for calculating optical properties from the chemical composition of oxide glass. The Na2O contains increases with decrease the quality of optical properties in the glass composition.

REFERENCES

[1] Rayan DA, Elbashar YH, Rashad MM. and El-Korashy A. J Non- Crystall Solids 2013;382: 52–56 .
[2] Elhaes H, Attallah M, Elbashar Y , Ibrahim M, El-Okr M. J Physica B: Condensed Matter 2014;449:251–254.
[3] Aly Saeed RM, El shazly YH, et al. J Radiat Physics Chem 2014 ;102:167-170.
[4] Nehal Aboulfotoh, Yahia Elbashar, Mohamed Ibrahem, Mohamed Elokr. J Ceramics Int 2014; 40 (7): 10395–10399.
[5] Hanan Elhaes, Mohamed Attallah, Yahia Elbashar, Ayser Al-Alousi, Mohamed El-Okr, and Medhat Ibrahim. J Comput Theor Nanosci 2014;11:2079-2084.
[6] DA Rayan, YH Elbashar, AB El Basaty and MM Rashad. Res J Pharm Biol Chem Sci 2015;6(3):1026-1030
[7] NM Bobkova and SA Khot'ko. J App Spectroscopy 2005;72(6): 853.
[8] A Speghini, et al. J Alloys Compounds 2000; 300-301:174.
[9] Bettinelli, Speghini A, Ferrari M and Montagna M. J Non- Crystall Solids 1996; 201(3): 211.
[10] Bettinelli M and Speghini A. Solid State Commun 1996;97(6): 521.
[11] AE Burns, DW Winslow, WJ Clarida, M Affatigato, SA Feller and RK Brow. J Non- Crystall Solids 2006;352(23-25):2364.
[12] Joseph Simmons and Kelly S. Potter, Optical Materials, Academic Press, 2000.
[13] SR Palit. Pure Appl Chem 1965;10(4):505-526.
[14] Sebastien Chenais, Frederic Druon, Sebastien Forget, Francois Balembois, Patrick Georges. Progr Quantum Electron 2006;30:89–153.
[15] Daniel Royer, Eugene Dieulesaint, S.N. Lyle, Elastic Waves in Solids II: Generation, Acousto-optic Interaction, Applications, Springer; 1 edition, 2000
[16] W Luis Mochan and Ruben G Barrera. Physical Review B 1985; 32(8):4989-5001.

[17] Wenjie Xiea, Siu-Chung Tam , Lam Yee-Loy , Jingang Liu , Hongru Yang , Jianhui Gu , Wilson Tan , Feng Zhou. Optics & Laser Technology 2000;32:199-203.
[18] DL Yu, DY Tang. Optics & Laser Technology 2003;35:37 – 42.
[19] E Safari, A Kachanov. Optics & Laser Technology 2006;38:534–539.
[20] Shandarov S, Burimov N, Veretennikov S. IEEE 10.1109LEOS.1996.565235
[21] Yu Lu, et al. IEEE Q M 10.1109/ISAF.2000.942380
[22] Johnson VR, Olson FA. IEEE 10.1109/PROC.1967.5652
[23] R El-Mallawany, A Abousehly, AA El-Rahamani and E Yousef. Mater Chem Physics 1998;52(2): 161
[24] JE Shelby, Introduction to Glass Science and Technology, Second Edition, the Royal Society of Chemistry 2005
[25] Joseph Simmons and Kelly S. Potter, Optical Materials, Academic Press, 2000
[26] SF Shaukat, Ya-ming Dong, R Farooq and PR Hobson, Journal of Shanghai University (English Edition), 2001; 5(3) 201-204.
[27] MY Nadeem, Waqas Ahmed. Turk J Phy 2000;24;651 – 659
[28] Walter Greiner. Classical Electrodynamics, Springer, 1998
[29] Daniel Royer, Eugene Dieulesaint. Elastic Waves in Solids II: Generation, Acousto-optic Interaction, Applications ,Springer, 1999
[30] Ralf Menzel. Photonics: linear and nonlinear interactions of laser light and matter, Springer, 2001
[31] Frank Träger. Handbook of lasers and optics, Springer, 2007.