Study of the correlation between optical properties and the variations of nano-scale free volume in bismuth borate glasses

A Thesis Submitted for the degree of Master of Science as a partial fulfillment for requirements of the Master of Science

(Applied Nuclear Physics)

To

Physics Department – Faculty of Science

Ain Shams University

By

Naglaa Fathy Osman Mansour

B.Sc. in Physics, 2006

Supervised by

Prof. Dr. Mona Mohamed Abd Latif Mohsen

Professor of Nuclear Physics - Physics Department

Faculty of Science – Ain Shams University

Prof. Dr. Ehsan A. H. Gomaa

Physics Department

Faculty of Science

Ain Shams University

Prof. Dr. Manal Abd El- Baki

Glass Department

National Research Center

Dokki

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Approval Sheet

Candidate Name : Naglaa Fathy Osman Mansour.

Thesis Title : Study of the correlation between optical properties and the variations of nano-scale free volume in bismuth borate glasses.

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Supervisors: **Signature**

1- Prof. Dr. Mona M. A. Mohsen.

2- Prof. Dr. Ehsan A. H. Gomaa.

3- Prof. Dr. Manal A. El. Baki.

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Title Sheet

Name : Naglaa Fathy Osman Mansour

Degree : M.Sc. in Physics

Department : Physics

Faculty : Faculty of Science

University : Ain Shams University

Graduation Year : 2006

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Abstract

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Name : ***Naglaa Fathy Osman Mansour***

Title : "Study of the correlation between optical properties and the variations of nano-scale free volume in bismuth borate glasses".

Submitted to: *Department of Physics, Faculty of Science, Ain Shams University.*

Abstract:

Bismuth borate glasses with compositions x (Bi_2O_3) – (100-x) (B_2O_3) (where x is in mol. % ranging from 25-50 in steps of 5) have been prepared by using melt quenching technique.

The glass transition temperature (T_g) of the tested samples has been measured in the temperature range 0˚C to 600˚C with heating rate of 10˚C/min by differential thermal analysis (DTA). It is found that the glass transition temperature (T_g) decreases with increasing Bi_2O_3 content, which indicates that the degree of disorder increases.

Furthermore, the density, molar volume and oxygen packing density have been studied. It has been found that the density increases as well as the molar volume. However, the oxygen packing density decreases by increasing the Bi_2O_3 content which gives an indication that the structure becomes loosely packed.

Positron Annihilation Lifetime (PAL), Fourier Transform Infra-Red (FTIR) and X-ray Diffraction (XRD) measurements

have been performed to study the amorphous and defect structure as well as the vibrating band structure. PAL results have revealed weak formation of ortho-positronium (o-Ps) at amorphous sites, where the positronium is the bound state of a positron and an electron. At low concentration, the pore size at these sites increases from 2.5 nm to 3.5 nm with increase of Bi_2O_3 content then shows weak decrease to 3 nm at higher concentration showing also a reduction in the relative pore fraction from 9.8% to 1% in agreement with XRD spectra, which indicates the presence of some peaks associated with Bi_2O_3 phase.

The correlation between the optical properties deduced from FTIR spectra, and the positron annihilation lifetime parameters has been investigated. The decrease of the annihilation lifetime τ_2 of trapped positrons at defects with Bi_2O_3, suggests a free annihilation of positrons at non-bridging oxygen (NBO) bonds, which is also evidenced by the positive correlation between I_1 and the number of NBO atoms.

FTIR spectra revealed the presence of bonds, that are assigned to vibrations of Bi-O bonds from [BiO_3] pyramidal and [BiO_6] octahedral units and B-O bonds from [BO_3] and [BO_4] units. On the other hand, increasing Bi_2O_3 up to 35% concentrations have led to increase in the optical basicity or polarizability because the ionic radii of Bi^{2+} is larger than those of B^{2+}. Consequently, a decrease in the optical band gap energy (E_g) with Bi_2O_3 is observed. Therefore it is to be expected that an increase in the refractive index will occur.

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