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Comparative studies between theoretical and experimental of elastic properties and irradiation effects of soda lime glasses doped with neodymium oxide

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HIGHLIGHTS

- Results show good agreement between experimental and theoretical of elastic moduli.
- Network bonding was distorted with the Nd_2O_3 was added and irradiated.
- Transformation of the glass network structure from Q_4 to Q_3 after irradiation.

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ABSTRACT

A comparative studies on the theoretical and experimental values of elastic moduli of $(90 - x)\text{RWG} - (10)\text{Na}_2\text{O} - (x)\text{Nd}_2\text{O}_3$ glass system, where RWG is recycled window glass and x is 0.001, 0.01, 0.1 and 1 mol%, was investigated. The radiation effects on structural properties and elastic moduli were evaluated by measuring the ultrasonic velocities. In addition, the FTIR spectra were measured to investigate the effects of irradiation on the structure of the glass. Moreover, the theoretical bond compression model was used to confirm the obtained results from the experiments. The results show that evidently changes in the structure of the glass depend on the concentration of the neodymium oxide and gamma irradiation. Furthermore, the experimental elastic moduli are in good agreement with the theoretical values.

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1. Introduction

Glasses materials are receiving extensive attention due to their unique properties such as hardness, transparency at room temperature, high strength and excellent corrosion resistance. Continued effort for the improvement of new glassy materials and the study of their properties is highly relevant because of the potential in various technological fields. Glassy systems have physical isotropy, the absence of grain boundaries, continuously variable composition and good work ability over their crystalline counterparts (Joseph et al., 2002). Moreover, the radiation damage processes which emerge in glass are generically the same as those which occur in crystals. In the simplest provision, there are three basic processes: (i) radiolysis, (ii) displacement (or knock on) damage, and (iii) electron rearrangement. In all processes, what we define as damage is the existence of after irradiation local structures (either atomic or electronic) which differ from the structure

present before irradiation (Ezz-Eldin et al., 1996). Irradiation affects the structure of the glass matrix, resulting in changes in the optical, physical and electrical properties. Therefore, the scientific information of the glass structure before and after irradiation is a requirement for understanding the structural evolution of nuclear glasses under long term irradiation during storage of radioactive wastes or isotopes sources, radiation shielding, radiation detection by using glass dosimeter, etc. (Neuville et al., 2003). Studies on irradiated glasses have been previously published on simple glass systems such as silicate glasses (Devine, 1994) or on multi-component glasses such as borosilicate glasses (Kaur et al., 2013; Abdelghany et al., 2014; AbdelAziz et al., 2014).

Glasses containing rare-earth ions have attracted a great deal of interest due to their important properties. For examples, the glasses are heat-resistant, present interesting optical and magnetic behavior (Clare, 1994; Lemerrier et al., 1996; Clayden et al., 1999). The properties of rare-earth glasses include greater glass transition temperatures, greater hardness and elastic modulus, and greater chemical durability than many other glasses (Lemerrier 1996; Clayden et al., 1999). Therefore, the rare-earth glasses have been successfully used as laser

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ion hosts, optical lenses, seals, and vivo radiation delivery vehicles (Lin and Hwang, 1996; Shelby and Kohli, 1990). Among all the rare-earth ions doped in glasses, the neodymium (III) ion has been distinguished as one of the most efficient ones for obtaining laser emission, frequency up-conversion and optical fiber amplification (Jayasimhadir et al., 2007). Thus, the effects of gamma irradiation on structural properties of rare-earth glasses have been interested to investigation.

The properties of glass are closely related to the inter-atomic forces and potentials in the lattice structure. Therefore, changes in the lattice, due to doping and/or irradiation, can be directly noted. The elastic properties and other related parameters are of great interest, in order to study the linear and anomalous variations as a function of composition of glass, and have been interpreted in terms of the structure or transformation of cross-linkages in the glass network (Rajendran et al., 2001; Sharma et al., 2009). To study the structural properties of glass, the coordination numbers of the network structure and the change of oxygen bonds in the network former, induced by the cation modifiers and/or irradiation, need to be investigated. The information can be obtained from FTIR spectroscopy. Furthermore, many researchers use ultrasonic techniques for investigation the effects of irradiation on structural properties of glass (Sharma et al., 2009; Zahran, 1998; El-Mallawany et al., 1998; Laopaiboon and Bootjomchai 2014a, 2014b). Therefore, the ultrasonic technique is an appropriate tool for characterizing the microstructure, the deformation process and the structural properties of materials after successive irradiation. Moreover, the depth scientific results of structural properties by using bond compression model were reported (Abd El-Moneim, 2001; Marzouk and Gaafar, 2007). Thus, the theoretical values of elastic moduli were calculated by using the bond compression model to compare between the experimental and theoretical modulus (Gaafar and Marzouk, 2007; Abd El-Moneim, 2003).

Therefore, the investigation of the influence of rare-earth oxides (ROs) contents and gamma irradiation on the structural properties of silicate glasses has been interested. In this article, the effects of rare-earth oxides contents and irradiation on structural properties of glass samples were studied via ultrasonic techniques and FTIR spectroscopy. The elastic moduli of the glass samples before and after irradiation with different concentration of neodymium oxide will be discussed. Information about the structure of the glass samples can be deduced after calculating the number of network bonds per unit volume, the average cross-link density, the number of vibrating atoms per unit volume, the average stretching force constant and the average ring size. Moreover, the theoretical and experimental of elastic moduli have been compared.

2. Experimental work

2.1. Glass Preparation

The glass samples were prepared in rectangular shapes from the $(90 - x)\text{RWG} - (10)\text{Na}_2\text{O} - (x)\text{Nd}_2\text{O}_3$ glass system (where RWG

is recycled window glass and x are 0.001, 0.01, 0.1 and 1 mol%) using the melt-quenching method. The oxides of Na_2O and Nd_2O_3 used in this work were of an analytical reagent grade. The RWG was common window glass sold in Ubon Ratchathani, Thailand. The chemical composition of RWG was determined in my previous work (Bootjomchai and Laopaiboon, 2014). Preparation of recycling glass from window glass to be used in this work is to thoroughly clean and grind until powdery. To prepare the glass samples, appropriate amounts of Na_2O , Nd_2O_3 and RWG powders were weighed using an electronic balance with the accuracy of the order of 0.0001 g. The starting materials were mixed thoroughly in ceramic crucibles. The mixture was preheated at 573 K for 1 h to remove H_2O and CO_2 . The preheated mixture was then melted in an electric furnace whose temperature was controlled at 1523 K to ensure homogeneity. The melted glass was then poured into preheated stainless steel molds at about 723 K and then annealing was carried out for a period of 2 h at 773 K. Bulk glass samples of about $1.5 \times 1.5 \times 1.0 \text{ cm}^3$ were thus obtained. The glass samples were polished using different silicon carbide grades. The sample thicknesses were measured to the micrometer.

2.2. Density and molar volume measurements

The density (ρ) of each sample was measured by using Archimedes' principle with n -hexane as immersion liquid. The experiments were repeated three times for accurate value of the density. The estimated error in these measurements was approximately $\pm 0.001 \text{ g cm}^{-3}$. The molar volume (V_a) was calculated for each glass from the expression; $V_a = M/\rho$, where M is the molecular weight of the glass, calculated according to the relation (1) (Abd El-Moneim et al., 2006).

$$M = \sum_i x_i M_i \quad (1)$$

where x_i is the mole fraction of the component oxide i and M_i is its molecular weight. The glass packing density can be calculated from the following Eqs. (2)–(3) (Hager, 2012)

$$V_t = \frac{\rho}{M} \sum_i x_i V_i \quad (2)$$

where V_i is given by,

$$V_i = \frac{4\pi N_A}{3} (x r_M^3 + y r_O^3) \quad (3)$$

where N_A is Avogadro's number, and where r_M and r_O are the ionic radii of the cation and anion of the oxide M_xO_y , respectively. The errors in molar volume and packing density were acquired from experiments repeated three times of densities. The estimated error in these results was $\pm 0.021 \text{ cm}^3 \text{ mol}^{-1}$ and $\pm 0.0013 \times 10^{-6} \text{ m}^3$, respectively and shown in Table 1.

Table 1

Glass composition, density (ρ), molar volume (V_a) and packing density (V_t) of the glass samples before and after gamma irradiation.

Sample no.	Composition (mol%)			ρ (g cm^{-3}) ± 0.001		V_a ($\text{cm}^3 \text{ mol}^{-1}$) ± 0.021		$V_t \times 10^{-6}$ (m^3) ± 0.0013	
	RWG	Na_2O	Nd_2O_3	Before	After	Before	After	Before	After
G-0	90	10	0	2.567	2.565	23.351	23.3747	0.4592	0.4588
G-1	89.999	10	0.001	2.572	2.558	23.313	23.4391	0.4609	0.4584
G-2	89.990	10	0.01	2.570	2.554	23.340	23.4911	0.4690	0.4660
G-3	89.900	10	0.1	2.575	2.560	23.416	23.5458	0.5530	0.5500
G-4	89	10	1	2.656	2.647	23.837	23.9225	1.3838	1.3789

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