Theoretical analysis for ultrasonic properties of vanadate-phosphate glasses over an extended range of composition: Part II

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ABSTRACT

Makishima-Mackenzie's theory and Abd El-Moneim's semi-empirical formulas were used to predict the compositional dependence of ultrasonic properties in binary V_2O_5-P_2O_5 (45 mol% ≥ V_2O_5 ≤ 85 mol%) glasses at room temperature and at 8 MHz frequency. Anomalous behavior between the calculated dissociation energy per unit volume of the glass and ultrasonic properties was discussed in terms of the basic structural units that constituting the glass network. Values of the dissociation energy per unit volume of the glass were calculated from the average single bond strengths proposed by Dimitrov and Komatsu for chemical bonds in the basic structural units of V_2O_5 and P_2O_5 oxides. The ring deformation model has also been used to estimate the mean atomic ring size of the glass network from data of bulk modulus and average first-order stretching force constant of V-O-P linkages. It has been found that, the average single bond strengths of P—O bonds in PO_4 groups and V—O bonds in VO_4 and VO_5 groups play a dominant role in correcting the anomalous behavior between the calculated dissociation energy per unit volume of the glass and ultrasonic properties. Values of the theoretical elastic moduli, which have been calculated on the basis of Makishima-Mackenzie's theory, are in a very good agreement with the corresponding experimental ones. Moreover, Abd El-Moneim's semi-empirical formulas, which correlate ultrasonic attenuation coefficient with the corrected dissociation energy per unit volume, mean atomic ring size, oxygen density and packing density, appear to be valid for the investigated glass samples.

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1. Introduction

Phosphate glasses are interesting materials especially in connection with their diverse applications. Recently, phosphate-based glasses found a variety of technological and optical applications, due to their specific properties, such as good thermal and mechanical stabilities, high transparency, low refractive index and low melting temperature [1–3]. In particular, binary V_2O_5-P_2O_5 glasses exhibit semiconducting properties arising from electron transfer between V^{+4} and V^{+5} ions [4,5]. A review of literature indicated that a lot of studies have been made, with different characterization methods, on the structure and physical properties of P_2O_5- and V_2O_5-based glasses [6–13]. Results of an X-ray photoelectrons spectroscopy (XPS) and magnetic susceptibility identified the presence of primarily P—O—P, P—O—V and V—O—V structural bonds in binary V_2O_5-P_2O_5 glasses [6]. Wright and his co-workers [7] investigated some V_2O_5-based glasses by using neutron diffraction technique. It has been found that the vanadate network of P_2O_5-V_2O_5, BaO-V_2O_5 and PbO-V_2O_5 glasses is composed of distorted, interconnected, VO_5 trigonal bipyramids/tetragonal pyramids. In case of binary P_2O_5-V_2O_5 glasses, all phosphorus atoms are coordinated by four oxygen atoms and the PO_4 tetrahedra share corners with VO_5 bi-pyramids. XANES (X-ray Absorption Near Edge Structure) study of the valence state of vanadium in ternary Li_2O-V_2O_5-P_2O_5 glasses also identified the presence of both V^{4+} and V^{5+} ions glass samples having high V_2O_5 concentration [10]. Furthermore, the relative abundance of vanadium V^{4+} valence state (V^{4+} / $[V^{4+} + V^{5+}]$) is a decreasing function of V_2O_5 in the glass. Recently, the atomic structures of vitreous V_2O_5 and binary V_2O_5-P_2O_5 glasses were investigated by X-ray and neutron diffraction [11]. Results revealed that the short-range structure of vitreous V_2O_5 and $73V_2O_5$-$27P_2O_5$ glass sample is composed of mixtures of VO_5 and VO_4 structural units.

The study of ultrasonic/acoustical properties of glasses by ultrasonic techniques is also very significant for characterization and understanding their structure. The measurement of ultrasonic properties, as a function of composition, can produce considerable information about the microstructure of glasses and behavior of the network formers and modifiers. In recent years, there are interesting reports in the literature, which deal with the study of ultrasonic properties of binary V_2O_5-P_2O_5 glasses over a wide range of composition by using ultrasonic techniques [12–14]. Mukherjee et al. [12] measured the elastic moduli and ultrasonic attenuation coefficient of V_2O_5-P_2O_5 (47.69 mol% ≥ V_2O_5 ≤ 82.27 mol%) glasses as a function of composition and temperature. Farley and Saunders [13] also

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reported the experimental data of elastic moduli for V_2O_5-P_2O_5 (45 mol% ≥ V_2O_5 ≤ 85 mol%) glasses at room temperature. The results revealed that the substitution of P_2O_5 by V_2O_5 leads to a reduction in the rigidity (weakness) and loose packing of the glass network.

Attempts [14–28] have been made, in the few last years, to predict the composition dependence of ultrasonic properties in inorganic glasses at room temperature. In case of ultrasonic attenuation, the most widely used model is the one proposed recently by Abd El-Moneim [15,16], which expressed the coefficient of longitudinal ultrasonic attenuation in terms of the dissociation energy per unit volume, packing density, oxygen density, first-order stretching force constant, mean atomic ring size and bulk modulus of the glass. In Ref. [14], we interpreted the effect of the transition metal oxide V_2O_5 on the structure, physical and ultrasonic properties of binary V_2O_5-P_2O_5 (45 mol% ≥ V_2O_5 ≤ 85 mol%) glasses. Many significant compositional parameters, such as molar volume, excess molar volume, number of network bonds per unit volume, dissociation energy per unit volume, packing density and first order stretching force constants of P—O and V—O bonds were evaluated for each glass sample and correlated with ultrasonic parameters. The correlation has been carried out on the basis of Abd El-Moneim's semi-empirical formulas [15,16] for ultrasonic coefficient and Makishima-Mackenzie's theory [17,18] for elastic moduli. However, the following negative results were reported, due to the anomalous behavior between calculated dissociation energy per unit volume of the glass and ultrasonic properties:

i- The agreement between theoretical and experimental values of elastic moduli is unsatisfactory for all the investigated V_2O_5-P_2O_5 glass samples; and

ii- Abd El-Moneim's semi-empirical formula [15,16], which correlates the ultrasonic attenuation coefficient with the first-order stretching force constant, dissociation energy per unit volume and packing density, appears to be invalid for this type of glasses.

The goal of the present study is to complete our previous work on the correlation between ultrasonic and compositional properties of binary V_2O_5-P_2O_5 glasses [14]. An attempt has been made to correct the anomalous behavior between the calculated dissociation energy per unit volume of the glass and ultrasonic properties. The dissociation energy per unit volume of the glass was calculated from the average single bond strength of chemical bonds that are present in the basic structural units of the glass network. The mean atomic ring size of the glass network has also been estimated from data of bulk modulus and average first-order stretching force constant of V-O-P linkages. The obtained data of dissociation energy per unit volume and mean atomic ring size, beside those of packing density, average first-order stretching force constant and oxygen density were used to predict the composition dependence of ultrasonic attenuation coefficient on the basis of Abd El-Moneim's model [15,16]. Furthermore, the theoretical values of elastic moduli were calculated from Makishima-Mackenzie's theory [17,18] and compared with the corresponding observed values.

1.1. Makishima-Mackenzie's theory [17,18] for elastic moduli

Makishima and Mackenzie [17,18] have worked out a theoretical model to calculate the packing density, dissociation energy per unit volume and elastic moduli of multi-component inorganic oxide glasses from the molar fractions, packing factors and dissociation energies per unit volume of the oxide constituents. On the basis of this model [17,18], the above mentioned parameters can be expressed as

Packing density $\quad V_t = \dfrac{\rho}{M} \sum\limits_i x_i \ V_i$ (1)

Dissociation energy per unit volume $\quad G_t = \sum\limits_i G_i x_i$ (2)

Bulk modulus $\quad K_{th.} = 10\, G_t V_t^2$ (3)

Young's modulus $\quad E_{th.} = 8.36\, G_t V_t$ (4)

where $M = \sum x_i M_i$ and ρ are the respective molecular weight and density of the glass, whereas x_i, M_i, V_i and G_i are the molar fraction, molecular weight, packing factor and dissociation energy per unit volume of oxide component i, respectively. The dissociation energy per unit volume and packing factor can be calculated for an oxide A_yO_z from the following equations:

$$V_i = \frac{4}{3}\pi N_a \left(y R_A^3 + z R_O^3 \right)$$ (5)

$$G_i = \rho_i U_i / M_i$$ (6)

where N_a is Avogadro's number, R_A and R_O are the respective ionic radius of metal and oxygen, whereas ρ_i and U_i are the respective density and molar dissociation energy of oxide component i.

1.2. Abd El-Moneim's semi-empirical formulas [15,16] for ultrasonic attenuation coefficient

Recently, Abd El-Moneim [15,16] reported a model, known as Abd El-Moneim's model [15,16], to predict the composition dependence of ultrasonic attenuation coefficient in inorganic oxide glasses at room temperature. On the basis of this model, the ultrasonic attenuation coefficient (α) can be expressed in terms of oxygen density ($[O]$), average first-order stretching force constant (F), means atomic ring size (ℓ), dissociation energy per unit volume (G_t), packing density (V_t) and experimental bulk modulus (K) of the glass according to the following semi-empirical formulas:

$$\alpha = \frac{\chi_1}{F} (F/K)^{m/4}$$ (7)

$$\alpha = \chi_2 \frac{[O]}{F} \ell^m$$ (8)

$$\alpha = \frac{\chi_1}{F} \left(F/10 G_t V_t^2 \right)^{m/4}$$ (9)

where χ_1 and χ_2 are two frequency dependent constants, whereas m is a positive power, its value depends upon the type of the glass. Meanwhile, the average first-order stretching force constant of a multi-component glass can be estimated from an equation reported by Higazy and Bridge [19] in the form

$$F = \frac{\sum\limits_i x_i\, n_i f_i}{\sum\limits_i x_i\, n_i}$$ (10)

where n_i is the number of network bonds per cation (coordination number of cation) in oxide component i with cation-anion bond length r_i and first-order stretching force constant $f_i = 17/r_i^3$.

Gopal et al. [20] and Rajendran et al. [21] proposed the following equation, which correlates the experimental bulk modulus (K) with molar volume of the glass,

$$K V_M^b = C$$ (11)

where b and C are two constants, their values depend on the type of glass and its composition. Very recently, Abd El-Moneim [14] has used Eqs. (3) and (11) to eliminate V_t^2 and G_t from Eq. (9) and reported the following semi-empirical relationship, which relates the ultrasonic attenuation coefficient with both the average first-order starching force