Properties and Structure of ROR2ONa2OAl2O3P2O5 Glasses

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Properties and Structure of RO-R_2O-Na_2O-Al_2O_3–P_2O_5 Glasses

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Abstract. The properties and structural features of RO-R_2O-Na $_2O$-Al_2O_3–P_2O_5 (R= Mg, Ca, Ba and RO= Li) glasses in the system have been investigated. The properties of those glasses seem to depend on the field strength of the alkali or alkali-earth ions in glasses as in silicate glasses. Infrared (IR) spectroscopy indicates that the glass network is dominated by bridging P-tetrahedral present in glasses with O/P $\approx$3.0. The variation in physical properties of the glasses seem to be closely related to the variation in structure of the glasses and could be explained by simple mechanism such as field strength and differences in mass.

Keywords: Density, glass transition, molar volume, alkali, alkaline-earth, IR spectroscopy, phosphate glasses.
PACS: 71.23.Cq

INTRODUCTION

Phosphate glasses have been well received because of their special properties and applications compared with their silicate counterparts, they have low glass transition temperatures and are well suited for doping with rare-earth ions for the production of laser amplification glass or Faraday rotators [1]. The high thermal expansion coefficient and low glass transition temperature of alkali aluminophosphate glasses make them useful for hermetic sealing technology [2,3]. The chemical durability of iron phosphate glasses is better than that of the borosilicate glasses and up to 50 wt% of certain nuclear waste can be vitrified in these glasses, as a result they are potential candidates as a host matrix to vitrify certain high level nuclear wastes [4]. Even though there have been many studies of phosphate glasses, there have been limited studies of RO-R_2O-Na $_2O$-Al_2O_3–P_2O_5 glasses in term of the properties and the glass structure.

The properties of alkali or alkali-earth phosphate glasses have been studied by many researchers [5]. Most of the properties of those glasses seem to depend on the field strength of the alkali or alkali-earth ion in glasses as in silicate glasses.

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Therefore, one can expect that RO-R_2O-Na $_2O$-Al_2O_3–P_2O_5 glasses will follow a similar trend in properties and structure as RO-R_2O-Na $_2O$-Al_2O_3–SiO_2 glasses.

However it is important to verify this assumption because the structure of phosphate glasses is quite different from that of silicate glasses. It has been shown that the alkali or alkaline-earth phosphate glasses generally have a linear chain structure, which differed from the silicate structure [6]. The aim of this investigation was to study the structure and properties of RO-R_2O-Na $_2O$-Al_2O_3–P_2O_5 glasses in terms of variation of the alkali or alkaline-earth oxide.

EXPERIMENTAL TECHNIQUES

Preparation of Sample

Glasses were synthesized by melting dry mixtures of 25 g according to the composition 20(RO-R_2O)-5Na_2O-5Al_2O_3–70P_2O_5 (R = Mg, Ca, Ba and RO = Li). To react the constituents, the mixed powders were heated in an electrical furnace at 350°C for 1h, and then melted in another furnace at 1300°C. To ensure proper mixing and homogeneity, the molten liquid was shaken frequently and vigorously. After being checked, the melt was cast by pouring as fast as possible into hot steel split mould to quench it to form a glass. The glass was immediately transferred to an annealing furnace at 250°C where it was kept for 3 h to relieve any residual stress which could cause embrittlement. At the end of this annealing process, the furnace was switched off and the glass left to cool down to the room temperature gradually by controlled thermal treatment at cooling rate of 0.5°C/min. The sample were selectively cut, ground, and polished. After preparation, samples were stored in plastic containers in desiccators until the FTIR and DTA measurement was performed. The amorphous nature of the samples was checked by X-ray diffraction. The density, D, of the glass samples was measured at room temperature using the Archimedes method with toluene as an immersing liquid.

Measurements of DTA

The equipment used to carry out the thermal measurement was a Perkin-Elmer Pyris Diamond TG/DTA Series system, which was operated under standard atmospheric conditions. The maximum temperature that could be reached by the instrument was approximately 1400°C. The same weight of fine standard and sample (± 5-20 mg) were loaded in an alumina crucible and were heated at a rate of 10°C/min for all samples. With the combination of built-in computer and UNIX operating system. It was possible to obtain DTA curves and the required data for analysis.

Measurements of IR Spectra

A Perkin Elmer 1600 Fourier Transform infra red (FTIR) have been used to investigate all sample prepared using the KBr pellet technique. Typically around 2 mg

of the finely ground sample is mixed with 200 mg of KBr powder and the mixture then pressed for 4 minutes, in evacuable die under 10 tons of pressure to give a transparent disk with a surface area of 1 cm^3. The FTIR spectra were recorded in the spectral range of 4000 – 400 cm^{-1} resolution and 64 scans to ensure a good signal to noise ratio.

RESULTS AND DISCUSSION

As shown in Table 1, the densities of the $20(RO\text{-}R_2O)\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ glasses with no substitution, where R is Ba, Ca, Mg and R_2O is Li increased in the order of Li < Mg< Ca < Ba, as expected from the relative masses of the alkaline-earth and alkali ions.

TABLE 1. Composition and some measured parameters of $20(RO\text{-}R_2O)\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ glasses.

RO (mol)	R_2O (mol%)	Na_2O (mol%)	Al_2O_3 (mol%)	P_2O_5 (mol%)	Density (gcm^{-3})	Molar Volume (cm^3/mole)	Glass Transition(°C)
20	-	5	5	70	3.12	44.29	370
20	-	5	5	70	2.56	46.44	405
20	-	5	5	70	2.52	45.87	440
	20	5	5	70	2.38	47.69	330

R= Ba, Ca, Mg
R_2= Li

The molar volumes of the glasses have also shown a similar trend. The variation in the molar volume as well as the density in this glass system is very hard to explain using a simple mechanism. It should be noted that the molar volume $20CaO\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ glass was lower than that the $20MgO\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ glass, which is discussed below in terms of the structure of the glass.

The glass transition temperature of the above mentioned glass system, as shown in Table 1, the glass transition temperature decreased in order of MgO>CaO>BaO>Li_2O. This is also attributed mainly to the lower field strength of the Na^+ than that of the alkali and alkaline earth ion, resulting in a loosely bonded structure. A similar trend in variation of properties in the alkali, alkali-earth metaphosphate glasses have been observed previously [7].

The IR spectra of $20(RO\text{-}R_2O)\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ glasses is shown in Fig. 1. The spectra are similar to those that reported for other metaphosphate glasses [8,9]. In general, there are seven major bands observed at around 1365, 1268, 1062, 954, 864, 744, and 470 cm^{-1}. These bands can be assigned to the P-O-P sym.str unperturbed, P-O-P bending $\nu_{as}PO_2$, $\nu_s PO_2$, POP, ν_sPOP, and δPO_2 modes of $(PO_3)_n$ chain groups, respectively [9]. The intensity of strong bands observed around 1365, 1268,1062 and 954 cm^{-1} for the glasses of $20(RO\text{-}R_2O)\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ decreases as the relative mass of alkali or alkali – earth increases, and their frequencies shift to lower values. However, there are no significant structural changes to the metaphosphate network and there is no evidence for the presence of significant concentrations of

terminal PO_3 groups, these observations are consistent with the analyzed compositions which yield O/P ratio of ≈ 3.0.

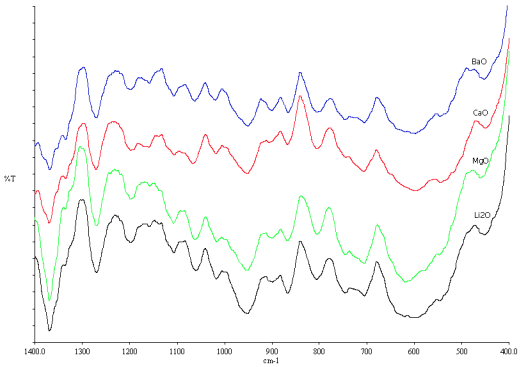

FIGURE 1. IR spectra of $20(RO\text{-}R_2O)\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ (R= Mg, Ca, Ba and RO= Li) glasses.

CONCLUSIONS

The properties and structure of glasses in the $20(RO\text{-}R_2O)\text{-}5Na_2O\text{-}5Al_2O_3\text{–}70P_2O_5$ has been investigated. IR spectroscopy reveals the glass networks are dominated by bridging P-tetrahedra that constitute the metaphosphate chains, with O/P ≈ 3.0. The variation in physical properties of the glasses seem to be closely related to the variation in structure of the glasses and could be explained by simple mechanism such as field strength and differences in mass.

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