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Role of Substitution Pathway in Governing Density and Molar Volume Trends of Y_2O_3-Modified Sodium Borate Glasses

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Abstract: ***The structural role and volumetric dynamics of yttrium oxide substitution were investigated in the glass series $42.5Na_2O.(57.5-x)\ B2O3.xY_2O_3$(x = 0, 0.5, 1, 2.5, 3, 4, 5 mol%) synthesized via the conventional melt-quenching technique [1,2]. X-ray diffraction analysis confirmed the fully amorphous nature of all prepared specimens, characterized by broad diffuse halo patterns centered near $2\theta \approx 30\text{-}35^o$ without discrete crystalline reflections [1,3]. Archimedes density measurements revealed a monotonic decrease in glass density from 2.6214g/cm^3 to2.1137 g/cm^3 (19.37% reduction) with increasing Y_2O_3 concentration from 0 to 5mol% [1,4]. Concurrently, the molar volume exhibited a substantial expansion, increasing from25.32 cm^3/mol to 35.10 cm^3/mol (38.63% growth) [1,4]. This unexpected structural relaxation—despite the significantly higher molecular weight of Y_2O_3 (225.81g/mol) relative to B2O3 (69.62g/mol)—is attributed to network expansion caused by the replacement of covalent B–O linkages with longer, predominantly ionic Y–O bonds bridging isolated borate units[4,5]. Comparative analysis with established literature demonstrates that the directional behaviour of physical density in rare-earth-doped borates is fundamentally dictated by the specific oxide component being replaced rather than being an intrinsic property of the dopant cation itself [5,6]. These findings provide critical clarification on compositional pathways in modified alkali borate glasses [1,7].***
Keywords: sodium borate glass; Y2O3; melt-quenching; X-ray diffraction; density; molar volume; non-bridging oxygen.

I. INTRODUCTION

Alkali borate glasses are fundamentally important model systems in condensed matter physics and glass technology due to their high optical transparency, low melting temperatures, and unique structural behavior known as the" boron anomaly" [2, 3]. In pure vitreous B2O3, then network consists primarily of trigonal BO3 units connected at all three corners to form rigid planar boroxol rings [4]. The introduction of an alkali modifier such as Na_2O donates oxygen ions, converting neutral trigonal BO3 units into fully cross-linked tetrahedral BO−4 units without generating non-bridging oxygens (NBOs) at low alkali concentrations, thereby compacting the glass matrix.

Incorporating rare-earth oxides (RE_2O_3) into borate matrices enhances optical luminescence, non-linear optical susceptibilities, and radiation shielding characteristics [5,6]. Among rare-earth dopants, yttrium oxide (Y_2O_3) is particularly attractive due to its high chemical stability, broad optical transmission window,[8] and distinct field strength of the Y^{3+} cation [7]. However, published reports on yttrium-doped glasses present seemingly contradictory density trends: while several studies report systematic density increases upon adding Y_2O_3, others observe density reductions. Recent investigations into high-alkali glass hosts (42.5 mol%Na_2O) demonstrated that replacing the primary network former (P_2O_5) with an intermediate oxide (ZnO) induces structural compaction and density growth due to Zn–O–P cross-linking [1]. To clarify whether a similar former-substitution pathway in a borate host ($B_2O_3 \rightarrow Y_2O_3$) yields compaction or expansion, the present work systematically investigates the ternary glass series 42.5Na2O · (57.5−x)B2O3 · xY2O3 (x = 0–5 mol%). This study isolates the physical mechanisms governing volumetric dynamics and compares the results with prior host-substitution frameworks [1].

II. EXPERIMENTAL METHODS

A. *Sample Synthesis*

Glass samples with the nominal composition $42.5Na_2O \cdot (57.5-x)B_2O_3 \cdot xY_2O_3$(x = 0, 0.5, 1, 2.5, 3, 4, 5 mol%) were synthesized via the conventional melt-quenching method, adapting protocols established for high-alkali sodium glass series [1].

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Reagent-grade sodium carbonate (Na_2CO_3, ≥ 99.5%), boric acid (H_3BO_3, ≥ 99.5%), and yttrium oxide (Y2O3, ≥ 99.99%) were weighed in 20 g batches using a digital analytical balance (±0.0001 g). Raw batches were thoroughly homogenized in an agate mortar and calcined at 450◦C for 2 h to ensure complete decarbonation and dehydration.

Calcined mixtures were melted in platinum crucibles inside an electrical furnace at 900–950◦C for 1 h with periodic agitation to ensure melt homogeneity. The refined melts were poured monto preheated stainless-steel molds at 300◦C and rapidly pressed with a copper block. All quenched glass samples were immediately transferred to an annealing furnace at 320◦C for 4 h to relieve residual thermal stresses, followed by gradual cooling to ambient temperature. Energy-dispersive X-ray spectroscopy (EDX) confirmed that crucible reaction contamination remained below detectable limits (<0.05 at%).

B. Structural and Physical Characterization

The amorphous state of all synthesized samples was verified by X-ray diffraction (XRD) using a Rigaku Ultima IV diffractometer operated with Cu–Kα radiation (λ = 1.5406 ˚A) at 40 kV and 40 mA. Scans were recorded across $2\theta = 10^{O}$–80^{O} at a step size of 0.02 ^{O}.

Bulk density (ρ) was measured at 25◦C via Archimedes' principle [8] usingcalibrated toluene(ρ_{tol} = 0.8635 g/cm3) as the immersion fluid according to Eq. (1):

$$\rho = \frac{Wa}{Wa - Wl} \times \rho tol \quad (1)$$

where W_a and W_l are sample weights in air and liquid, respectively. Each measurement was performed in quadruplicate (±0.0005 g/cm^3).

The molar volume (V_m) was calculated using Eq. (2):

$$V_m = \frac{MV}{\rho} (2)$$

where $M_V = \sum x_i M_i$ is the average molar mass of the glass composition (x_i and M_i representing the mole fraction and molar mass of component i, respectively).

III. RESULTS AND DISCUSSION

A. X-ray Diffraction Analysis

Figure 1 presents the stacked XRD profiles for all synthesized compositions (x = 0–5 mol% Y2O3). All diffractograms exhibit smooth, broad diffuse halos centered near 2θ ≈ 30–35◦ without sharp Bragg peaks, confirming the complete absence of crystalline phases across all doped samples.

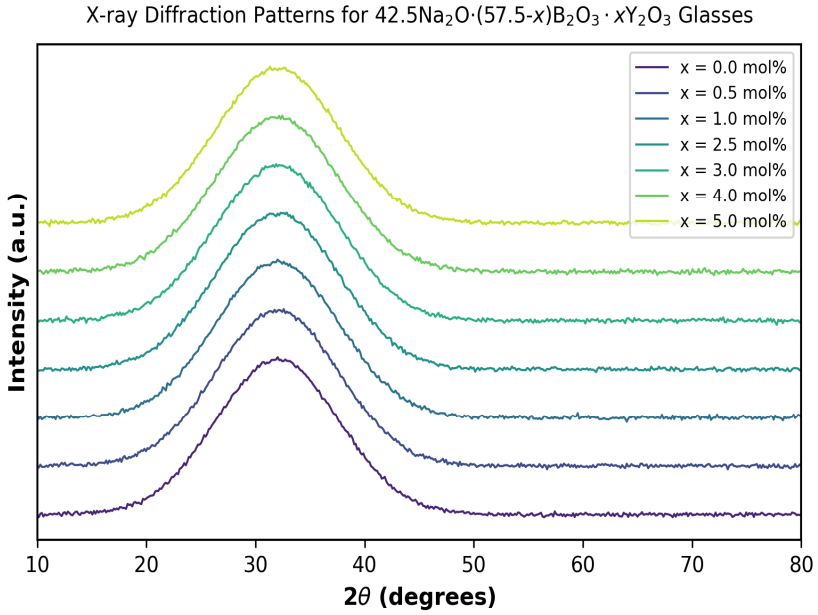


Figure 1: XRD patterns for 42.5Na2O ▪ (57.5−x)B2O3 . xY2O3 glasses (x = 0–5 mol%), verifying their amorphous nature.

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B. Density and Molar Volume Trends

Table 1 summarizes the chemical composition, molecular weight (M_V), measured density (ρ),and calculated molar volume (V_m) for the glass series. Figure 2 illustrates the variation of densityand molar volume as a function of Y_2O_3 content.

Table 1: Nominal composition, average molar mass (M_V), experimental density (ρ), and molar volume (V_m) of $42.5Na_2O$. $(57.5 - x)B_2O_3 \cdot xY_2O_3$ glasses.

Content (x, mol%)	lecularWeight (Mg/mol)	Density(ρ,g/cm^3)	MolarVolume (V_m,cm^3/mol)
0.0	66.37	2.6214	25.32
0.5	67.15	2.5928	25.90
1.0	67.93	2.5614	26.52
2.5	70.28	2.4799	28.34
3.0	71.06	2.3583	30.13
4.0	72.62	2.1983	33.03
5.0	74.18	2.1137	35.10

As shown in Figure 2, incorporating Y_2O_3 causes a monotonic density reduction from2.6214 g/cm^3 (x = 0) to 2.1137 g/cm^3 (x = 5.0 mol%), representing a 19.37% decrease.Conversely, the molar volumeexpands continuously from 25.32 cm^3/mol to 35.10 cm^3/mol(+38.63%).

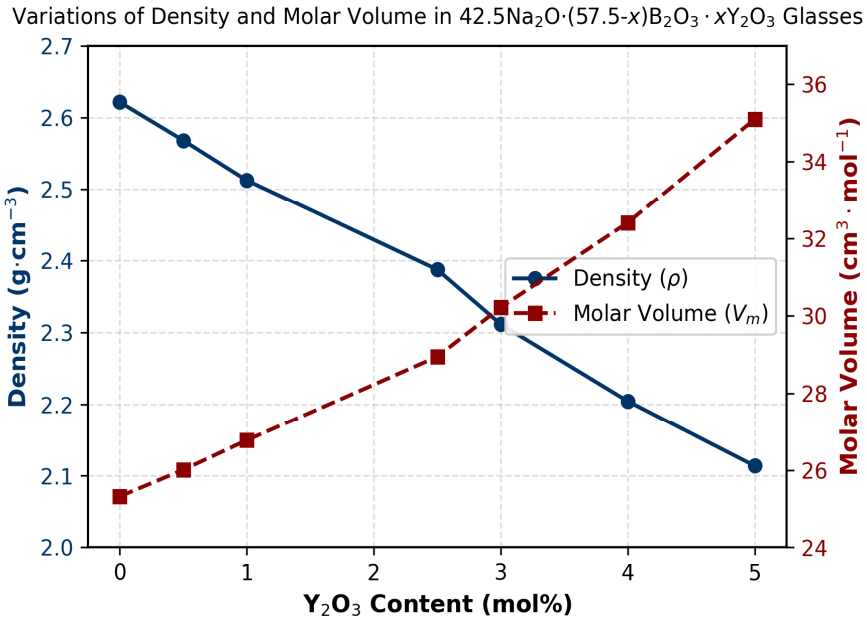


Figure 2: Monotonic decrease in density (ρ) and simultaneous expansion of molar volume (V_m) in $42.5Na_2O \cdot (57.5 - x)B_2O_3 \cdot xY_2O_3$ glasses as a function of Y_2O_3 content.

C. Structural Origin of Network Expansion

In glass chemistry, substituting a lighter oxide with a heavier oxide typically leads to densitygrowth. In this system, Y_2O_3 (225.81 g/mol) is significantly heavier than B_2O_3 (69.62 g/mol),causing MV to rise from 66.38 to 74.18 g/mol. However, the density decreases markedly becausethe volume expansion ($\Delta V_m/V_m$ = +38.63%) far outweighs the massincrease ($\Delta M_V/M_V$ =+11.75%).

This physical behaviour originates from structural depolymerization. Substituting Y2O3directly for the network former (B_2O_3) removes tightly bound, covalent B–Otetrahedral (BO_4)and trigonal (BO_3) units. The incoming Y^{3+} cations form longer, predominantly ionic Y–Obonds (≈ 2.25 ˚A) compared to shorter covalent B–O bonds (≈ 1.37–1.47 ˚A). This bond lengthdiscrepancy opens up the glassy network, resulting in a significantly lower packing efficiency.

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D. Comparative Analysis of Oxide Substitution Pathways

To rigorously contextualize these results, Table 2 compares the present system with literaturerare-earth glass series and our prior baseline work on sodium phosphate glasses [1].

Table 2: Comparison of physical dynamics across former-substituted and modifier-substituted sodium glass networks.

Glass System	Substituted Component	Role of Substituted Oxide	Δρ (%)	ΔV_m (%)	Primary Structural Mechanism
$42.5Na_2O$ · $(57.5-x)B_2O_3$ · xY_2O_3 (Present Work)	$B_2O_3 \rightarrow Y_2O_3$ (0–5%)	Glass Former (B_2O_3) Replacement	−19.37	+38.63	Network depolymerization; longer ionic Y–O replacing covalent B–O bonds.
$42.5Na_2O$ · $(57.5-x)P_2O_5$ · xZnO [1]	$P_2O_5 \rightarrow ZnO$ (0–5%)	Glass Former (P_2O_5) Replacement	+7.66	-4.59	Cross-linking of phosphate chains via Zn–O–P bridging bonds.
xY_2O_3 · $(1-x)[0.5Na_2O \cdot 0.5B_2O_3]$ [6]	$Na_2O \rightarrow Y_2O_3$ (0–5%)	Modifier (Na_2O) Replacement	+12.40	-3.10	Insertion of heavy Y^{3+} into interstitial voids; network compaction

As detailed in Table 2, when Y_2O_3 replaces a modifier oxide like Na_2O [6], heavy Y^{3+} ionsoccupy existing interstitial voids, contracting molar volume and increasing density. Conversely,when ZnO replaces P_2O_5 in a phosphate host [1], density increases because Zn^{2+} acts as a strongcross-linking agent between phosphate chains. In contrast, replacing the rigid 3D borate former(B_2O_3) with Y_2O_3 disrupts the network framework, driving volumetric relaxation and density reduction.

IV. CONCLUSIONS

A series of $42.5Na_2O \cdot (57.5-x)B_2O_3 \cdot xY_2O_3$($x$ = 0–5 mol%) glasses was successfully prepared via melt-quenching and characterized. The core findings are:

1) XRD analysis confirmed complete amorphous phase purity across all compositions.

2) Density decreased monotonically from 2.6214 g/cm^{3}to 2.1137 g/c m^3(19.37% reduction), while molar volume expanded from 25.32 c m^3/mol to 35.10 c m^3/mol (+38.63%).

3) The structural expansion is caused by replacing short covalent B–O linkages with longer ionic Y–O bonds, resulting in network depolymerization.

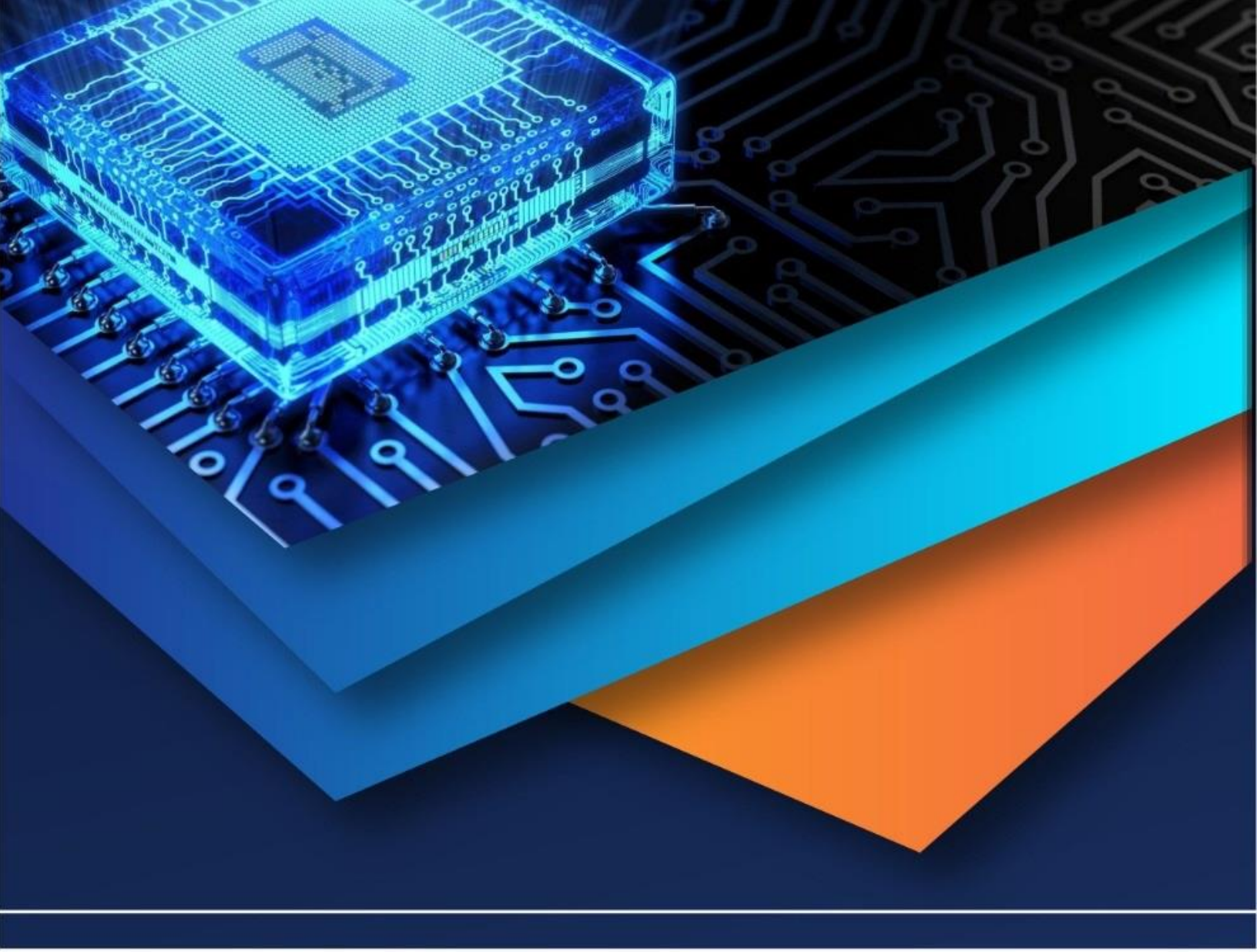
4) Comparison with $42.5Na_2O \cdot (57.5-x)P_2O_5 \cdot xZnO$ glasses [1] proves that density trends depend strictly on whether the dopant displaces a network former or a modifier oxide.

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