Structural and Optical Band Gap of Dy3+ doped P2O5-CaO-BaO-Gd2O3 Glasses

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Abstract. This study aims to determine the influence of variations in the composition of quartz sand on the physical properties and structure of phosphate glass medium doped with dysprosium ions (Dy^{3+}). Phosphate glass is known to have good glass network forming ability, high optical transparency, and compatibility against doping of rare-earth metals such as Dy^{33}, thus potentially being used in optoelectronic applications and luminescent materials. In this study, glass medium was synthesized using the melt quenching method, with a base composition of P_2O-CaO-BaO-Gd_2O_3 and addition of Dy_2O_3 by 0.5 mol%. Variations were made on the content of quartz sand as a source of silica to study its changes to the physical properties and structure of glass. Characterization of samples was performed using X-ray Diffraction (XRD) for amorphous structure analysis and phase transformation, Fourier Transform Infrared (FTIR) spectroscopy was utilized to detect chemical bonds, in conjunction with density and thermal resistance assessments to examine their physical attributes. This research demonstrates that variations in quartz sand are crucial for regulating the physical properties and structural features of phosphate glass, while also creating prospects for advancing glass-based materials in upcoming optical technology applications.

Keywords: Phosphate Glasses, Quartz Sand, Dysprosium (Dy^{3+}), Amorphous, Melt Quenching.

1 Introduction

In recent years, scientific interest in phosphate glass compositions has surged considerably, fueled by their broad applicability in advanced technological fields, with particular emphasis on optical and electronic devices. The exceptional optical transparency and thermal stability exhibited by these glasses have positioned them as key materials in the development of solid-state lasers, diagnostic imaging technologies, and precision sensing platforms. A highly effective strategy for enhancing both the optical and physicochemical characteristics of phosphate glasses involves the incorporation of rare-earth ions, which significantly boosts their

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overall luminescent efficiency. [1]. Quartz sand is widely utilized as a primary raw material in glass-making due to its superior transparency across a wide spectral region and favorable thermal conductivity. Incorporation of quartz sand into the phosphate glass network substantially modifies several fundamental physicochemical properties, notably density, melt viscosity, and a range of mechanical characteristics. [2-3]. Glass is defined as an amorphous solid substance synthesized through thermal melting of various minerals, especially silica (SiO_2), which then undergoes a rapid cooling process. There are four main classifications of glass, Of the major oxide glass families (silicate, phosphate, borate, and tellurite), phosphate-based compositions were chosen as the host material owing to their superior rare-earth doping capacity relative to silicate and borate glasses, resulting in substantially higher luminescence intensities. Despite this, an important disadvantage of phosphate glass lies in its relatively inadequate resistance to aqueous environments and aggressive chemical conditions. As a result, quartz sand incorporation is anticipated to add to the chemical stability of phosphate glass against degradation [4]. The doping of Dy^{3+} ions into the phosphate glass network is performed to markedly improve the emission efficiency across specific wavelength ranges, thereby rendering the material highly suitable for optical display technologies and as a gain medium in solid-state laser systems. [5]. Trivalent dysprosium (Dy^{3+}) ions are widely recognized for their outstanding photoluminescence characteristics, rendering them highly valuable in numerous optical applications, such as solid-state lasers, radiation dosimetry systems, and fluorescence-based sensing devices. [6]. Variations in the relative proportions of phosphate and silica components lead to appreciable changes in fundamental optical properties-particularly the refractive index and absorption coefficient-which in turn critically determine the suitability and efficiency of the resulting glasses for optoelectronic applications [7]. This investigation is expected to offer novel perspectives on compositional optimization of glass systems for targeted functional applications. The reported results are anticipated to serve as an important reference for future research in optical and electronic materials and to support the ongoing development of rare-earth-doped photonic and electronic technologies. [8]. The study will use a method of cooling (melt quenching). The title of this study is “Effect of Quartz Sand on physical properties and structure of phosphate glass medium doped with dysprosium ion (Dy^{3+})”. There are two main compositions used: $74.5P_2O_5$ - 15CaO- 5BaO - $5Gd_2O_3$ - $0.5Dy_2O_3$ without quartz Sand composition, suitable for applications with high optical emission requirements. 15QS - $59.5P_2O_5$ - 15CaO- 5BaO - $5Gd_2O_3$ - $0.5Dy_2O_3$ the addition of 15 mol% quartz sand adds stability and chemical resistance without much compromising its optical properties.

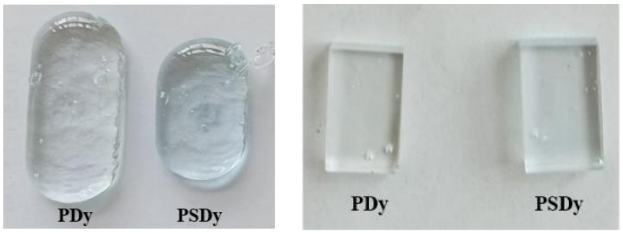
2 Experimental Method

Phosphate-based glasses were prepared using high-purity quartz sand sourced from the Huta Ginjang deposit. The raw sand was first thoroughly cleaned to remove surface impurities, rinsed with distilled water, and subsequently air-dried under sunlight. The dried quartz sand was then subjected to ball-milling for 4 hours to obtain a fine powder. All starting materials were accurately weighed according to the batch compositions listed in Table 1 (samples containing quartz sand designated as PSDy, while quartz-free samples were label PDy). The powdered constituents were carefully mixed to ensure homogeneity using a spatula, after which each batch was transferred into an alumina crucible for melting. The alumina container was placed in a jar filled with silica gel to minimize the moisture content in the material, and it was allowed to

remain for 24 hours inside a vacuum chamber. The thoroughly mixed materials were then loaded into a furnace and heated to 1200°C for 3 hours to facilitate the melting of the glass composition, resulting in complete melting that yielded homogeneous and crack-free glass material, which was subsequently poured into a rectangular stainless steel mold. The resulting sample underwent annealing by heating it for 3 hours at 500°C, followed by gradual cooling to room temperature. Afterward, the glass sample was cut to dimensions of 1 cm × 0.3 cm × 1.5 cm. The polished samples were then analyzed using FTIR spectroscopy, XRD, data processing and analysis, and the display glass show in Fig 1.

Table 1. Composition of PDy and PSDy glasses

Label	Composition of Glass
PDy	74,5P_2O_5-15CaO -5BaO - 5Gd2O3 - 0.5Dy_2O_3
PSDy	15QS - 59,5P_2O_5 - 15CaO - 5BaO - 5Gd_2O_3 - 0.5Dy_2O_3



(a) (b)

Fig. 1. PDy and PSDy glasess (a) before cutt and polish (b) after cut and polished

3 Results and Discussion

3.1 Physical Properties

A comprehensive set of physical parameters- namely density, refractive index, molar volume, Dy^{3+} ion concentration, polaron radius, inter-ionic distance, field strength, dielectric constant, molar refractivity, oxide-ion polarizability, metallization criterion, and reflection loss—were calculated for the PDy and PSDy glass series. The corresponding values are summarized in Table 2.

Table 2. The physical Properties glasses

Measurement parameters	**Glass Samples**	
	PDy	PSDy
Weight molar, *M* (g)	141.8154	129.5365
Density (g/cm^3)	2.8623	2.8738
Molar volume (cm^3/mol)	49.5459	45.0750
Ion concentration, N x 10^{20} (ion/cm^3)	6.0773	6.6801
Polaron radius x10^{-8} (Å)	1.0248	9.9304
Inter nuclear distance x 10^{-7}	2.5435	2.4646
Field strength, F x 10^{16} cm^2	5.62	5.98
Refractive index (n)	1.5426	1.5435
Molar refractivity (R_m)	15.6074	14.2186

Molar electronic Polarization x 10^{-24}	6.1903	5.6394
Metallization Criteria (M)	0.6850	0.6846
Reflection loss (R) %	4.5541	4.5660
Dielectric constant (Ɛ)	2.3796	2.3824

The incrise in density resulted from the greater molecular weight of Dy_2O_3 relative to SiO_2. Furthermore, The molar volume of the synthesized glasses shows a consistent upward trend as the Dy_2O_3 content is progressively increased.. This evidently indicated that the elevated dopant levels boosted the quantity of non-bridging oxygens (NBOs), thereby causing the glass network structure to expand. A progressive rise in Dy_2O_3 concentration leads to a corresponding increase in the number density of Dy^{3+} ions within the glass network, suggesting a uniform dispersion of Dy^{3+} ions across the fabricated glass samples [9-10].The incorporation of silica compounds into the material resulted in a decrease in molar volume, molar electron polarization, and internuclear distance due to the formation of a denser and more compact silica network. Although electron polarization can be enhanced through cation modification, its mobility remains constrained by the dominant silica structure. Pure silica glass exhibits relatively high electron polarization; however incorporation of supplementary cations from the alkali or alkaline-earth groups, further increases the Si–O polarization. Nonetheless, the molar volume remains low due to the prevailing compactness of the silica network. Additionally, the internuclear distance decreases with increasing silica content, reflecting the denser and more compact nature of the silica structure compared to other oxides[11-14].

3.2 Structural Properties

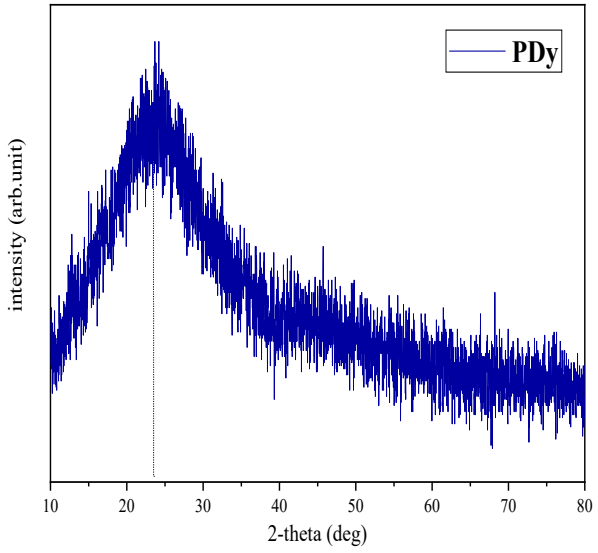


Fig. 2. XRD spectra of PDy glasses

The structural nature and phase purity of the prepared glasses were examined using X-ray diffraction (XRD) analysis. The room-temperature XRD pattern of the Dy^{3+}-doped samples, displayed in Figure 2, reveals the characteristic amorphous hump with no evidence of crystalline peaks. A wide hump was evident in the 2θ range of 20–35°, peaking at 2θ = 24°, indicative of

the typical feature of amorphous glass materials, with no additional crystalline peaks appearing across the entire pattern. These observations verify that the synthesized glass exhibits an amorphous nature [15].

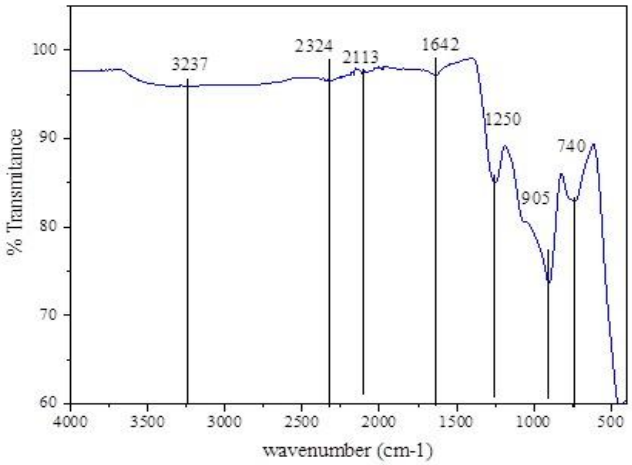


Fig. 3. FTIR spectra of PDy glasses

This FTIR spectrum is found in phosphate glass or oxide-based amorphous materials, especially those with added metal ions or dopants (such as Dy^{3+}). It indicates that the material contains hydroxyl groups (–OH), phosphate groups (P–O–P), and possible traces bound to carbonate compounds or air [15]. Explanations of the infrared absorption peaks identified in the image, along with their interpretations, are shown in Table 3.

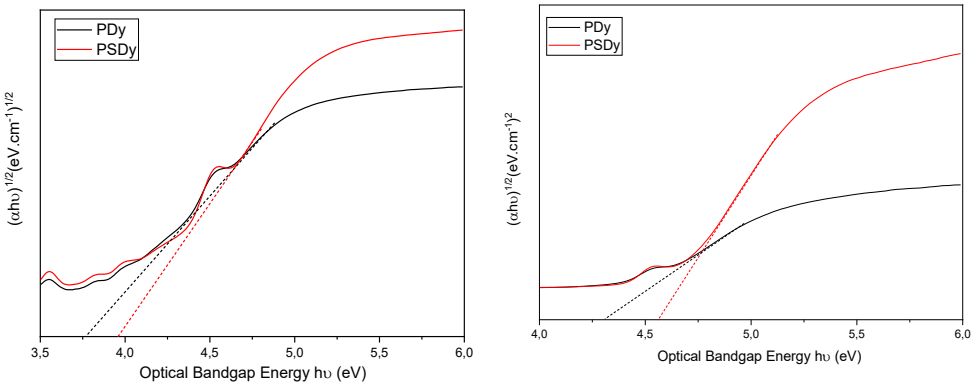
Table 3. Description of waves based on functional groups

Wavenumber (cm^{-1})	Assignment	Reference
3237 cm^{-1}	The observed peak reflects the basic stretching mode of OH groups present in the produced glass samples. Its strength gradually weakens with higher Dy_2O_3 concentration due to the simultaneous drop in P_2O_5 proportion.	[19]
2324 cm^{-1}	Hydroxyl groups strongly bonded to phosphorus atoms within the glass matrix.	[20]
2113 cm^{-1}	The band arises from either the symmetrical stretching of B–O bonds in triangular BO_3 structural units or the symmetric vibration of non-bridging oxygen atoms linked to phosphorus in Q^2 tetrahedral configurations.	[21]
1642 cm^{-1}	This feature is linked to O-H vibrations originating from both phosphate and borate networks, manifesting as P-OH and B-OH linkages in the prepared glasses	[19]
1250 cm^{-1}	Spectral signals between 1400 and 1500 cm^{-1} correspond to connections between trigonally coordinated boron and non-bridging oxygen ions	[21]
905 cm^{-1}	P-O-P bridges connecting Q^2 tetrahedra in metaphosphate-like $(PO_4)^{-1}$ unit.	[21]

740 cm^{-1}	The absorption in the 735-766 cm^{-1} region is associated with symmetric stretching of P-O-P bridges or bending vibrations of O-P-O groups within pyrophosphate ($P_2O_7^{4-}$) entities belonging to Q^1 phosphate units.	[21]

3.3 Optical Properties

Analysis of the UV absorption edge allows precise determination of the optical band gap energy, a key indicator for understanding electronic band structure and optical transitions in both amorphous and crystalline solids. In typical insulating systems, this energy gap surpasses 5 eV, leading to strong electron localization and negligible electrical conductivity [18]. The direct and indirect band gap values obtained for the Dy^{3+} containing phosphate glasses are displayed in Figure 5.



(a) (b)

Figure 5. (a) Indirect optical gap and (b) Direct optical gap of Dy^{3+}glass sample.

The band gap values of both indirect and direct optical gap samples are shown in Table 5.

Table 5. Band gap values of glass samples

Sampel	Indirect (eV)	Direct (eV)
PDy	3.76	4.30
PSDy	3.95	4.56

4 Conclusion

The resulting phosphate glass medium are significantly influenced by the incorporation of quartz sand as a silica source in the synthesis of Dy^{3+}-doped phosphate glasses. Quartz sand (SiO_2) the addition of quartz sand represents a common and effective strategy to enhance the thermal resistance and mechanical strength of phosphate glass systems.. Variations in quartz sand composition directly impact key physical properties, including density (ρ), where the addition of SiO_2 tends to decrease the density due to the lower atomic mass of Si compared to P or Dy, while simultaneously promoting a more rigid silicate network that improves structural stability. Furthermore, SiO_2 variations affect the transparency and color of the glasses, particularly in the visible and ultraviolet spectra; Structurally, the crystalline quartz sand undergoes a phase transformation upon integration into the phosphate glass matrix, resulting in

an amorphous Q sand-Phosphate glass, as confirmed by the absence of crystalline peaks in X-ray diffraction (XRD) spectra. These findings underscore the role of quartz sand in optimizing the performance of Dy^{3+}-doped phosphate glasses show considerable promise for a wide range of applications in optical devices and luminescent materials, suggesting avenues for further investigation into compositional tuning for enhanced luminescent properties and durability.

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