Exploring the Physical Properties and Tauc's Plot Analysis of Nd^{3+} Doped Telluroborate Glass

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Abstract

In the present work, the investigation begins with the synthesis of telluroborate glass samples doped with Nd^{3+} rare earth ion using established melt quenching techniques with composition $(50–x)B_2O_3 \cdot 20TeO_2 \cdot 15Mg_2CO_3 \cdot 15K_2CO_3 \cdot xNd_2O_3$ (where x varies as 0, 0.5, 1, 1.5, 2 and 2.5 mol %). All samples were found to be in glassy form with a broad hump in XRD spectra which is characteristic of amorphous nature. The physical parameters including the optical dielectric constant, polaron radius, interatomic separation, molar refraction, and metallization criterion are also analyzed based on molar density and molar volume. The Tauc's plot reveals that the band gap energy rises as the dopant concentration increases. Similarly, the refractive index shows an upward trend with higher dopant concentrations. Optical absorption spectra were measured at room temperature over a wavelength range of 180 nm to 1000 nm. In conclusion, the comprehensive exploration of physical properties in Nd^{3+} doped telluroborate glass offers valuable insights into the potential applications of these materials in advanced optical and photonic devices. This work also contributes to the expanding knowledge base in the field of glass science, fostering advancements in materials engineering and device development.

Keywords: Telluroborate glass, Physical parameters, rare earth ion, Tauc's plot.
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Introduction

Telluroborate glasses, known for their thermal and chemical stability, high refractive index, and broad spectral transparency, are ideal for harsh environments and advanced optical applications [1-2]. Nd^{3+}-doped telluroborate glasses, in particular, are valued for their unique electronic transitions, which enhance fluorescence lifetime, emission cross-sections and quantum efficiency, making them suitable for lasers, amplifiers, sensors and photonic devices [3-7]. However, despite reported advancements, such as near-infrared emission studies, there is limited understanding of their structural and physical properties. This study explores the impact of varying Nd_2O_3 concentrations on the physical, optical and theoretical properties of these glasses, emphasizing their potential in optical technologies.

Method

The telluroborate glasses with composition of $(50–x)B_2O_3 \cdot 20TeO_2 \cdot 15Mg_2CO_3 \cdot 15K_2CO_3 \cdot xNd_2O_3$ (where x varies as 0, 0.5, 1, 1.5, 2 and 2.5 mol %) were prepared by melt quenching method. To prepare a sample for study analytical reagent grade chemicals consist of B_2O_3, TeO_2, Mg_2CO_3 and K_2CO_3 were used. The rare earth oxides added to the glasses were 99.99% pure.

Discussions

The physical properties of doped telluroborate glasses discussed in table 1. The analysis highlights the impact of Nd^{3+} ion incorporation on the optical and physical properties of TEB glasses:

1. Physical Parameters: The introduction of Nd_2O_3 increases density and molar volume due to its role as a network modifier, generating non-bridging oxygens (NBOs) and enhancing structural

randomness.

2. Refractive Index and Derived Parameters: Nd^{3+} ions modify the glass network by expanding it, decreasing inter-ionic distances and polaron radius, and increasing field strength, leading to significant structural and optical changes.

3. Optical Absorption Spectra: UV-Vis-NIR spectra reveal ten absorption bands of Nd^{3+} transitions, with the 582 nm band being hypersensitive to environmental changes and indicative of increased covalency in bonding.

4. Bandgap and Urbach Energy: Higher Nd^{3+} concentrations raise the optical bandgap, reflecting reduced NBO content and structural compactness. Concurrently, decreasing Urbach energy suggests fewer defects and improved structural integrity.

Overall, Nd^{3+} doping significantly enhances structural coherence, optical properties, and the performance of TEB glasses.

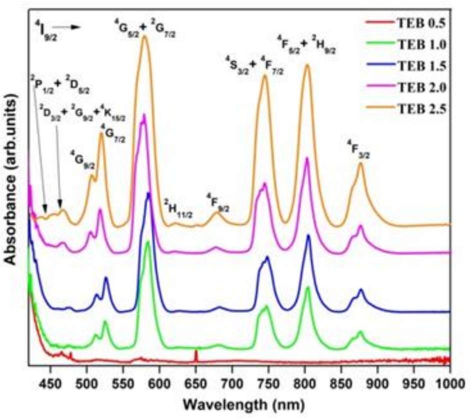

Figure 1: UV-VIS absorption spectra of Nd^{3+}: TEB glasses

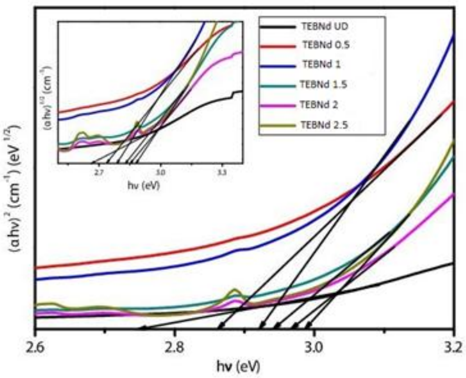

Figure 2: Tauc's plot for direct allowed transition of the Nd^{3+}: TEB glasses

Conclusion and Future Prospective

This study successfully prepared Nd^{3+}-doped telluroborate glasses using the melt quenching technique and characterized them for physical and optical properties. XRD analysis confirmed their amorphous nature. Density, refractive index, molar volume, polarizability, and optical basicity increased with higher Nd_2O_3 doping, indicating network expansion and enhanced ionic properties. A correlation between refractive index, density, and electronic polarizability was established. Optical spectra revealed that bandgap values increased with Nd^{3+} concentration, attributed to the formation of non-bridging oxygen (NBO), while Urbach energy showed an inverse relationship with the bandgap.

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Table 1: Physical properties of doped Telluroborate Glass

Physical properties	UD sample	0.5 Doped	1.0 doped	1.5 doped	2.0 doped	2.5 doped
Average molecular weight M (g)	103.7524	105.0866	106.4209	107.7552	109.0895	110.4238
Density (g/cm^3)	2.9817	2.9920	3.0292	3.0545	3.0901	3.1255
Refractive index (n)	1.639	1.641	1.658	1.665	1.686	1.690
Rare earth ions concen- tration N (X 10^{22}ions/cms)	-	0.8574	1.7144	2.5609	3.4122	4.2620
Dielectric constant (∈)	2.6863	2.6929	2.7490	2.7722	2.8426	2.8561
Optical dielectric constant (pdt/dp)	1.6863	1.6929	1.7490	1.7722	1.8426	1.8561
Molar Volume V_m (g/cm^3)	34.7964	35.1225	35.1317	35.2775	35.3025	35.3299
Reflection losses (R)	0.0586	0.0589	0.0612	0.0622	0.0652	0.0658
Molar refractivity (R_m)	12.5197	12.6687	12.9390	13.0985	13.4326	13.5031
Polaron radius (r_p)	-	0.4241	0.3366	0.2945	0.2676	0.2485
Interatomic distance (r_i)	-	1.0526	0.8355	0.7309	0.6643	0.6167
Electronic polarizability (α_e)X (10^{-22} ions cm^{-3})	0.1427	0.1430	0.1460	0.1473	0.1509	0.1516
Field strength F (cm^3)	-	1.2840	1.3239	2.2491	2.9050	3.7601
Molar electronic polarizability (α_m)	4.9681	5.0273	5.1345	5.1978	5.3304	5.3584
Metallization criterion (M)	0.6402	0.6393	0.6317	0.6287	0.6195	0.6178
Oxide ions polarizability	1.5677	1.6802	1.8838	2.0041	2.2561	2.3093
Optical basicity	0.5400	0.5472	0.5544	0.5615	0.56887	0.5759