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OPTICAL, ELASTIC, ELECTRICAL, AND RADIATION SHIELDING PROPERTIES OF $x\mathrm{BaF_2} - (50 - x)\mathrm{CaF_2} - 50\mathrm{B_2O_3}$ MIXED ALKALINE EARTH BORATE GLASSES

NOOR FADHILAH BINTI MUHAMAD SAHAPINI

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ABSTRACT

Borate glass with fluoride ions has diverse applications in solar energy converters, lasers, infrared fibre optics, and electronic devices. Exploring the mixed alkali effect in borate glass is crucial for identify its potential. Therefore, this study aims to investigate the optical, elastic, electrical, and radiation shielding properties of $x$$BaF_2$–$(50 - x)$$CaF_2$–$50B_2O_3$ (x = 5 – 35 mol%) mixed alkaline earth borate glass. Glass samples were synthesised via melt-quenching technique, confirmed as amorphous through X-ray diffraction (XRD) analysis. FTIR spectroscopy revealed BO_3 conversion to B_4 units. The addition of BaF_2 increased molar volume (V_m) and density (ρ) except at 25 mol% BaF_2, due to mixed alkaline earth effect (MAEE) and extensive non bridging oxygen (NBO) formation, supported by the abrupt decrease of N_4. The increase in the optical band gap (E_{opt}), describing the weakening of the glass structure. Anomaly at 20 mol% BaF_2 in refractive index (n) and optical band gap (E_{opt}) variation, linked to the role of MAEE. The elastic velocities, shear (S) and young (Y) modulus decreased with ($x \leq 30$ mol%), aligned with structural findings. However, the longitudinal (L) and bulk (K_e) modulus had minima at 10 and 25 mol%, coincided with Urbach Energy (E_u) maxima, indicating increased in structural randomness. Makishima-Mackenzie Model aligned with the experimental values, exhibiting a sudden drop at 25 mol%, due to dissociation bond energy decrease. Bulk compression model proposed isotropic deformation, affecting network bond lengths and sizes while keeping interatomic bond angles unchanged. The ring deformation model indicated isotropic ring compression due to bending between structural units. The anomaly at 25 mol% correlated with the variation of σ_{DC} against composition. The conductivity initially decreased ($x < 20$ mol%) due to the blocking effects of larger Ba^{2+} ions against Ca^{2+}. However, an abrupt increase occurred at 25 mol%, indicating enhanced charge mobility. The temperature and frequency dependence of σ_{AC} suggested the Overlapping Large Polaron Tunneling (OLPT) model dominated as the main transport mechanism. Besides, the dielectric constant (ε') was more prominent in low-frequency regions, signifying that the space charge polarisation as main polarisation. Anomalies at 10 mol% and 25 mol% on ε', supported the elastic data. In the radiation shielding study, adding BaF_2 to the glass samples increased the effective atomic number, thereby enhancing their potential for radiation attenuation. Among the various glass samples, the composition containing 25 mol% BaF_2 displayed the smallest values for MFP and HVL, indicating its superior effectiveness in photon attenuation. Therefore, this composition can be considered as a preferable option among the glass samples for gamma protection applications.

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CHAPTER 1

INTRODUCTION

1.1 Research Background

Glasses are considered non-crystalline materials or amorphous solids as they lack the long-range order of an atomic structure [1]. The diversity of glass usage and applications depends on its properties, which are determined by the compositions and modifying components in the glass former [2]-[3]. Oxide glasses have been extensively investigated as amorphous materials due to their exceptional physical properties, high potential for industrial applications, and excellent radiation protection properties. The network former, modifier, and intermediate are the three significant components of oxide glasses. Network former, such as tellurite, borate, silicate, germanate, and phosphate, act as a backbone of the glass structure and have some unique characteristics depending on their types.

Borate (B_2O_3) is among the best oxide glass former due to its high glass formation capability, low melting temperature, high thermal stability, wide glass-forming range, compatibility with transition metals and rare earth elements, and high chemical durability [4]. The B_2O_3 compound also has a small cation size and high bond atomic strength, which increases its durability and stability [2], [5]. Pure borate oxide-based glasses (B_2O_3) consist of boroxol rings, while doped B_2O_3 is generally formed with three and four coordinated boron units, which can be arbitrarily combined to form different B_xO_y superstructural units, such as pentaborate, triborate, diborate, and others [4], [6]. Besides, outstanding properties like transparency and high density possessed by borate glasses make it a good glass host for radiation protection glass.

Incorporating fluoride ions (F^-) in oxide glass as a glass modifier has gained attention because of its advantages in various applications, such as solar energy converters, lasers, infrared fibre optics, and electronic devices [7]-[9]. Glasses with fluorine are relatively moisture resistant [10] and possess high mechanical strength [11]-[12] compared to the other alkali oxide borate glasses. It was due to the fluoride compounds in oxide glass assisting in the removal of the OH^- group and ultimately