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UNVEILING THE STRUCTURAL FEATURES OF MGO-ZNO-CR_2O_3-$K_2B_4O_7$ GLASSES

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Abstract : Glassy materials became more important in the day to day life in various application such as the materials that gives protection from radiation, optical fiber materials for communication, etc. In the current work, MgO-ZnO-Cr_2O_3-$K_2B_4O_7$ glasses are prepared and characterized to know more about the structural features about the prepared glasses. Melt quenching was used to make the samples. In this method, the high pure required chemical were weighed, heated them to melt congruently and then quenched to form the glass samples. The so formed glasses were then exposed to XRD, FTIR, and Raman spectroscopy were used to examine the glass samples. The lack of distinct peaks in the samples' XRD spectra helped to demonstrate the non-crystalline phase of the produced samples. Density values are measured for all the samples using the Archimedes principle and it is measured for three pieces of samples for each composition and averaged to get accurate values. The density data revealed that the values of the glass samples show clear increase from 2,343 to 2.406g/cc when MgO increases at the expense of $K_2B_4O_7$. As a result of the transformation of BO_3 units into BO_4 units, the density has increased. FTIR data is taken from 400 cm^{-1} to 4000 cm^{-1}, however the spectra drawn between 400 cm^{-1} to 1600 cm^{-1}, since the data above 1600 cm-1 shows only the OH band. Metal cation vibrations were detected in the lower wavenumber side of the FTIR spectra, with BO_4 units in the 800–1200 cm^{-1} range and BO_3 units beyond the 1200 cm^{-1} range. The rises in the density of the samples are confirmed using FTIR spectra as well with the help of rising in the using BO_4 units. Raman spectra recorded in the range of 200 to 1800 cm^{-1}. Several borate groups, including diborate and penta borate, are visible in Raman spectra.

IndexTerms **– Borate glasses, XRD, FTIR, Raman spectra.**

1. INTRODUCTION

In recent decades, technologies have been used to carry out a significant advancement in science. Glass and other amorphous materials are highly recommended for their high inherent transparency, quick reaction time, and exceptional resistance to variations in the environment. Glass is therefore a crucial component of communication. With oxygen, borate glasses can change their coordination number from three to four. This contrasts with glasses made of silicate and phosphate. Glasses of silicate and phosphate only need oxygen to form tetrahedral units. The material's endurance is mostly determined by its structural characteristics. [1-3].

Magnesium oxide (Mgo) has the ability to modify the structure, chemical stability, and durability of borate glasses. The glass transition temperature can be lowered by Mgo.Depending on its content, ZnO-B_2O_3 glasses can either function as a network former or a modifier. Zno creates B-O-Zn bonds at low concentrations, which increases fracture toughness and scratch resistance .B-O-Zn bonds increase chemical resistance against bases, acids, and moisture by lowering the availability of non-bridging oxygen atoms (NBOs)[4 - 6].

A transition metal oxide called Chromium oxide (Cr_2O_3) is added to glass to enhance its mechanical, chemical strength[7. 8]. Some glasses have $K_2B_4O_7$ as a component. Containing glasses of alkali tetra borate ($K_2B_4O_7$) can change the electrical, optical, and physical characteristics of glasses[9, 10]. Glasses of alkali tetra borate are created by melting and quenching them at temperatures of about 1150 degrees Celsius. Unless there are equivalent levels of alkali oxides, the density of these glasses rises as the amount of $K_2B_4O_7$ increases. These glasses have broad, peak less X-ray diffraction, which suggests that they are amorphous. BO_3 triangular and BO_4 tetrahedral structural units make up borate glasses. Oxides such alkali oxides and metal oxides can be used to modify borate glasses. In order to look into the structural alterations in the glasses, the authors would like to examine the XRD, FTIR, and Raman spectrum characteristics associated with Mgo-Zno-Cr_2O_3-$K_2B_4O_7$ glasses.

2. EXPERIMENTAL

The precise glass composition for alkaline zinc potassium tetra borate (MZCK) glasses is xMgo-10Zno-0.5Cr_2o_3-(89.5-x)$K_2B_40_7$.The range of x numbers in this composition is 0, 10, 20, 30, and 40. A mono pan balance was used to measure these substances. These chemicals were added to the composition in the necessary amounts, and they were crushed until the mixture was homogenous. These substances were subsequently placed in crucibles made of porcelain and heated. For one hour, the furnace's temperatu re was kept at 1000 degrees Celsius. The melt is swirled three times over the course of an hour to ensure that it is well mixed. First, the samples were quenched on a prepared steel plate to remove any internal tensions and strains.

By first quenching the samples on a steel plate that had been heated to 200°C and then annealing them, the interior tensions and strains were removed for a duration of 12 hours. Fig. 1 shows the flow chart for the sample preparation. The MZCK glass sample images are shown in Fig. 2, where the X-ray diffraction spectra were captured on. The X'Pert Pro X-Ray diffractometer from Phyilps. If these samples' XRD spectra show no distinct peaks that would have indicated the samples' amorphous phase. When calculating the density of samples, the Archimedes principle is applied. Additionally, FTIR spectra were obtained from these samples using a Perkin Emler Frontier FTIR within the wavelength range of 400–1600 cm^{-1} with a resolution of 3 cm^{-1}. On the J. Y. H. LABRAMHR Raman spectrometer, Raman spectra were captured in the 200–1800 cm^{-1} range. Every measurement used in this study was taken at room temperature.
The density of the samples is determined using the Archimedes technique, which involves calculating the density of three pieces f rom each sample and averaging them to obtain an exact density values.

Table1 Sample code, the glass compositions, density(g/cc) and molar volume(cc/mol) composition in mol %

Sample code	Mgo	Zno	Cr_2O_3	$K_2B_4O_7$	Density	Molar volume
MZCK-0	0	10	0.5	89.5	2.343	92.949
MZCK-10	10	10	0.5	79.5	2.346	84.575
MZCK-20	20	10	0.5	69.5	2.373	75.475
MZCK-30	30	10	0.5	59.5	2.380	67.168
MZCK-40	40	10	0.5	49.5	2.405	58.424

3. RESULTS AND DISCUSSIONS

3.1 X-ray diffraction

In order to comprehend the basic characteristics of glasses and create novel materials, XRD is a useful tool for the advancement of research in the glass sector. Any crystalline states or particles that may be embedded in bulk glass and could result in flaws or change the glass's characteristics can be found and described with the aid of XRD. One method for examining the structure of glasses is X-ray diffraction, or XRD. Figure 1 shows the xMgo-10Zno-0.5Cr_2O_3-(89.5-x)$K_2B_4O_7$ glasses' XRD patterns. The XRD spectra make it evident that there were no distinct crystalline peaks with defined features; instead, a broad hump was observed in the 25–35 degree region. This demonstrates the amorphous nature of the MZCK glasses.

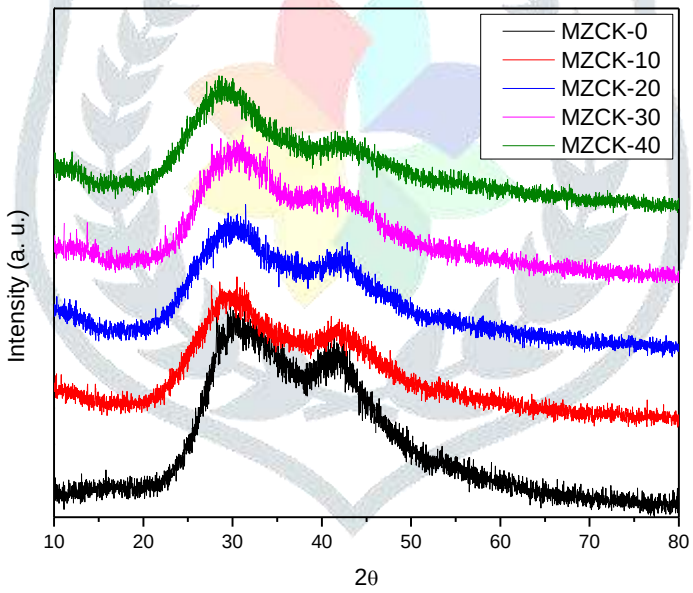

Figure 1 XRD spectra of MZCK glasses

3.2. Density

Density affects glass's ability to withstand pressure and negative effects, preserving its structural soundness. Because it affects the effectiveness and usability of glass for a variety of purposes, density is a crucial consideration in business and manufacturing settings. Glass samples are compared using density readings, and it is unlikely that two samples from the same source came from the same origin if their densities differ considerably. When there are multiple shards in a sample, density readings can be used as a screening method to detect the many glass sources present.[11, 12]. Table 1 shows the obtained density values for the MZCK glasses. It is evident that the density value increases from MZCK-0 to MZCK-40 upon the introduction of MgO. According to the density data, when MgO grows at the expense of $K_2B_4O_7$, the values of the glass samples rise from 2.343 to 2.406g/cc. The density has grown as a result of the conversion of BO_3 units into BO_4 units.

3.3. Spectra of FTIR

By measuring how much infrared light is absorbed by molecules, FTIR spectroscopy may identify the different vibrational patterns of chemical connections in glass. Investigators can identify the kinds and configurations of chemical bonds, such as B-O-

B bonds in borate glasses, by examining the locations and strengths of these vibrational modes. Because of its exceptional sensitivity to the local structure of glasses, FTIR enables researchers to examine compositional and bonding arrangement fluctuations.

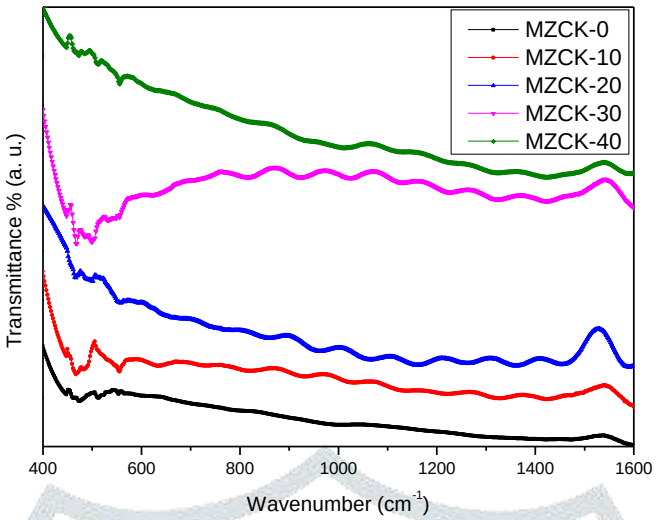

Figure 3 FTIR spectra of MZCK glasses

Wave numbers obtained from FTIR are 447, 513, 563, 622, 707, 806, 902, 1011, 1107, 1214, 1313 1426 and 1490cm^{-1}. These wave numbers obtained analysis of the material MZCK. Generally, these wave numbers corresponding to the vibrational frequencies of different chemical bonds with in the material. These wave numbers tell us the molecular structure and composition. Region I: Generally this region 400 to 700cm^{-1} associating with bending vibrations of metal ions bonds like Mg-O, Zn-O, Cr-O and network vibrations of the borate glass matrix B-O the peaks at 447, 513, 563 and 622cm^{-1} arise from these types of vibrations [13, 14]. Region II:: The second region, between 700-1100cm^{-1}, is characteristic of stretching vibrations in the borate network , specially B-O stretching in BO_3 and BO_4 units. The peaks at 707, 806, 902 and 1011 cm-1 can attributed to these vibrations with variations depending on the specific bonding environment. The peak at 1107 cm^{-1} might indicate the presence of B-O stretching[15, 16]. Region III: The third region, between 1200-1500 cm^{-1}, corresponds to asymmetric stretching of B-O bonds in BO_3 units the peaks at 1214, 1313, 1426 and 1490 cm^{-1} are likely these vibrations with shifts in position reflecting changes in the borate network structure and the influence of the added oxides MgO, ZnO, Cr_2O_3 [17, 18].

The present case the numbers from 447 – 563 cm^{-1} are arised due to metal cation (Mg^{2+} , Zn^{2+}) vibrations. The O-B-O vibrations are due to 622 cm^{-1} wavenumber while the stretching B-O-B in BO3 units are raised from the wavenumbers 707 to 806 cm^{-1}. The numbers from 902 to 1011 cm-1 are due to B-O stretching's in borate groups while the 1107 cm^{-1} is assigned to B-O-B elongations in [BO_4] tetrahedron. Stretching vibrations of tetragonal BO_3 units raised due to the wavenumbers 1214 to 133 cm^{-1} whereas the wavenumbers above 1400 cm^{-1} are ascribed due to Anti-symmetrical stretching vibrations of B–O–B groups.

3.4 Raman spectra

The presence of NBO ions in oxide glasses can be detected by Raman spectroscopy, which is essential for comprehending the structure and characteristics of glass networks. It facilitates comprehension of the atomic configuration in silicate, borate, and other glass systems, as well as the kinds of structural units (such as rings and tetrahedra) that are involved. Raman spectroscopy can assist describe the material makeup of glass by revealing the kinds and amounts of various ions or elements that are present. It can be used to examine how various modifiers or additives affect the structure and characteristics of glass, such as how alkali metals affect silicate glasses. Figure 4 displays the Raman spectra of the present MZCK glasses, which were measured in the 400–1800 cm^{-1} wave number range.

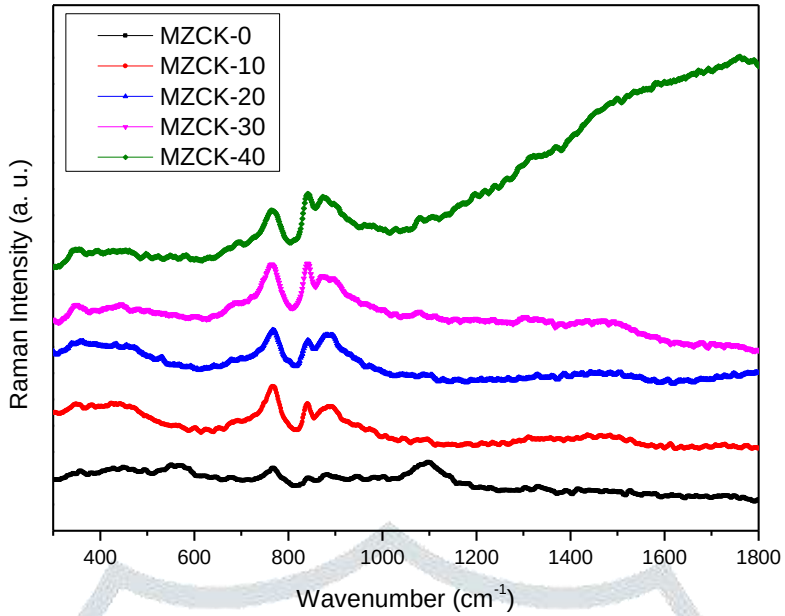

Figure 4 Raman spectra of MZCK asses

For MZCK samples, the exact band positions were at approximately 351, 452, 583, 693, 766, 843, 876, 979, 1078, 1321, and 1495 cm^{-1}. Low Wavenumber Region (300-600cm^{-1}), bands in this region may be associated with vibrations of the network modifying cations Mg+,Zn+,K+ and bending modes of the borate network. The wavenumber 351cm^{-1} could be related to Mg-O Vibrations or network bending modes. The wavenumber 452 cm^{-1} might be correspond to Zn-O vibrations or borate network bending. The wavenumber 583 cm^{-1} could be due to B-O vibrations in BO3 or network vibrations. Mid Wavenumber Region 600-1100cm^{-1} is often dominated by stretching vibration of the borate network. The wavenumber 693cm^{-1} could be associated with B-O-B bending or ring vibration in borate groups. The wavenumbers 766cm^{-1} and 843cm^{-1}peaks likely correspond to stretching vibrations of BO_3 units. The wavenumber 876cm^{-1}may be related to vibrations of BO_4 units[19, 20]. The wavenumbers 979cm^{-1} and 1078cm^{-1} could be attributed to asymmetric stretching of BO_4 units. High Wave number Region 1100-1500cm^{-1} can contain the combinations of the other vibrations. The wavenumbers 1321cm^{-1} and 1495cm^{-1} peaks might be due to B-O stretching vibrations in specific borate arrangements or combinations of other modes. By analyzing the changes in Raman spectra with varying MgO content, it's possible to understand how the addition of MgO modifies the borate network structure and the material's properties.

4. CONCLUSIONS

The glasses with the combination xMgo-10Zno-0.5Cr_2o_3-(89.5-x)$K_2B_4O_7$ were made the range of values for x was 0 to 10, 20, 30, and 40, and their structural characteristics were examined using FTIR and Raman spectra. Density values are calculated using the Archimedes principle, and it was found that as the Mgo % of the glasses increased, so did the density values. It might be feasible to employ glasses with a greater MgO % and density as shielding materials. By analyzing these materials using FTIR spectroscopy, several distinct borate groups, bismuthate groups, and metal cation vibrations were found. It was determined that the density had grown given that the FTIR bands on the higher wave number end had widened. The various vibrational modes present in the glasses' structure were examined using the Raman spectra.

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