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INSIGHTS INTO THE GLASS NETWORK STRUCTURE OF COAL FLY ASH-BASED GLASS

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Abstract
Coal fly ash is the by-product of coal combustion in thermal power plants. The chemical composition of coal fly ash allows it to be utilized as a secondary raw material for glass production. Na_2CO_3 and $CaCO_3$ were introduced in the batch as raw materials for glass network modification. Dark homogenous glass was obtained by melting the batch and quenching it on the stainless steel in the air. This research investigates the relative share of structural units of the glass network by deconvolution of the part of the FTIR spectra. Results show that most dominant structural units contain one and two bridging oxygen per [SiO_4] tetrahedral indicating low glass network connectivity.

***Keywords**: Coal fly ash, Glass, FTIR, Deconvolution*

1. INTRODUCTION

The global reliance on coal for electricity generation has resulted in the large-scale production of coal fly ash, raising significant environmental concerns. Coal fly ash, a fine particulate residue generated during the combustion of pulverized coal in thermal power plants, represents one of the most abundant industrial by-products worldwide. Traditionally viewed as waste, coal fly ash is typically disposed of in landfills or ash ponds, posing long-term environmental and economic challenges [1]. However, due to its rich chemical composition- primarily consisting of silicon dioxide (SiO_2), aluminum oxide (Al_2O_3), calcium oxide (CaO), and other oxides- fly ash is increasingly being recognized as a valuable secondary raw material for various industrial applications. It can be utilized as a secondary raw material in applications such as cement additives, road construction, filter and adsorbent synthesis, geopolymer production, etc [2-4]. Among these applications, the utilization of fly ash in the production of glassy materials has gained considerable attention. The high content of glass network-forming oxides makes fly ash an attractive alternative to conventional raw materials. Through appropriate thermal processing, fly ash can be melted and vitrified to form homogeneous glass. Recycling fly ash into glass products not only reduces the environmental burden associated with its disposal but also supports the principles of the circular economy by converting industrial waste into high-value materials. This approach offers a sustainable pathway for the development of new construction materials, coatings, insulating components, and other functional products [5]. The present study investigates the potential of coal fly ash as a primary component in glass synthesis. Modifying cations were introduced in the batch to reduce the amount of bridging oxygen in [SiO_4] tetrahedra. The lower amount of bridging oxygen per tetrahedra implies the lower viscosity of the melt which benefits glass formation. Using

Fourier Transform Infrared Spectroscopy (FTIR) analysis and deconvoluting the part of the spectra gives information on the types of structural units of the glass network and the amount of bridging oxygen in the produced glass.

2. EXPERIMENTAL

The glass was prepared using coal fly ash, Na_2CO_3, and $CaCO_3$ as raw materials as described in the previous research [1]. The chemical composition of the glass was determined using an Atomic Absorption Spectrometer (AAS) Perkin Elmer 703. The structural characteristics of the produced glasses and glass-ceramics were analyzed using Fourier Transform Infrared Spectroscopy (FTIR). The measurements were conducted with a Nicolet iS50 spectrophotometer (Thermo Fisher Scientific, Waltham, MA, USA) over the wavenumber range of 4000 to 400 cm^{-1}.

3. RESULTS AND DISCUSSION

The chemical composition of the obtained glass is presented in Table 1.

Table 1. Chemical composition of the glass

Oxide	SiO_2	Al_2O_3	CaO	MgO	Na_2O	K_2O	TiO_2	Fe_2O_3
mol %	49.95	11.99	21.92	2.18	10.69	0.57	0.70	2.00

Dark homogenous glass was produced with a high amount of modifying oxides which enabled good pourability of glass melt. The structure analysis of the glass by FTIR method is presented in Figure 1.

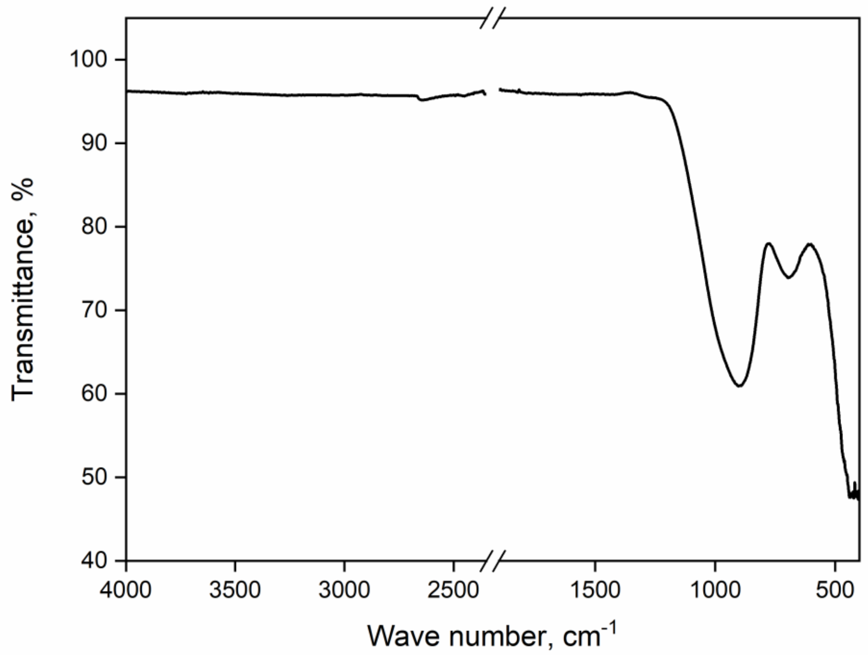

Figure 1. FTIR analysis of the glass sample

Figure 1 shows three absorption zones typical of aluminosilicate glasses. The first zone, at about 470 cm^{-1}, corresponds to bending vibrations of bridging oxygen in Si-O-Si or Si-O-Al bonds within tetrahedral structures. The second one, at approximately 710 cm⁻¹, corresponds to symmetric stretching vibrations in X-O-X structures (X=Si, Al or Fe). The third and broadest zone, between 1200 and 800 cm^{-1}, represents strong absorption bands related to asymmetric stretching of bridging oxygen in Si-O-Si or Si-O-Al bonds, and stretching vibrations of non-bridging oxygen in O-Si-O linkages [6, 7]. Deconvolution of the third zone of the spectra can give insights into a glass network structure. The band at 1200-800 cm^{-1} can be divided into five individual bands, Q^n (n=0-4), where n represents the number of bridging oxygen in the tetrahedral [SiO_4] structure. Figure 2 presents the deconvoluted part of the spectra.

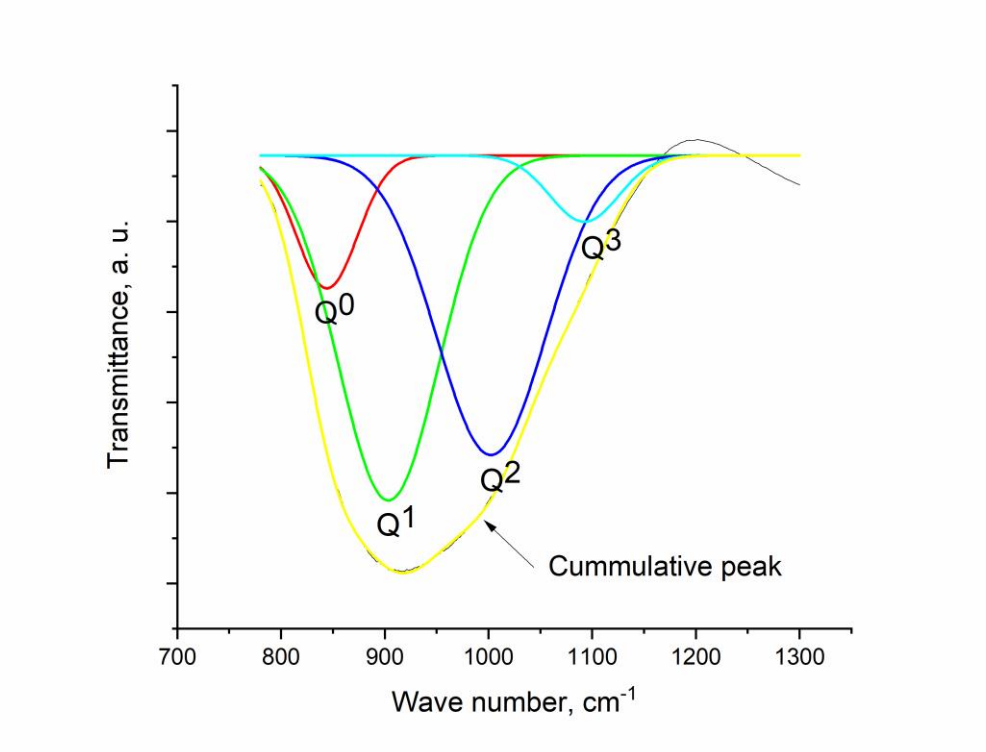

Figure 2. Deconvolution of the part of FTIR spectra

It can be observed that the glass sample does not contain structural units with all four bridging oxygens (Q^4 units), indicating that the introduction of modifying cations in the glass batch has disrupted the silicate network. These modifiers break Si–O–Si bonds and generate structural units containing non-bridging oxygens, most dominantly Q^2 and Q^1 species, which are characterized by silicon tetrahedra containing two and one bridging oxygen atoms, respectively. Table 2 presents Q-units and their corresponding Infrared (IR) band wave numbers [8].

Table 2. IR bands of Q^n structural units

Name of the structural unit	Number of non-bridging oxygen	IR band according to literature [8], cm^{-1}	IR band (this research), cm^{-1}
Q^0	4	840-890	844
Q^1	3	900-950	903
Q^2	2	960-1030	1002
Q^3	1	1050-1100	1092
Q^4	0	1160-1190	/

The relative distribution of tetrahedral structural units within the glass network is as follows: Q^0 units comprise 10.12%, Q^1 units 43.33%, Q^2 units 40.84%, and Q^3 units 5.7%. This distribution indicates a predominantly disrupted silicate network, with a high proportion of Q^1 and Q^2 units. Number of bridging oxygen per tetrahedra (BO/T) was calculated according to equation 1 [7]:

$$BO/T = 0 \cdot Q^0 + 1 \cdot Q^1 + 2 \cdot Q^2 + 3 \cdot Q^3 + 4 \cdot Q^4 \quad (1)$$

The number of bridging oxygen per tetrahedral is 1.42 indicating low glass network connectivity. The introduction of CaO and Na_2O into the glass batch composition acts as a network modifier, disrupting the continuous silica network by breaking Si–O–Si bonds. This disruption results in the formation of non-bridging oxygen. The presence of these non-bridging oxygens reduces the overall connectivity of the silicate network, thereby lowering the glass's viscosity. This reduction in viscosity is crucial during the melting process, as it enables optimal conditions for the glass melting process. The low amount of bridging oxygen per tetrahedra is expected knowing that a high amount of modifying cations were introduced in the batch.

4. CONCLUSION

The dark homogenous glass was produced by melting and quenching on the stainless steel batch that contains coal fly ash, Na_2CO_3, and $CaCO_3$. FTIR analysis showed spectra typical of aluminosilicate glasses. Deconvolution of the part of the spectra between 1200 and 800 cm^{-1} gave insights into glass network structure. There was no detected Q^4 structural unit and 1.42 bridging oxygen per [SiO_4] tetrahedral indicating low glass network connectivity.

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REFERENCES

[1] V. Savić, M. Dojčinović, V. Topalović, I. Cvijović-Alagić, J. Stojanović, S. Matijašević, S. Grujić, Int. J. Environ. Sci. Technol., 21 (2024) 6065–6074.
[2] E. Ercenk, T. Yasar, S. Demirkiran, S. Yilmaz, J. Therm. Anal. Calorim., 148 (10) (2023) 4015–4031.
[3] X. Zhao, H. Zhao, X. Huang, L. Wang, F. Liu, X. Hu, et al., Ecotoxicol. Environ. Saf., 223 (2021) 112550.
[4] Z. Hussain, N. Chang, J. Sun, S. Xiang, T. Ayaz, H. Zhang, et al., J. Hazard. Mater., 422 (2022) 126778.
[5] E. Worrell, M.A. Reuter., Handbook of Recycling: State-of-the-art for Practitioners, Analysts, and Scientists, Elsevier, Waltham, MA, 2014.
[6] E. Montoya-Quesada, M.A. Villaquirán-Caicedo, R.M. De Gutiérrez, Bol. Soc. Esp. Ceram. Vidr., 61 (4) (2022) 284–299.
[7] C. Zou, J. Cao, M. Zhao, Z. Wang, J. Lu, J. Eur. Ceram. Soc., 39 (15) (2019) 4979–4987.
[8] W. Xu, K. Shen, Z. Cao, F. Liu, Y. Zhang, T. Zhang, N. Wu, S. Ouyang, Mater. Chem. Phys., 263 (2021) 124334.