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Non-bridging oxygen and high-coordinated aluminum in metaluminous and peraluminous calcium and potassium aluminosilicate glasses: High-resolution ^{17}O and ^{27}Al MAS NMR results

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Abstract

Change in configuration and structure with composition are important components of thermodynamic and transport properties of most aluminosilicate melts, but the complex interactions, particularly in metaluminous and peraluminous compositions, are not yet well understood. In this paper, we present high-resolution ^{27}Al and ^{17}O MAS and 3QMAS NMR data on several calcium and potassium aluminosilicate glasses prepared at several SiO_2 isopleths, ranging from peralkaline to peraluminous compositions. In all calcium aluminosilicate glasses, the ^{V}Al content increases with increasing Al content, while the NBO content decreases (in one series, below the limit of detection), consistent with other recent NMR studies of calcium aluminosilicate glasses. An increase in ^{V}Al content per total Al is also observed as the glass approaches the calcia-silica binary. In the potassium aluminosilicate glasses, NBO is directly quantified for the first time in metaluminous and peraluminous compositions; ^{V}Al is below the detection limit. We discuss possible mechanisms for the incorporation of alumina into the melt structure and show how changes in the ^{V}Al content as a function of composition may be used to eliminate mechanisms that do not fit the observed data. We also explore reactions, which show the difficulty of explaining the NBO present on the metaluminous join with only the observed ^{V}Al, implying the necessity of multiple reactions producing NBO in such compositions.

Keywords: Aluminosilicate glasses, non-bridging oxygen, high-coordinated aluminum, NMR spectroscopy, oxygen-17, aluminum-27