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Moesgaard, Mette; Keding, Ralf; Skibsted, Jørgen; Yue, Yuanzheng

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Structural heterogeneity in calcium aluminosilicate glasses

Mette Moesgaard [a], *Ralf Keding* [a], *Jørgen Skibsted* [b], *Yuanzheng Yue** [a]

[a] Section of Chemistry, Aalborg University, DK-9000 Aalborg, Denmark
[b] Department of Chemistry, Aarhus University, DK-8000 Århus, Denmark

The physical and chemical properties of glasses are determined largely by their microstructure in both short- and intermediate-range. Despite numerous studies on the intermediate-range order (IRO), some key questions still remain unanswered. In this work, we investigate the IRO of peralkaline glasses within the calcium aluminosilicate system. This is performed by structural modeling and solid-state ^{29}Si and ^{27}Al nuclear magnetic resonance (NMR) spectroscopy. Two structural modeling approaches are proposed to describe the IRO. One model assumes a random spatial arrangement of Al, whereas the other allows clustering of regions rich in highly polymerized AlO_4 and SiO_4 units and other regions rich in highly depolymerized SiO_4 units. The clustering is described as IRO heterogeneity and this modeling approach provides a good description of the NMR spectra for all glasses. In contrast, the first approach can not convincingly model the NMR data. Thus, structural heterogeneities in the IRO do exist in the studied glasses.

Key words:

Calcium aluminosilicates

Structural modeling

Intermediate-range order

MAS NMR spectroscopy