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Structural heterogeneity in calcium aluminosilicate glasses

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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 ²⁹Si and ²⁷Al 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 AlO₄ and SiO₄ units and other regions rich in highly depolymerized SiO₄ 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