



The interplay of microscopic dynamics, structure and mass transport in silicate melts

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We use inelastic neutron scattering to study the mechanisms of mass transport in alkali silicates and sodium aluminosilicate melts at temperatures up to 1600 K. Binary alkali silicates show evidence for the existence of alkali diffusion channels in the static structure. These channels percolate in the Si-O network and serve as preferential alkali ion conducting pathways. The non-homogeneous distribution of the alkali ions in the disrupted tetrahedral Si-O network on length scales of 6-8 Å strongly influences the structural relaxation, i.e. the viscosity, of the network. By systematically replacing Na₂O by Al₂O₃, albite and jadeite as well as their 75 % per-alkaline compositions exhibit a significant decrease in the Na mobility and an increase in the viscosity. This goes along with a disruption of the channel structure found in binary alkali silicates with the addition of Al₂O₃. Neutron scattering on water bearing silica, sodium trisilicate and albite glasses reveals, that although dissolved water has a drastic impact on the melt viscosity, the structure is barely affected by the presence of OH groups. Vibrational spectra, that are dominated by the scattering of the hydrogen atoms, strongly depend on the anhydrous silicate composition, whereas the vibrational densities of states do not exhibit systematic changes in the concentration range of the dissolved water between 1 to 5 wt%.