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The impact of Al_2O_3 and Fe_2O_3 on relaxation and structure in sodium silicates disclosed by inelastic neutron scattering.

F. Kargl (1), A. Meyer (1), M. M. Koza (2) and H. Schober (2)

(1) Physik Department, Technische Universität München, 85747 Garching, Germany, (2) Institut Laue-Langevin, 38042 Grenoble, France

The composition of silica based melts and their microscopic structure are known to determine properties of molten rock and thus bear important influence on geological processes. Moreover, the composition and resulting properties determine whether a glass is feasible for technological applications. Thus it is obviously important to develop an understanding of the relationship of microscopic dynamics and structure with mass transport and its implications for properties of silica based melts. We present inelastic neutron scattering investigations of binary and ternary compositions. Time-of-flight spectroscopy allows to observe sodium self diffusion in silica based melts at magmatic temperatures. The transport mechanism and the number of modifier ions participating in the transport process are quantified within our investigations. Furthermore, the microscopic origin of the relaxation processes in such melts is revealed. Addition of alumina is observed to alter the dynamical behaviour of the modifier ions and medium range order. We observe a drastic slowing down of relaxation processes at a given temperature. Besides Al_2O_3, Fe_2O_3 plays an important role in most of the natural melts. Iron is known to feature two different oxidation states depending on temperature and composition. However, the position and coordination of iron with respect to the surrounding alkali silicate structure is not unambiguously resolved. From our investigations we conclude that iron is not homogeneously distributed in sodium iron silicates. A comparison with the elastic structure factors of the binary compositions indicates that iron seems to prefer a location within the sodium diffusion channels found in binary sodium silicates.