

# Effect of pressure on the structure of albite liquid near glass transition

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The network structure and density of albite glasses recovered from high pressure (to 7.2 GPa) and annealing temperatures across the liquid-glass transition region ( $T_g$ ) were analyzed *ex situ* using high-field  $^{27}\text{Al}$  magic-angle-spinning nuclear magnetic resonance (NMR) spectroscopy. For each pressure,  $^{27}\text{Al}$  NMR spectra show only subtle changes in the Al-O bonding environment at temperatures ranging from  $T_g-100\text{K}$  to  $T_g+50\text{K}$ . From these data, we calculate robust values for average aluminium coordination number and the mean quadrupolar coupling constant ( $C_q$ )-a proxy for the distortion and distribution of Al-O bonding environments- at fictive temperatures ( $T_f$ ) near  $T_g$ . While  $C_q$  increases linearly with density and pressure, the average Al number only increases above 2.6 GPa. Interestingly, in samples annealed in the vicinity of  $T_g$ , the fraction of  $^{16}\text{Al}$  is consistent with the results of MD simulations with pressure<sup>[1,2]</sup>. However, we find that the fraction of  $^{15}\text{Al}$  is greater in MD simulations, reflecting the structure at temperatures  $>1000-3000\text{K}$  higher than what is measured experimentally in glasses, where  $T_f$  is much closer to  $T_g$ . In albite and other sodium aluminosilicate liquids, high pressure-temperature simulation and experimental studies correlate maxima in  $\text{O}^{2-}$  diffusivity with either critical fractions of high-coordinated Al + Si<sup>[1]</sup> or the onset of increasing fraction of high-coordinated Al<sup>[3]</sup>. The possible role of such structural controls on transport properties with pressure will be discussed over all temperatures where liquid-like behavior exists.

[1] Bryce et al. (1999) *Am Min.* **84**, 345-356 [2]Suzuki et al. (2002) *Phys. Chem. Min.*, **29**, 159-164. [3] Wang et al. (2014) *Nat. Commun.* **5**, doi:10.1038/ncomms4241.