Structure of aluminate liquids and glasses under extreme conditions

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Abstract

In contrast to pure silica, SiO2, liquid alumina Al2O3 does not form a glass. This is in accordance with Zachiariasen's rules, since a significant fraction of aluminium atoms exhibit a coordination number of more than four and share edges. However, the introduction of CaO increases the O:Al ratio, allowing the formation of corner-shared AlO4 tetrahedra that facilitate glass formation. Liquid calcium aluminates are important components of natural magmas and their glasses have important applications for infrared-transmitting optics. A detailed and accurate description of the structural role of Al and Ca in high temperature CaO-Al2O3 liquids is important for understanding glass-forming mechanisms. Furthermore, pressure-induced structural transformations in calcium-aluminosilicate melts, and associated changes in physical properties (e.g. compressibility and viscosity), have a profound impact for the rheology of natural magmas and geophysical processes, from planetary formation to present-day volcanism.

In this communication, I will summarise recent progress in using the containerless high-temperature technique of aerodynamic levitation with CO2 laser heating, in combination with synchrotron x-ray diffraction, neutron diffraction with isotope substitution, and state-of-the-art molecular dynamics computer simulations, to reveal unique insight into dramatic and unexpected structural transformations on local and intermediate-range length-scales which take place during vitrification of these non-traditional glass-forming liquids [1,2,3]. I will also discuss the results of *in situ* laser-heated diamond anvil cell experiments with synchrotron x-ray diffraction of calcium-aluminate liquids and glasses, which reveal pressure-induced Al-coordination change and the development of short-range topological ordering [4].

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