Characterization of borate glasses, crystals and minerals

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Simple lead borates are common glasses used in many applications, but the addition of small amounts of aluminum has been found to confer favourable mechanical and processing properties. The intent of this work is to determine the structural origins of these physical properties in boroaluminates, and compare them with the corresponding properties in borogallate glasses. While some aspects of this project are awaiting the construction of a boron-free probe – which was given the green light in November 2008 –we have moved ahead with ^{27}Al and ^{71}Ga MAS NMR experiments in boroaluminate and borogallate glasses to quantify the populations of four-, five- and six-coordinate species. ^{27}Al MAS NMR of glasses at moderate magnetic fields such as 14.1 T provides adequate spectral resolution amongst these units, but greater precision can be obtained at 21.1 T. By contrast, ^{71}Ga MAS NMR at 14.1 T yields unresolved peaks obscured by overlapping spinning sidebands, from which speciation cannot be reliably derived. Only by using very fast magic-angle spinning at 21.1 T can lineshape features be detected which permit estimates of the concentrations of different Ga species in the glass (Figure 1). In combination with ^{11}B MAS NMR data (collected at 14.1 T), these populations provide valuable information about cation short-range order which can be used in charge-balance calculations to determine the degree of network polymerization, a key contributor to various materials properties. Once higher-field ^{11}B MAS NMR data become available, these calculations can be confirmed by direct measurement of borate network depolymerization.

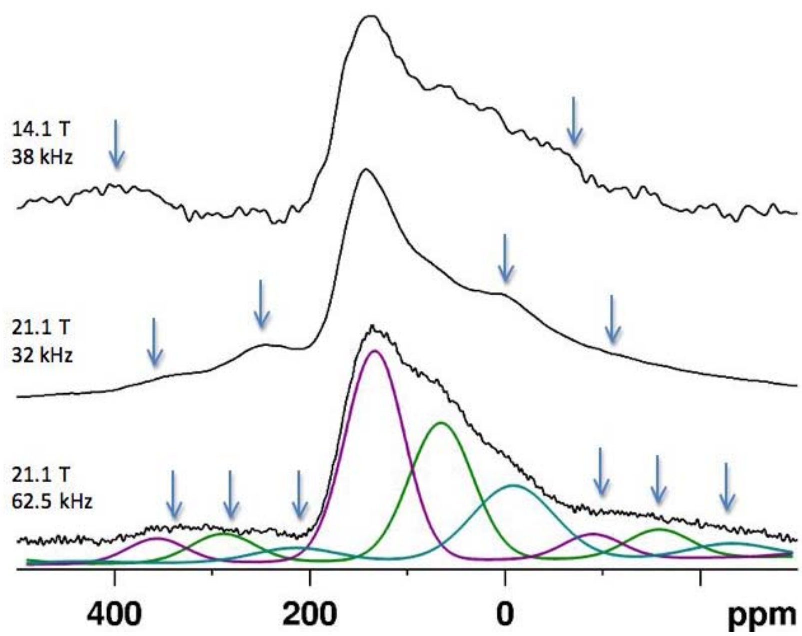

Figure 1: ^{71}Ga MAS NMR spectra of lead borogallate glass, showing the importance of high field and fast spinning. Arrows mark the spinning sidebands. Coloured subspectra indicate the fits employed to estimate four-, five- and six-coordinate Ga.