# NMR-Driven Reverse Monte Carlo Study of Sodium Borate Glasses

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Borate glasses are known to have a large fraction of the boron atoms involved in superstructural units like boroxol or pentaborate rings, in addition to the double coordination of boron atoms (3 and 4). This generates the boron's anomaly, which is a non-linear evolution of properties upon the addition of sodium oxide.[1] For example the glass transition temperature reaches a maximum for alkali content around 25%. In this work, we investigate theoretically and experimentally the structure of sodium borate glasses using $^{11}B$ and $^{23}Na$ NMR, molecular dynamics (MD) simulations and neutron diffraction.

Comparison of classical MD (CMD) with ab-initio MD (aiMD) shows that only aiMD produces structural models with a non-negligible fraction of super-structural units (6 membered rings) but still below the one determined by two-dimensional $^{11}B$ MQMAS NMR spectroscopy.[2] With the help of DFT-GIPAW computation of NMR shifts,[3] the NMR fingerprint of the various boron and sodium environments could be predicted and are found to be in good agreement with experimental data. These calculations improve our understanding of the impact of the structural disorder on the distribution of NMR parameters, typically the effect of the bond angle distribution (BAD) on the isotropic chemical shift of boron-11.

In order to improve our structural models, in particular to include a larger fraction of superstructural units, we develop a hybrid reverse monte carlo (HRMC) scheme combining MD with NMR and neutron data. The fraction of superstructural units is taken as an adjustable parameter and we observe that neutron data are not sufficiently sensitive to discriminate the various structural models, in contrast to $^{11}B$ NMR for both $BO_3$ and $BO_4$ units (i.e., ring and non-rings species). Simulated $^{11}B$ and $^{23}Na$ 2D MQMAS NMR are found to be in good agreement with experiments but the DFT-GIPAW NMR calculations limits the size of systems that can be studied (from 500 to 1000 atoms). In order to overcome this limitation, we have recently developed a Machine Learning (ML)[4] approach for computing NMR shifts and first applications of these emerging methodologies to borate glasses will be presented.

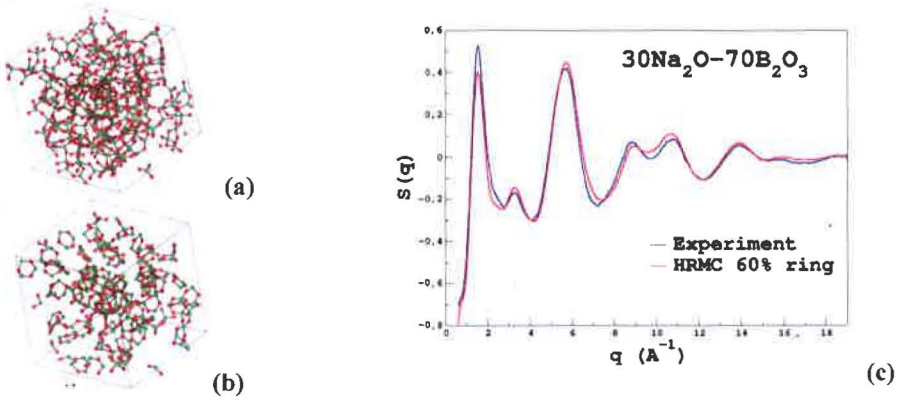


**Figure 1. (a) Structural model of $30Na_2O-70B_2O_3$ glass, highlighting rings (b). (c) Experimental and theoretical neutron structure factors.**

**References**

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