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To cite this version:

Erwan Chesneau, Thibault Charpentier, Gregory Tricot, Sylvain Cristol. Structural study of sodium borate glasses combining molecular dynamics and NMR. 15th International Conference on the Physics of Non-Crystalline Solids, Jul 2018, St Malo, France. cea-02340332

HAL Id: cea-02340332

https://cea.hal.science/cea-02340332

Submitted on 30 Oct 2019

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Structural study of sodium borate glasses combining molecular dynamics and nuclear magnetic resonance

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Abstract

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. For example the glass transition temperature reaches a maximum for alkali content around 25%.
In this study, we used an approach combining Molecular Dynamics (MD) with Nuclear Magnetic Resonance (NMR) to examine the evolution of the glass structure with the increase of alkali content. Structural models were generated by Classical MD (CMD) and ab-initio MD (aiMD) to compare the reliability/performance of both methods to reproduce NMR properties which were computed using the GIPAW method.

Only aiMD permits to generate superstructural units whereas CMD models are free of any 6-membered ring. With those MD-GIPAW data, correlations between NMR parameters could be highlighted, especially between the quadrupolar coupling constant CQ and the isotropic chemical shift δiso for boron and sodium. Accounting for those, the fitting model used for the analysis of experimental 1D and 2D spectra could be significantly improved.

Comparison of MD NMR results with experimental ones shows that boron-11 chemical shifts range obtained on the aiMD models reproduce almost perfectly the experimental one. Our calculations reveal chemical shift variations for BO3 and BO4 when boron atoms are inside or outside a superstructural unit. Moreover, NMR parameters are less distributed for boron inside a ring, as a result of the stronger geometrical constraints inside a superstructural unit. In addition, correlations between local structural features and NMR parameters were investigated such as the dependence of boron-11 isotropic chemical shift with the average angle B-O-B.

Keywords: solid state NMR, molecular dynamics, borate glasses, superstructural units

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