Structure-Property relationships in barium silicate glasses & crystals: Preliminary results

B. J. A. MOULTON[1,2*] D. V. SAMPAIO[1,2], A. M. RODRIGUES[2], C. DOERENKAMP[3], L. D. SILVA[2], A. PICININ[1], H. ECKERT[3,4], J. P. RINO[1,2], E.D. ZANOTTO[2], P. S. PIZANI[1,2]

[1] Physics Department, Federal University of São Carlos, Rod. Washington Luis, Km 235 13565-905 São Carlos, SP, Brazil, benmoul@df.ufscar.br, davidvsampaio@gmail.com, pizani@df.ufscar.br

[2] CERTEV - Center for Research, Technology, & Education in Vitreous Materials, Department of Materials Engineering, Federal University of São Carlos, 13565 - 905 São Carlos-SP, Brazil: www.certev.ufscar.br, dedz@ufscar.br

[3] Institute of Physics in São Carlos, University of São Paulo, São Carlos, SP 13560-590, Brazil. cdoerenkamp@gmail.com

[4] Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstrasse 28/30, 48149 Münster, Germany. E-mail: eckerth@uni-muenster.de

This study focuses on the structure-property relationships in the baria-silica system. We have synthesized and simulated a series of barium silicate glasses and minerals covering the compositional range $xBaO\text{-}(1\text{-}x)SiO_2$ where x_{glass} = 0.27-0.45 & $x_{crystal}$ = 0.33-0.66. Raman spectroscopy, ^{29}Si NMR, Ba L_3-edge XANES, and molecular dynamics simulations are correlated with changes in the density and refractive index of these glasses and their crystalline equivalents.

^{29}Si NMR results have been used to calibrate the Raman Q^n band deconvolution. NMR and MD results show that the network connectivity increases with silica content, as expected. These results are compared with other alkaline-earth silicate glasses in terms of both their Q^n and oxygen speciation.

Detailed comparison between the Raman spectra of barium-silicate glasses and crystals shows some unexpected behaviours. For instance, in minerals, the Si-O-Si bending mode (535-550 cm^{-1}) does not appear to correlate with inter-tetrahedral angle. The origin of this behaviour is currently under investigation, as these modes display a much more diverse behaviour in barium silicate glasses and supercooled liquids.