Network Topology and Diffusion in Soda Lime Borate Glass Systems
Smedskjær, Morten Mattrup; Mauro, John C.; Sen, Sabyasachi; Yue, Yuanzheng

Publication date:
2010

Document Version
Early version, also known as pre-print

Link to publication from Aalborg University

Citation for published version (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

? Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
? You may not further distribute the material or use it for any profit-making activity or commercial gain
? You may freely distribute the URL identifying the publication in the public portal

Take down policy
If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from vbn.aau.dk on: december 29, 2018
NETWORK TOPOLOGY AND DIFFUSION IN SODA LIME BORATE GLASS SYSTEMS

Morten M. Smedskjaer1*, John C. Mauro2, Sabyasachi Sen3, Yuanzheng Yue1

1* Section of Chemistry, Aalborg University, Sohngaardsholmsvej 57, DK-9000 Aalborg, Denmark – morten04@bio.aau.dk
2 Science and Technology Division, Corning Incorporated, Corning, NY 14831, USA
3 Department of Chemical Engineering and Materials Science, University of California at Davis, Davis, CA 95616, USA

In this paper, we have investigated the structure, transport properties, and network topology of the borate glass series (in mol%): (89-x)B2O3 – xNa2O – 10CaO – 1Fe2O3 with x = 5, 10, 15, 20, 25, 30, and 35. By using a temperature-dependent topological constraint model, we have predicted the scaling of the glass transition temperature, fragility, and boron speciation with composition (x). Experimental results are in good agreement with the predicted ones, and this provides insights into the correlation between the glassy dynamics and the structure of soda lime borate glasses. Through this correlation, we attempt to clarify the origin of the correlation between the inward cationic diffusion and the glass composition. The inward cationic diffusion is induced by reducing ferric ions to ferrous ions in the glasses near the glass transition temperature. The extent of inward diffusion varies with composition and this variation depends on the boron speciation and the electrostatic environments of the involved modifying ions. This work also provides information on the microstructural origin of fragility of oxide liquids.

Keywords: Borate glasses; diffusion; network topology; topological constraint model; boron speciation; fragility; glass transition