

## **Aalborg Universitet**

## Statistical Mechanical Modeling of Lithium Borate Glass Structure and Topology

Bødker,	Mikkel Sandfeld;	; Mauro, John C.	; Youngman,	, Randall E.;	Smedskjær,	Morten
Mattrup			_		_	

Publication date: 2019

Link to publication from Aalborg University

Citation for published version (APA):

Bødker, M. S., Mauro, J. C., Youngman, R. E., & Smedskjær, M. M. (2019). Statistical Mechanical Modeling of Lithium Borate Glass Structure and Topology. Poster presented at 25th International Congress on Glass, Boston, United States.

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 ?

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.

## Statistical Mechanical Modeling of Lithium Borate Glass Structure and Topology

M. Bødker\*1; J. C. Mauro2; R. Youngman3; M. M. Smedskjaer1

1. Aalborg University, Denmark 2. Pennsylvania State University, USA 3. Corning Incorporated, USA

Predicting the compositional evolution of the atomic-scale structure of oxide glasses is important for developing quantitative composition-property models. In binary borate glasses, the addition of network modifiers will either increase the connectivity by converting three-fold into four-fold coordinated boron, or decrease the connectivity by creating non-bridging oxygens. Here, based on 10B nuclear magnetic resonance spectroscopy data from literature, we present a statistical description of the compositional evolution of both intermediate range superstructures (e.g., boroxol rings) and short range Qn species in lithium borate glasses. This is done by accounting for the relative enthalpic and entropic contributions to the bonding preferences. We show that the entire glass structure evolution can be predicted based on experimental structural information for only a few glass compositions in each series. The developed structural model can be combined with a previously established constraint theory model to also predict the glass transition temperature.