



Aalborg Universitet

AALBORG UNIVERSITY  
DENMARK

## Nature and Quantification of Stress in Over-Constrained Glasses

Li, X.; Smedskjær, Morten Mattrup; Mauro, John C.; Sant, Gaurav; Bauchy, Mathieu

*Publication date:*  
2019

[Link to publication from Aalborg University](#)

*Citation for published version (APA):*

Li, X., Smedskjær, M. M., Mauro, J. C., Sant, G., & Bauchy, M. (2019). *Nature and Quantification of Stress in Over-Constrained Glasses*. 15. Abstract from 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 ?

### Take down policy

If you believe that this document breaches copyright please contact us at [vbn@aub.aau.dk](mailto:vbn@aub.aau.dk) providing details, and we will remove access to the work immediately and investigate your claim.

## **Nature and Quantification of Stress in Over-Constrained Glasses**

X. Li<sup>1</sup> ; M. M. Smedskjaer<sup>2</sup> ; J. C. Mauro<sup>3</sup> ; G. Sant\*<sup>1</sup> ; M. Bauchy<sup>1</sup>

*1. University of California, Los Angeles, USA 2. Aalborg University, Denmark 3. Pennsylvania State University, USA*

Topological constraint theory classifies network glasses into three categories, viz., flexible, isostatic, and stressed–rigid, where stressed-rigid glasses have more topological constraints than atomic degrees of freedom. Such over-constrained glasses are expected to exhibit some internal stress due to the competition among the redundant constraints. However, the nature and magnitude of this internal stress remain poorly characterized. Here, based on molecular dynamics simulations of a stressed-rigid sodium silicate glass, we present a new technique allowing us to directly compute the internal stress present within a glass network. We show that the internal stress comprises two main contributions: (i) a residual entropic stress that depends on the cooling rate and (ii) an intrinsic topological stress resulting from the over-constrained nature of the glass. Overall, these results provide a microscopic picture for the structural instability of over-constrained glasses.