



Aalborg Universitet

AALBORG UNIVERSITY  
DENMARK

## Origin of the Mixed Alkaline Earth Effect on the Hardness of Silicate Glasses

Yu, Yingtian; Krishnan, N. M. Anoop; Smedskjær, Morten Mattrup; Mauro, John C.; Bauchy, Mathieu

*Publication date:*  
2017

*Document Version*  
Publisher's PDF, also known as Version of record

[Link to publication from Aalborg University](#)

*Citation for published version (APA):*

Yu, Y., Krishnan, N. M. A., Smedskjær, M. M., Mauro, J. C., & Bauchy, M. (2017). *Origin of the Mixed Alkaline Earth Effect on the Hardness of Silicate Glasses*. Poster presented at 12th Pacific Rim Conference on Ceramic and Glass Technology, Waikoloa, Hawaii, 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.

# Origin of the Mixed Alkaline Earth Effect on the Hardness of Silicate Glasses

Yingtian Yu<sup>1</sup>, Anoop N. Krishnan<sup>1</sup>, Morten M. Smedskjaer<sup>2</sup>, John C. Mauro<sup>3</sup>, Mathieu Bauchy<sup>1</sup>

<sup>1</sup>Civil and Environmental Engineering, University of California, Los Angeles, Los Angeles, CA, USA

<sup>2</sup>Aalborg University, Aalborg, Denmark

<sup>3</sup>Corning Incorporated, Corning, NY, USA

Most oxide glasses containing a combination of two (or more) types of alkali or alkaline earth cations tend to exhibit non-additive variations of their properties, when one cation is gradually substituted by the other one. This behavior, known as the mixed alkali effect (MAE), has remained an enigma in glass science. In particular, hardness – a property of primary interest for applications such as protective screens, can exhibit a positive or negative deviation from linearity with respect to the fraction of mixed ions. Here, based on molecular dynamics simulations, we investigate the hardness of mixed calcium/magnesium aluminosilicate glasses. We observe a minimum of hardness for mixed glasses, in agreement with micro-indentation experiments. Such anomalous behavior is found to arise from an increase propensity for shear flow relaxation under load, which is stimulated by the presence of internal stress in the atomic network. Finally, we demonstrate that the internal stress originates from a mismatch between the alkaline earth cations and the rest of the silicate network for mixed compositions. The present results offer a clear atomic picture of the origin of the MAE on hardness and highlight the potential for the nano-engineering of high-performance glasses.

**KEYWORDS:** Mixed ion effect, hardness, molecular dynamics.