



AALBORG UNIVERSITY
DENMARK

Aalborg Universitet

Topological control on glasses' dissolution kinetics

Invited Talk

Bauchy, Mathieu; Smedskjær, Morten Mattrup

Publication date:
2018

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Bauchy, M., & Smedskjær, M. M. (2018). Topological control on glasses' dissolution kinetics: Invited Talk. Abstract from 15th International Conference on Physics of Non-Crystalline Solids & 14th European Society of Glass Conference , Saint Malo, France.

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.

Topological control on glasses' dissolution kinetics

Mathieu Bauchy ^{*† 1}, Morten Smedskjær ²

¹ University of California, Los Angeles (UCLA) – United States

² Aalborg University – Denmark

Understanding and predicting the dissolution rate of silicate glasses is of primary importance for various applications, including bioactive glasses and borosilicate wastefoms. However, the mechanism of silicates' dissolution-and its rate-limiting step-remains poorly understood. In particular, present models linking the composition and structure of silicate glasses to their dissolution rate in a given solvent have remained largely empirical thus far. Here, based on vertical scanning interferometry (VSI) experiments and molecular dynamics (MD) simulations, we study the dissolution of a large variety of silicate glasses under various pH conditions. From a detailed analysis of the simulated structures, we demonstrate that the kinetics of the dissolution is controlled by the topology of the atomic network. We propose a new topological model of silicates' corrosion, which is shown to offer realistic predictions of dissolution rates and activation energies for a wide selection range of silicate glasses and crystals.

Keywords: Dissolution, Topological constraint theory, Molecular Dynamics

*Speaker

†Corresponding author: bauchy@ucla.edu