



Aalborg Universitet

AALBORG UNIVERSITY
DENMARK

Predicting Bond Switching and Fracture in Simulated Al₂O₃ Glass Using Machine Learning

Du, Tao; Liu, Han; Tang, Longwen; Sørensen, Søren Strandskov; Bauchy, Mathieu; Smedskjær, Morten Mattrup

Publication date:
2022

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Du, T., Liu, H., Tang, L., Sørensen, S. S., Bauchy, M., & Smedskjær, M. M. (2022). *Predicting Bond Switching and Fracture in Simulated Al₂O₃ Glass Using Machine Learning*. Poster presented at 26th International Congress on Glass, Berlin, Germany.

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.

Predicting Bond Switching and Fracture in Simulated Al₂O₃ Glass Using Machine Learning

Tao Du^{1*}, Han Liu², Longwen Tang², Søren S. Sørensen¹, Mathieu Bauchy², Morten M. Smedskjaer¹

¹ Aalborg University, ² University of California, Los Angeles
*taod@bio.aau.dk

Flaw-free amorphous alumina (a-Al₂O₃) samples have recently been found to exhibit excellent nanoductility at room temperature and under high strain rate. A better understanding of the underlying ductile deformation mechanism could help to facilitate the design of damage-tolerant glassy materials. In this work, based on atomistic simulations and classification-based machine learning, we reveal that the propensity of simulated glassy Al₂O₃ to exhibit nanoscale ductility is encoded in its static (non-strained) structure. The machine learning based softness metric trained from the spontaneous dynamics of the system (i.e., under zero strain) is able to readily predict the fracture behavior of the glass (i.e., under strain). Specifically, lower softness facilitates Al bond switching and the local accumulation of high-softness regions leads to rapid crack propagation. These results are helpful for designing oxide glass formulations with improved resistance to fracture.

References

[1] Du, T.; Liu, H.; Tang, L.; Sørensen, S. S.; Bauchy, M.; Smedskjaer, M. M. Predicting Fracture Propensity in Amorphous Alumina from Its Static Structure Using Machine Learning. *ACS Nano* 2021, 15 (11), 17705–17716.