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Predicting Bond Switching and Fracture in Simulated Al_2O_3 Glass Using Machine Learning

Tao Du[1*], Han Liu[2], Longwen Tang[2], Søren S. Sørensen[1], Mathieu Bauchy[2], Morten M. Smedskjaer[1]

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

Flaw-free amorphous alumina (a-Al_2O_3) 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 Al_2O_3 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

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