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

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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.