Predicting Fracture Propensity in Amorphous Alumina from its Static Structure using MD and Machine Learning

Du, Tao; Smedskjær, Morten Mattrup

Publication date:
2021

Predicting Fracture Propensity in Amorphous Alumina from its Static Structure using MD and Machine Learning

Tao Du, Morten M. Smedskjaer
Department of Chemistry and Bioscience, Aalborg University, Aalborg, Denmark

Based on MD simulations and classification-based machine learning, we reveal that the propensity of amorphous 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 under zero strain is able to readily predict its fracture behavior.

Reference: 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* **15**, 17705-17716 (2021).