Atomistic origin of network glass fracture

Franz Bamer*†[1], Zhao Wu[1], Bhagyashri Bachhav[1], Somar Shekh Alshabab[1], Michael Shields[2], and Michael Falk[2]

[1]RWTH Aachen University = Rheinisch-Westfälische Technische Hochschule Aachen – Germany
[2]Johns Hopkins University – United States

Abstract

Disordered network materials, such as silica glass, behave fundamentally differently than densely packed systems, such as metallic glass. Their network consists of corner-sharing SiO$_4$ tetrahedra (or SiO$_3$ triangles) that form rings of various shapes and sizes. Densely packed systems respond as an accumulation of local atomic-scale rearrangements occurring in point defects, also called shear transformation zones. After generating two-dimensional network glass models using a dual Monte Carlo bond-switching strategy, we perform rigorous mechanical investigations using the athermal quasistatic deformation method. We show that the onset of network glass fracture occurs in soft spots similar to shear transformation zones; however, in the case of network glasses, the local rearrangement picture in those zones can mainly identified as a bond-breaking type destroying the network topology locally. First, we will identify the peculiarities of these local fracture events. Then, we will present several prediction strategies to identify these zones in network glasses prior to mechanical loading. Hereby, we will identify local rearrangement spots presenting purely geometrical predictors and predictors using local probing techniques. Finally, we will show that neural network models can identify these zones if they are trained with sufficient data available.

*Speaker
†Corresponding author: bamer@iam.rwth-aachen.de