UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium SS 2023
Fr 21.04.2023, 14:00-15:30
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udue.de/TheoKoll

Predicting the failure of silica glasses

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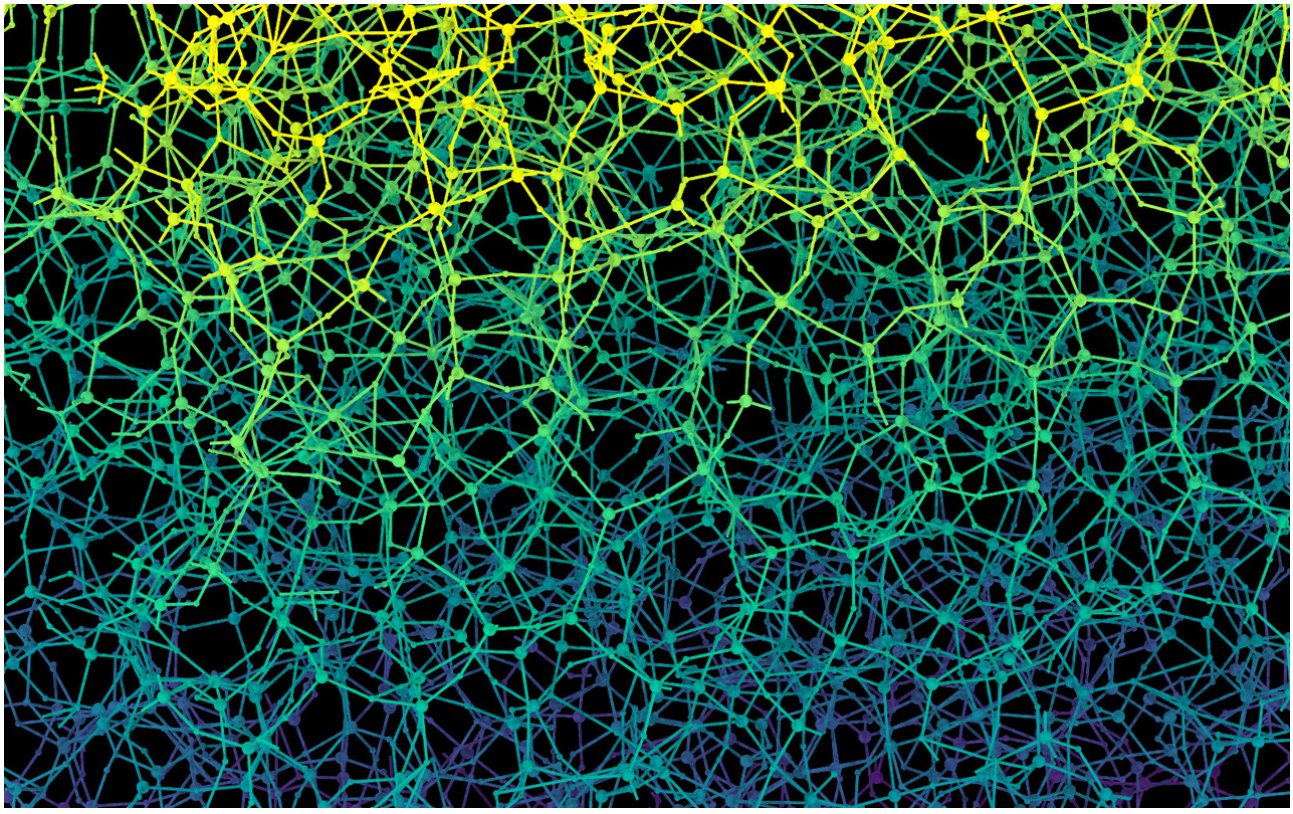

Glass represents the quintessential brittle material, shattering in pieces with little deformation. Yet at the nanoscale, silica glass becomes ductile and deforms plastically like metals. This behavior was observed experimentally in amorphous silica nanofibers, but its origin was unclear. We investigated the problem by extensive atomistic simulations. Our results show that the observed small sample size enhanced ductility is primarily due to diffuse damage accumulation. For larger samples, however, damage coalesce in extended cracks leading to brittle catastrophic failure. We then identify two distinct types of elementary plastic events, one is a standard quasilocalized atomic rearrangement while the second is a bond-breaking event that is absent in simplified models of fragile glass formers. Our results show that both plastic events can be predicted by a drop of the lowest nonzero eigenvalue of the Hessian matrix that vanishes at a critical strain. Finally, I will discuss our approach to predict the failure of two dimensional silica glasses by convolution neural networks.