

Statistical structural mechanism for shear localization in amorphous materials

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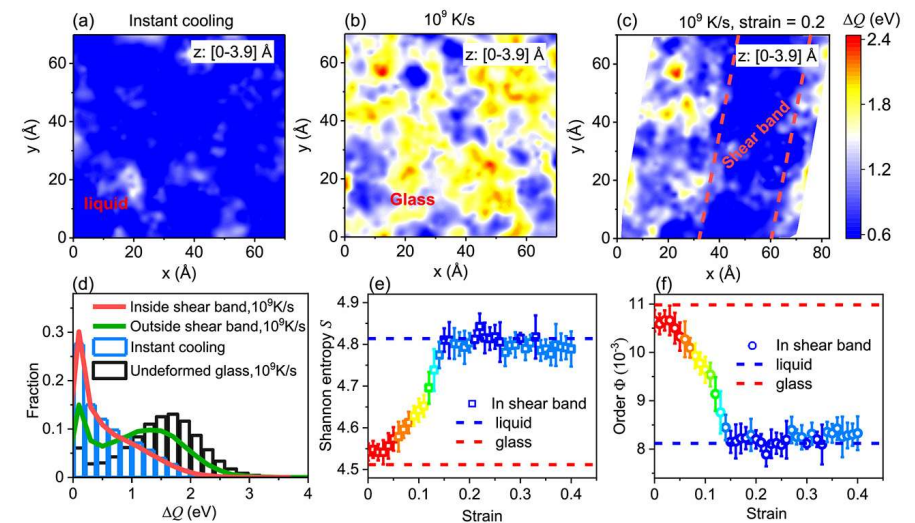
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Purpose Reveal the atomic scale structural mechanism of shear localization phenomenon in amorphous materials.

Outline Through introducing two fundamental physical parameters, a universal structure-property relationship is established.

Result Shear localization is a prevalent phenomenon in amorphous materials undergoing plastic deformation, yet its underlying structural mechanism at the atomic scale remains elusive. Here we introduce a quantitative approach to correlate structural order and disorder with the degree of shear localization in amorphous materials. This approach relies on two fundamental physical parameters: the statistical structural order, derived from Shannon entropy of local Voronoi structures, and the localization susceptibility, characterized by spatial correlations in atomic-scale von Mises strain. Extensive atomistic simulations validate our approach and reveal a universal relationship between structural order and shear localization across a wide range of amorphous solids, each with distinct chemical compositions and thermal histories. We interpret the correlation between structural order and shear localization within a framework of shear banding as a mechanically-driven glass transition, governed by a structural collapse analogous to thermodynamic glass transitions on the potential energy landscape.

A statistical mechanics perspective revealing shear banding as mechanically-driven glass-to-liquid transition



Computing system: SQUID General Purpose CPU nodes
node-hour 11435.2 node-hour
memory used 500 GB
parallelize 1 or 2 nodes