Evolution of the Fabric Tensor in Amorphous Silica: Via Molecular Dynamics Simulations

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Atomic Force Microscopy experiments and MD (Molecular Dynamics) simulations have revealed a process zone (PZ) near the crack tip in amorphous silica (a-SiO_2). Within this PZ pores nucleate and coalesce with one another up to 20 nm ahead of the crack tip. After which the cavities merge with the advancing crack to cause mechanical failure. Similarly, when a-SiO_2 sample is nanoindented one finds permanent damage under the indenter in the form of densified silica.

To shed light on the origin of irreversible deformation in amorphous media, where the notion of dislocations is irrelevant, MD simulations have been performed in a-SiO_2 systems which are subjected to (1) a cyclic loading and unloading of the hydrostatic pressure and (2) a shearing force at room temperature. In particular, the so-called fabric tensor commonly used in granular physics is computed and allows to evidence anisotropy setting in the structure silica.