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# XPDF and molecular dynamics analysis of the significance of bond angle change in the deformation of amorphous silica

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## Abstract

The deformation mode of amorphous materials differs from that of their crystalline counterparts in an important respect: whilst ordered materials possessing an atomic lattice arrangement deform in an affine way, glasses contain structural inhomogeneities down to Ångstrom length scales of interatomic bonds. Regions of denser packing exist alongside less dense domains, meaning that strain inhomogeneity manifests itself throughout structural scales. In this study we set ourselves the objective of elucidating how this non-uniform deformation is accommodated in amorphous silica: what mechanisms are responsible for different modes? With the help of X-ray Pair Distribution Function (XPDF) analysis and molecular dynamics simulation we were able to reveal that short range stretching of atomic bonds does not match the long range macroscopic strain. Instead, locally strain is accommodated by bond angle changes that we refer to as "scissoring" action. The relationships between macro and atomic level strains demonstrate that atomic rearrangement (bond angle change), rather than bond stretching, is the dominating strain accommodation mechanism up to length scales of approximately 15 Å in this material, even under moderate non-hydrostatic applied stress states down to ~100 MPa. <https://www.nature.com/articles/s41598-018-19900-2>

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