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The Origin of Deformation-Induced Topological Anisotropy in Silica Glass

Erik Bitzek[a,b], Achraf Atila[a,b], Sudeheer Ganisetti[a], Julien Guénolé[c], Arun Prakash[d], Jürgen Horbach[e], Lothar Wondraczek[f]

[a]*Department of Materials Science and Engineering, Institute I, FAU Erlangen-Nürnberg, Germany*

[b]*Computational Materials Design, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany*

[c]*Université de Lorraine, CNRS, Arts et Métiers, LEM3, Metz, France*

[d]*Micromechanical Materials Modelling, Technische Universität Bergakademie Freiberg, Germany*

[e]*Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Germany*

[f]*Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, German*

[a]*e.bitzek@mpie.de*

Silica glasses are due to their amorphous nature often seen as archetypal examples for isotropic materials. However, structural anisotropy can be induced through processing. The exact structural changes and the corresponding atomic-scale mechanisms responsible for anisotropic properties have so-far remained elusive.

Here we present recent results of atomistic simulations of silica glasses deformed under different conditions. By using novel analysis techniques, we were able to show that transient and persistent anisotropy induced by uniaxial deformations at room temperature have clearly different structural origins. We were furthermore able to directly visualize the atomic-scale mechanisms leading to the structural changes underlying the different types of anisotropy. We address the effect of network modifiers on the generation of anisotropy and discuss the impact of topological anisotropy on the mechanical properties of glasses. Or findings elucidate the relation between the deformation protocol and the resulting anisotropic structure of the silica network, and thus provide important insights for the design of oxide glasses with tailored materials properties.

Keywords: Silica; Anisotropy; Molecular Dynamics Simulation; Mechanical Properties