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2017 Alfred R. Cooper Young Scholar Award Presentation

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2017 Alfred R. Cooper Young Scholar Award Presentation

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Glass Relaxation is Controlled by the Topology of the Atomic Network

Abstract:

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Understanding, predicting, and controlling glass relaxation is of primary importance for the manufacturing of display glasses, as any small variation in volume can result in undesirable pixel misalignments. However, no clear atomistic mechanism of structural and stress relaxation is available to date, which limits our ability to identify optimal glass compositions featuring low relaxation. Here, based on modulated differential scanning calorimetry experiments and molecular dynamics simulations, we study the relaxation of a series of alkali-free calcium aluminosilicate (CAS) glasses with varying compositions. We observe that selected CAS compositions exhibit minimal relaxation. We investigate the structural origin of this behavior by means of topological constraint theory. Based on this analysis, we demonstrate that minimal relaxation is achieved for isostatic glasses, which are both free of eigenstresses and floppy modes. This highlights the crucial role of the atomic topology in controlling the propensity for glass relaxation.