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Topological Control on Glass Relaxation

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Understanding, predicting, and controlling glass relaxation is of primary importance for the manufacturing of substrate glasses used in display applications, as any small variation in volume can result in undesirable pixel misalignment. 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 molecular dynamics simulations, we study the relaxation of a series of alkali-free calcium aluminosilicate (CAS) and sodium silicate (NS) glasses with varying compositions. We observe that select glass 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 eigenstress and floppy modes. This highlights the crucial role of the atomic topology in controlling the propensity for relaxation.