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Mechanically informed identification of shear instabilities in disordered covalent network glass

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Abstract

Understanding the origins of plasticity in glasses is challenging due to their inherently disordered structure and the absence of clearly defined defects. Unlike crystalline solids, where dislocations govern plastic deformation, glasses lack long-range order, making it difficult to locate the microscopic origins of their irreversible deformation. However, it is hypothesized that plasticity initiates at localized regions structurally predisposed to atomic rearrangements, commonly referred to as Shear Transformation Zones (STZs). Identifying these zones in the undeformed state is a crucial step toward formulating a complete theory of glass deformation, yet it remains an elusive task. In this work, we investigate STZ identification in two-dimensional silica glass, a system characterized by its disordered covalent network. We generate glass structures using a Monte Carlo bond-switch algorithm and subject them to athermal quasistatic shear. By performing local shear simulations on subdomains of the system, we probe their local stress-strain behavior and demonstrate that STZs strongly correlate with regions of low local stress thresholds. Despite its accuracy, this approach is computationally intensive, requiring mechanical simulations at each atomic site. To address this limitation, we leverage the topological characteristics of the elastic structural response to develop purely geometrical indicators based on fabric tensors, which characterize the statistical directional distribution of silica-silica bond vectors. Our findings reveal a strong correlation between STZs and regions of maximal bond stretch variance when projected along the macroscopic deformation axis. While directional factors contribute to this relationship, bond stretch variance emerges as the predominant factor, underscoring the invariant nature of STZs in network glasses. Since our indicators rely exclusively on geometric measures, they offer an intuitive physical interpretation and can be extracted directly from structural images with minimal computational cost. In conclusion, we demonstrate that STZs in two-dimensional silica glass can be identified with high accuracy, laying the foundation for more precise macroscopic models that capture their yielding and fracture behavior.