Abstract

Recent progress in the acceleration of the athermal mechanical response identification of disordered solids

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The deformation mechanics of disordered materials, such as glasses and amorphous solids, are driven by elementary events on the nanoscale in material spots involving a few hundred atoms. Since every atom in the system has a unique atomic neighborhood, a physically meaningful description requires detailed information about the microscopic environment, making the simulation of larger samples a computational nightmare. We use the athermal quasistatic simulation (AQS) method, which is reasonable for ambient conditions far from the glass transition temperature but computationally costly the larger the sample at hand [1]. Our project targets two objectives: (i) detecting spots prone to rearrangements and (ii) generating athermal low-order descriptors enhanced by localization information. These simulations, which involve solving a multidimensional minimization problem at each step, are crucial for understanding the micro- and macroscopic mechanical properties of disordered materials. In this study, we offer new methods for rearrangement prediction to a priori localize plastic events based on structural information. We also present methods to accelerate the AQS procedure by improving initial optimization guesses [2] and employing parallel-in-time type computing [3].

References

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