Plasticity in fragile and strong bulk-metallic glasses during nanoindentation

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Abstract

Glass-forming liquids are known to change their thermodynamic and dynamical properties quasi-discontinuously as they transition from a fragile to a strong liquid upon cooling. Properties of "fragile" and "strong" glasses-obtained, respectively, by rapidly quenching an equilibrium melt from either above or below the fragile-to-strong transition (FTST) temperature-certainly depend on the initial temperature. However, it is not clear to what degree glasses reflect the discontinuity of the FTST after the quench. In this work, we address this question by conducting molecular dynamics simulations of a model bulk metallic glass with an FTST temperature of 830 K. We find the elastic properties to be relatively insensitive to the initial temperature. However, the yield stress of the strong glass cooled from 812 K is substantially 15 % higher compared to that of the fragile glasses, showing little dependence on the initial temperature all the way up to the highest investigated starting temperature of 1200 K. The larger yield strength correlates with more localized shear transformation zones (STZs) obtained during nanoindentation in the strong glass. Interestingly, the detailed topology of the STZs in the strong glass looks similar to the eye as those in the fragile glass, even when the melt had been relaxed twenty times the energy autocorrelation time and two hundred times the volume autocorrelation times. In contrast, the STZs produced in glasses quenched from stochastically unrelated melts show clearly distinguishable patterns. We conclude that shear-band formation is governed by the same mechanism in strong and fragile glasses, and that even fragile melts have a structural memory far longer than energy and volume auto-correlation times.

Keywords: Metallic glasses, Atomistic simulations, Nanoindentation

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