Dynamics of deeply supercooled liquids and glasses: From finite-time amorphous solids to brittle yielding

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Abstract

Molecular dynamics computer simulations of a model glassformer under shear are presented (1). The starting point for these simulations are deeply supercooled samples far below the critical temperature, Tc, of mode coupling theory. These samples are fully equilibrated with the aid of the swap Monte Carlo technique. For states below Tc, we identify a lifetime that measures the time scale on which the system can be considered as an amorphous solid. The temperature dependence of this lifetime can be well described by an Arrhenius law. The existence of transient amorphous solid states below Tc is associated with the possibility of brittle yielding, as manifested by a sharp stress drop in the stress–strain relation and shear banding. We show that brittle yielding requires, on theone hand, low shear rates and, on the other hand, the time scale corresponding to the inverse shear rate has to be smaller or of the order of the lifetime of the amorphous solid. Both conditions can only be met for a large lifetime, i.e., for states far below Tc. (1) K. Lamp, N. Küchler, and J. Horbach, *Brittle yielding in supercooled liquids below the critical temperature of mode coupling theory,* J. Chem. Phys. **157**, 034501 (2022).

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