

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Liquid-liquid phase transition and fragile-to-strong transition

LIMEI XU, SERGEY BULDYREV, H. EUGENE STANLEY — Using molecular dynamics simulations we study the dynamic properties for a model of liquid consisting of particles interacting via a spherically symmetric potential with repulsive and attractive ramps, first introduced by Jagla. The model displays anomalies similar to those found in liquid water, namely, expansion upon cooling and an increase of diffusivity upon compression as well as the liquid-liquid phase transition in the region of phase diagram easily accessible by simulations. At lower temperatures the low and high density liquids undergo glass transitions into correspondent glassy phases. We find that similarly to the behavior of water and silicon, the glass transition in the high density phase is fragile while in the low density phase it is strong. The difference is that in the present model, the co-existence line between low-density and high-density liquids as well as its Widom extension above the critical point have positive slopes. Thus, at constant pressure the behavior of diffusion coefficient changes upon cooling from strong to fragile, i.e. in the opposite way than in water and silicon.

Limei Xu

Date submitted: 14 Dec 2004

Electronic form version 1.4