MAR09-2008-005529

Abstract for an Invited Paper for the MAR09 Meeting of the American Physical Society

Simple scaling of the glass transition temperature with ${f pressure}^1$

NING XU, University of Pennsylvania and University of Chicago

Zero-temperature packings of frictionless spheres have been used as a starting point for understanding granular materials, foams, colloids and even glass-forming liquids. Such packings exhibit a jamming transition, known as Point J, with increasing packing fraction. This symposium presents recent work that explores the implications of Point J for systems at nonzero temperature, shear stress, or friction. In this talk, I present results that push beyond zero temperature to explore the connection between Point J and the glass transition. We performed molecular dynamics simulations of several three-dimensional models of glass-forming liquids, and measured the relaxation time from the intermediate scattering function along several trajectories to the glass transition, such as lowering temperature at fixed packing fraction, or raising pressure at fixed temperature. Along each trajectory, we extrapolated the relaxation time using the form $\tau = \exp(A/(T-T_0)^{\alpha})$ or $\tau = \exp(A/(p^r - p_0^r)^{\alpha})$. depending on whether temperature or pressure was varied, where p^r is the contribution to the pressure from repulsive forces, only. Here, A, α , T_0 and p_0^r are fit parameters. We find that T_0 is linear in the repulsive contribution to the pressure, p^r : $T_0 = vp^r$. The fit parameter v is approximately $0.035v_0 = (0.37\sigma)^3$, independent of potential, where v_0 is the average volume per particle and σ is the diameter of the particle. This linear scaling of T_0 with p^r holds very well at low p^r , which corresponds to the vicinity of Point J in purely repulsive systems where jamming transition at T=0 exists. This suggests that Point J marks the onset of a nonzero value of the glass transition temperature, T_0 . Experimental data for glycerol (K. Z. Win and N. Menon, Phys. Rev. E 73, 040501 (2006)) also show that T_0 is linear in pressure, with a prefactor of $0.04 \times$ the molecular volume.

¹Supported by DE-FG02-05ER46199 and DE-FG02-03ER46088.