Understanding the Glass Transition from Structural and Vibrational Properties of the Zero-temperature Glasses

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In the theory of simple liquids, repulsive part of the particle interaction determines the properties of liquids, while attraction only acts as a perturbation [1]. Recent studies questioned the perturbative role of attraction by showing that supercooled Lennard-Jones (LJ) and Weeks-Chandler-Andersen (WCA) liquids could have dramatically different dynamics even though their structures are similar [2-3]. We find that the nonperturbative effect of attraction can be understood from structural and vibrational properties of the zero-temperature (T=0) glasses [4]. There exists a crossover density ρ_s above which the T=0 LJ and WCA glasses have identical structures. The glass transition temperatures of both systems are also the same when the density ρ is greater than ρ_s. Below ρ_s, distinct structures lead to different vibrational properties between the two systems. LJ glasses have higher boson peak frequency and weaker low-frequency quasi-localization than WCA glasses, which make the LJ glasses more stable and therefore have higher glass transition temperatures than WCA glasses. Above ρ_s, both LJ and WCA glasses are isomorphic, leading to scaling collapse of their structures and vibrations. We derive a density scaling of the glass transition temperature from these scaling relations and dimension analysis, in excellent agreement with simulation results. We also propose an empirical expression of the glass transition temperature purely based on properties of the T=0 glasses, which fits the simulated glass transition temperature nicely over a wide range of densities.

References:

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