主論文の要約

論文題目: Effect of Mechanical and Thermal Annealing on the Yielding Transition of Cyclically Deformed Amorphous Solids (周期的に変形したアモルファス固体の降伏転移に対する機械的および熱的アニーリングの効果)

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We carry out the molecular dynamics simulation to investigate how protocols to prepare athermal amorphous solids affect the rheological and mechanical properties. Recent simulation studies revealed that the yielding behaviors of glassy systems depend sensitively on the extent of annealing of the amorphous solids. We employ two distinct annealing protocols to generate the jammed amorphous packings of frictionless spherical systems. One is the mechanical annealing (MA) in which a poorly annealed jammed system is stabilized by slowly deforming the system with cyclic oscillatory shear with small amplitudes. Other is to equilibrate a liquid at very low temperatures using the swap Monte Carlo simulation before its temperature is quenched to generate the jammed packing. We refer to this protocol as the thermal annealing (TA). We find that, while both annealing protocols make the yielding transition discontinuous, or brittle, instead of continuous, or ductile transition for poorly annealed system, the detailed natures of the transitions are distinct. In particular, the extent of MA depends crucially on the initial degree of TA. If the annealing temperature is not low enough, MA can bring system into a lower energy state, but the minimal inherent structures are present, which limits the extent of MA. In this regime, it is also found that even the energy of MA and TA system are similar, their mechanical properties are very different: the mechanical responses of MA system are anisotropic, depending on the shearing orientations it shows either softening or hardening compared to the system before MA. On the contrary, when the system is prepared below a threshold temperature, MA cannot stabilize the system anymore. The inherent structures become lower than the minimal inherent structures of the MA system, the yielding transition point is increased, and the brittleness of the system becomes substantially enhanced. A threshold temperature T_{c} separating these two regimes is identified, and its value turns out to be very close to the dynamic transition point, or the mode-coupling temperature, T_{MCT}. The T_{c} separating these two regimes is identified, and its value turns out to be very close to the dynamic transition point, or the mode-coupling temperature, T_{MCT}. Finally, persistent shear-bands are found after the yielding transitions, but its formation for systems prepared with temperature above or below T_{c} are different.