

Multiple glassy states and anomalous behavior of colloidal systems: Simulations and theory

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Dynamically disorder arrested states are studied in terms of glass transitions in different colloidal systems. In the context of glassy dynamics, the Mode Coupling Theory (MCT) gives a qualitative picture of the glass transition and its predictions are well supported by experiments and numerical simulations. For instance, the theory predicts a rich behavior (diffusion anomalies, multiple glass transitions, ...) for colloidal systems where hard-core repulsion is complemented by a short range attraction or by adding softness to the system. Recent MCT calculations have been done for the Square Shoulder (SS) model, a purely repulsive potential where the hardcore is complemented with a finite shoulder. For the one-component version of this model, MCT predicted [Sperl et. al., Phys. Rev. Lett. 104, 145701 (2010)] the presence of diffusion anomalies both upon cooling and upon compression and the occurrence of glass-glass transitions. In Molecular Dynamics (MD) Simulations, we focus on a non-crystallizing binary mixture, which, at the investigated shoulder width, verified the MCT predictions. We also perform novel MCT calculations using as input the partial structure factor obtained within MD simulations, confirming the simulation results. In the dynamical phase diagram, we encounter with a special locus of peculiar dynamics: invariant dynamics associated to the predicted glass line which has not been observed in any other system. An extensive study of SS system has revealed the presence of two hard sphere glasses, differing only in their hardcore length. The simple competition between the two repulsive length scales is sufficient for creating a rather complex dynamical behavior.

References:

M. Sperl, E. Zaccarelli, F. Sciortino, P. Kumar, and H. E. Stanley
Disconnected Glass-Glass Transitions and Diffusion Anomalies in a Model with Two
Repulsive Length Scales
Phys. Rev. Lett. 104, 145701 (2010)

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