

Molecular Dynamics Calculations of Intermediate Scattering Functions for Colloidal Fluids in Explicit Solvent

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Unimodal and bimodal colloidal suspensions are extremely useful model systems for the study of nucleation and vitrification. As the packing fraction of a unimodal colloidal solution is increased beyond the melting point, it crystallizes into a solid. But for the bimodal solution, polydispersity inhibits crystallization and therefore promotes a glass transition, where the system undergoes a transition to an amorphous solid [1]. Because of the convenient size and time scales of colloidal suspensions, colloidal crystallization can be studied using light scattering and microscopy [e.g. 1-3]. One of the main properties measured by light scattering is the intermediate scattering function (ISF) [e.g. 3], which is the auto-correlation function of the density-density fluctuations. Molecular Dynamics (MD) simulations of hard-sphere (HS) systems [e.g. 4], have been performed to provide a comparison with experiments, but to date none have taken into account hydrodynamic interactions (which are present in real colloidal systems) by simulating the solvent explicitly. We have used MD simulations with explicit solvent, to conduct a systematic study of the ISFs for both unimodal and bimodal colloidal suspensions near the melting point and in the metastable region. The aim of this study is to reveal new quantitative information about the causes of metastability, providing a better understanding of the processes that inhibit crystal formation and promote the glass transition.

References

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