Study of orientational relaxation of glass forming liquids

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ABSTRACT

As a liquid is allowed to cool down slowly, it attains minimum energy by searching through all the possible configurations; consequently forming a crystal at the freezing point. If there is an increase in the cooling rate, then system visits a lesser number of probable configurations, thus increasing the disorder in the solid. The tendency to reach the equilibrium gets further reduced with an increase in the complexity of the constituent particles, due to, their shape or relative change in the concentration of multi- component systems. The state of glass is highly disordered; as they are structurally similar to liquids, but mechanically behave like solids[1]. In our work with molecular dynamics simulations, we study pure Lennard-Jones, and Kob-Andersen model. Here we perform the variations in the composition of the minority components B in the range(0% − 15%) to analyze the effects of increment in B (impurity) on the relaxation dynamics. As, the glass transition is characterized by the dynamics, while studies on crystallization focus on the structure. Therefore, we perform both structural and dynamical studies to understand crystallization, vitrification, and the competition between them. To study glass transition, we generated low-temperature state points by a fast quenching and observed the structural variations for each composition at different temperatures. We noticed that as the composition of B increases, the violation of the Stokes-Einstein relation becomes pronounced in these systems.

References

[1] Phys. Rev. Lett. 73,1376 (1994)