سمینار هفتگی ماده چگال نرم

Journal Club: "Glass Formation in Mechanically Interlocked Ring Polymers: The Role of Induced Chain Stiffness"

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Abstract

"Polymer-related materials exhibit rich glassy behaviors at different length scales due to their various molecular structures and topological constraints. Recent studies have identified transient interpenetration of the long-chain rings contributing to dynamic arrest on the center-of-mass level. Interpenetration of rings is proposed as an approach to facilitate glass formation in polymer melts. In this work, inspired by recent advances in the synthesis of mechanically interlocked polymers, we investigate glass transition on the nanometer-scale segments influenced by permanent interpenetration of rings using molecular dynamics simulations. We find that decreasing chain length in the mechanically interlocked system is equivalent to inducing an effective chain stiffness on the subrings. The induced stiffness provides a unified explanation for these unique structural features and transient dynamic arrest in the system of interlocked rings with rather short chains. Further, a crossover is observed in the scaling relation between localization and glassy depth upon cooling. Our work reveals a dynamic transition from weak to strong caging at the crossover temperature. According to the localization model, we demonstrate that the chain stiffness increases the critical temperature and oscillation distance, which therefore leads to more fragile dynamics and a deeper glassy state. These findings are consistent with the predictions of molecular simulations and theories for polymers with real local stiffness. Our work deepens the understanding of the role of induced stiffness on glass transition, and it opens up a new direction to design rich glass materials by manipulating stiffness through mechanical bonds*."

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