Glass transition of ion-containing polymer melts

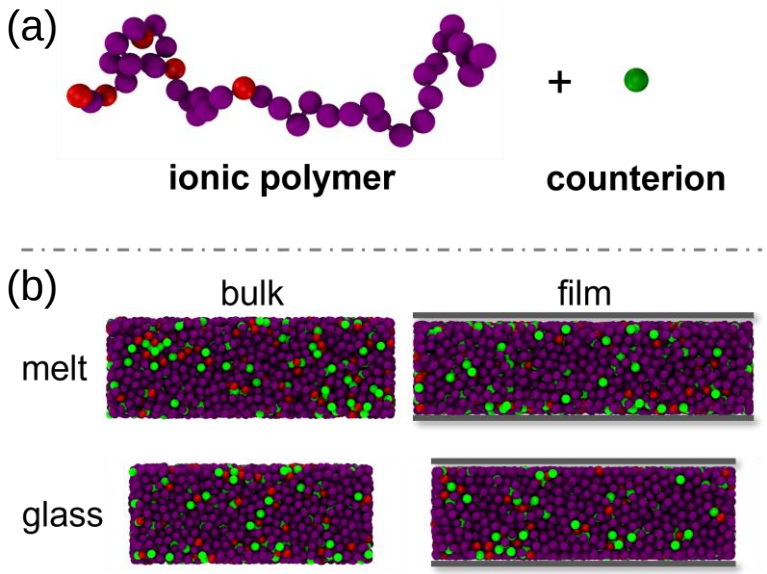

Figure 1: (a) Model system contains ionic polymers and counterions, which is charge neutral in total. The ionic polymer is depicted by a bead-spring model, consisting of neutral and charged beads (colored in purple and red, respectively). In the illustration, charged beads are randomly distributed along the chain. (b) Typical simulation snapshots of bulk and thin film systems in melt and glass states.

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Scientific Achievement

This work presents a systematic molecular dynamics simulation study about the coupling of ionic correlations with the glass transition. Our results reveal a few typical features about the glass transition process that are in qualitative agreement with previous studies, further highlighting the effects of counterion entropy at weak ionic correlations and physical crosslinking of ionic aggregates at strong ionic correlations.

Significance and Impact

This work provides an improved picture towards a comprehensive understanding of the glass transition in ion-containing polymeric systems from a molecular simulation perspective.

Research Details

- The variation of glass transition temperature is examined concerning the influence of electrostatic interaction strength, charge fraction, and charge sequence.
- The interplay with the film thickness effect is also discussed.
- Detailed parametric dependencies are displayed, which demonstrate that introducing strong ionic correlations promotes vitrification while adopting a precise charge sequence and applying strong confinement with weak surface affinity reduce the glass transition temperature.