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Effects of chain stiffness and shear flow on nanoparticle dispersion and distribution in ring polymer melts

Key words:

Ring Polymer, Nanocomposites, Chain Stiffness, Shear Flow, Molecular Dynamics

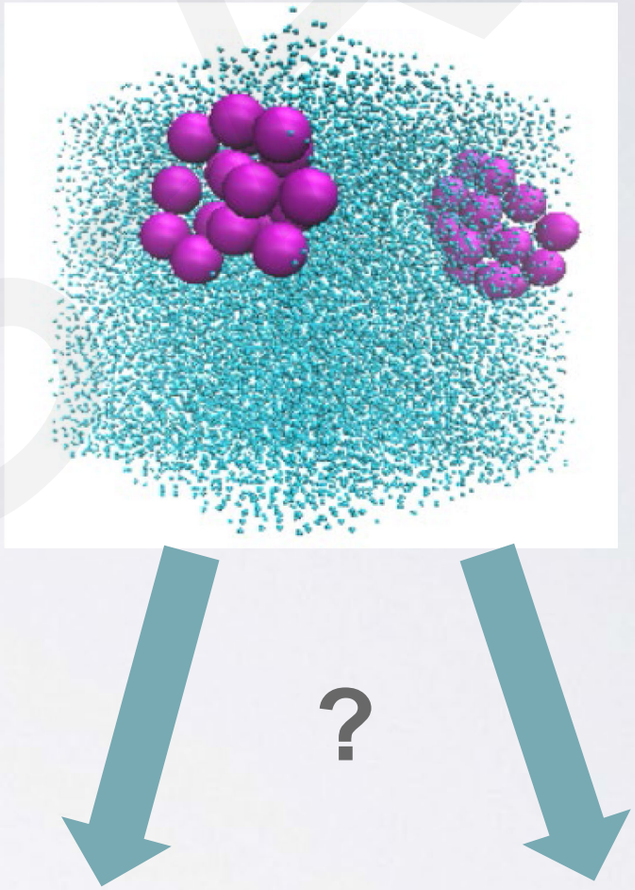
Found the problem

Existing problems

- Nanoparticles(NPs) are aggregated and phase-separated in ring polymer melt.
- The spatial distribution of nanoparticles is disordered and non-oriented.

Desire outcome

- Achieve good dispersion of NPs in ring polymer melt.
- The spatial distribution of NPs is orderly based on the good dispersion of NPs.



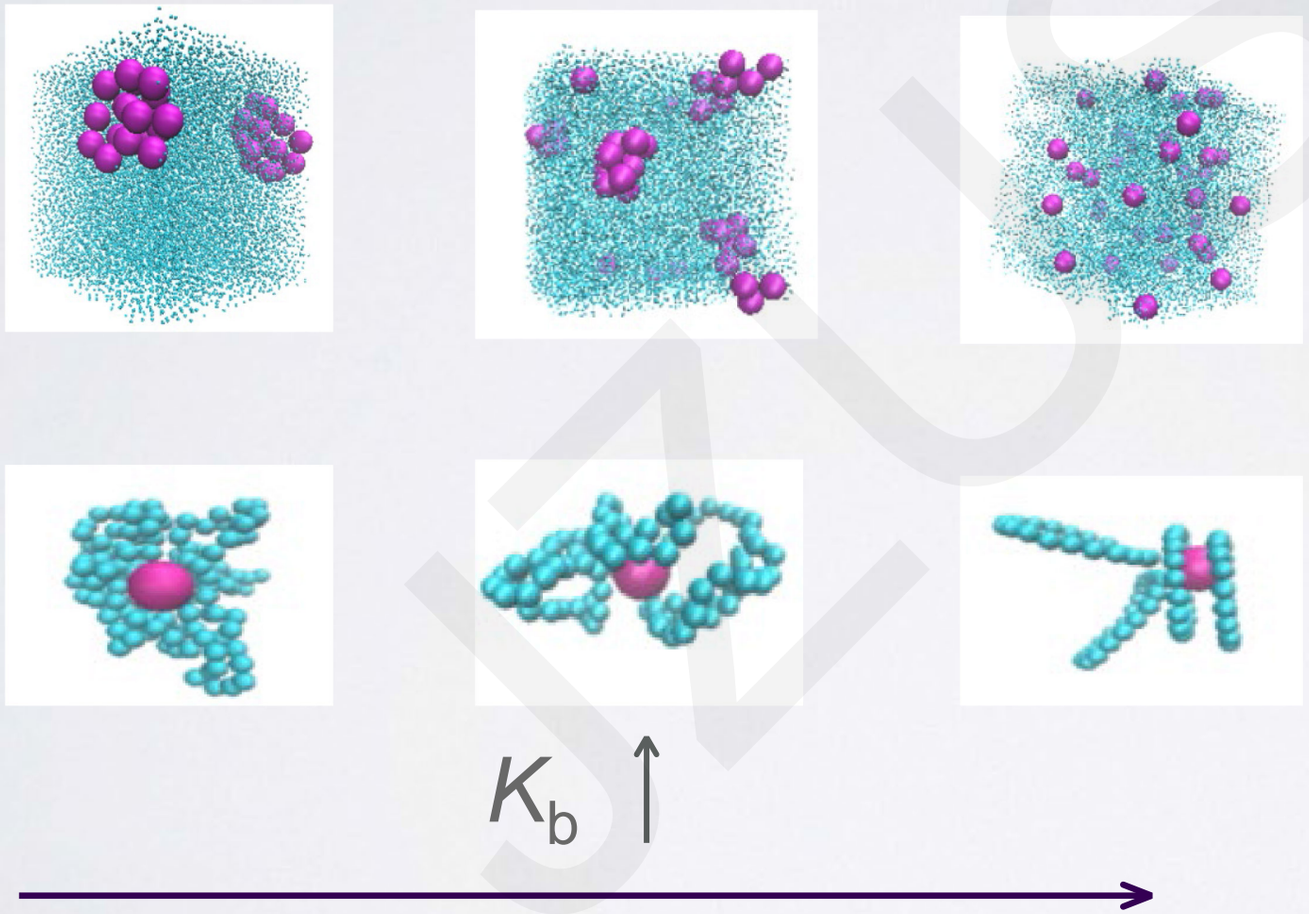
The solution to the problem

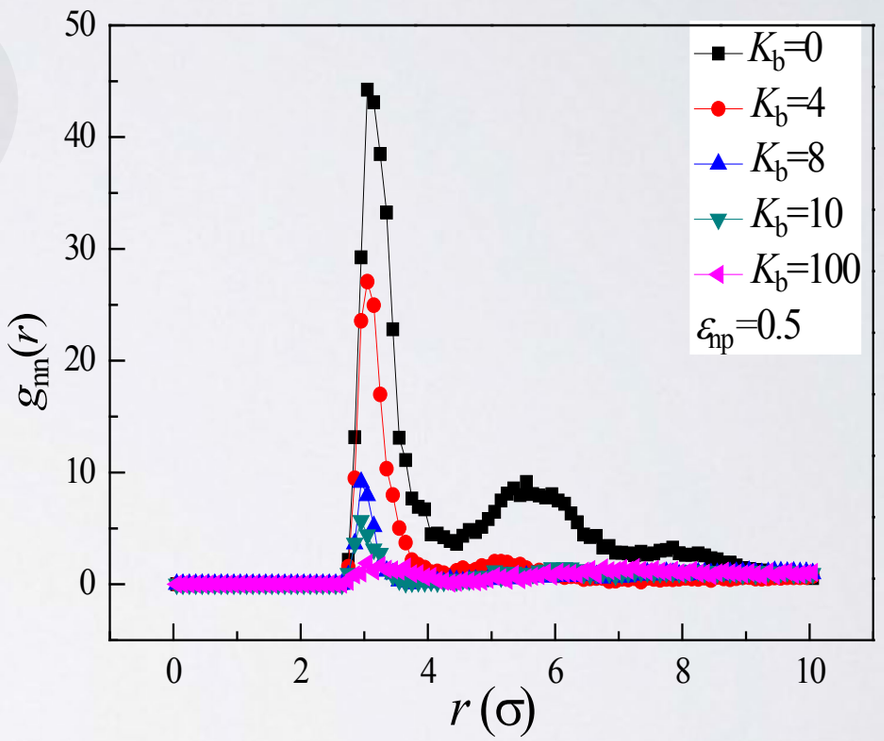
Realize the dispersed details of NPs are discussed under following sections:

- Change the stiffness of the ring polymer chain
- Applied shear flow on ring polymer chain
- Shear flow and chain stiffness are considered at the same time

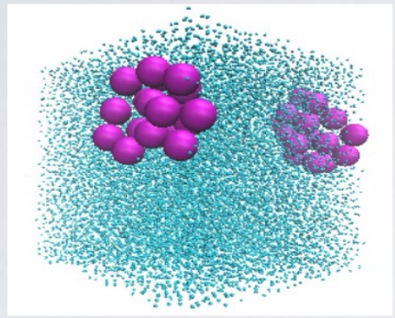
Demonstration of simulation results

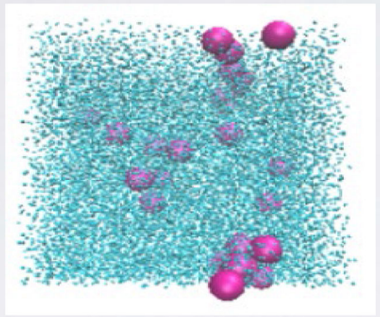
Change the stiffness of the ring polymer chain

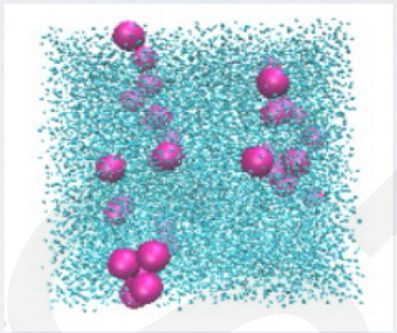




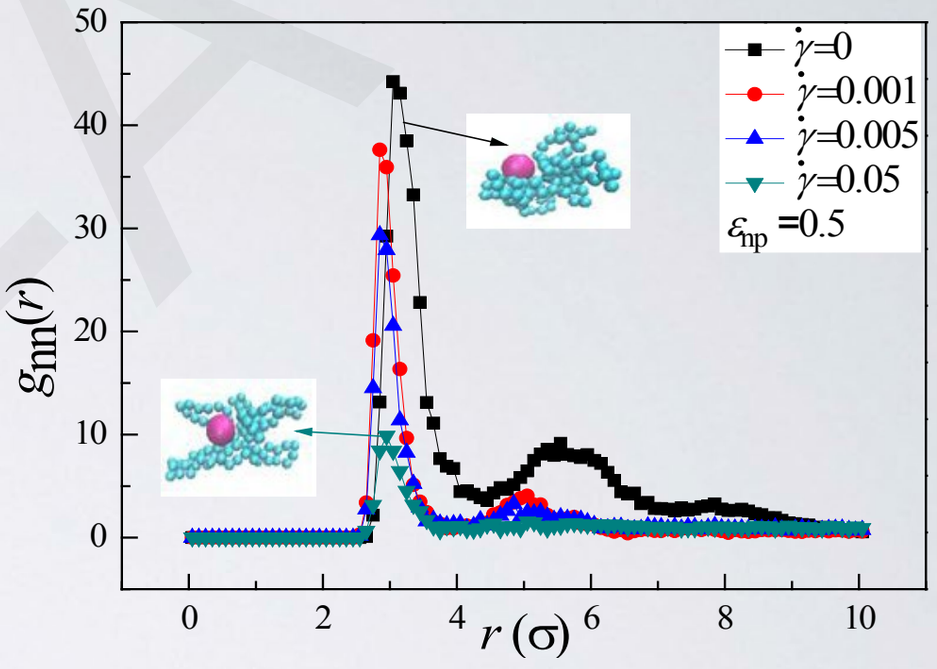
Applied shear flow on ring polymer chain

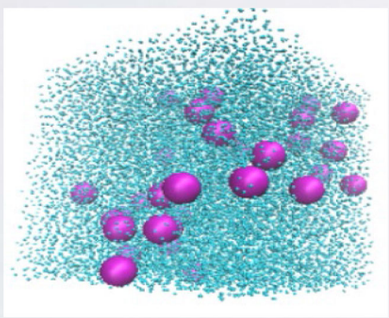


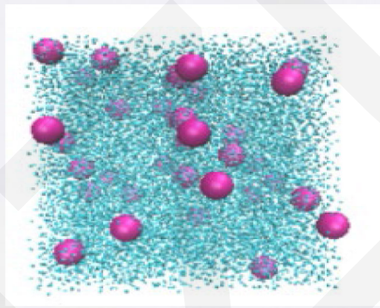


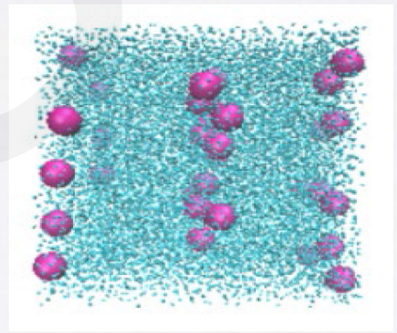


ε_{np}=0.5 $\dot{\gamma}$ ↑

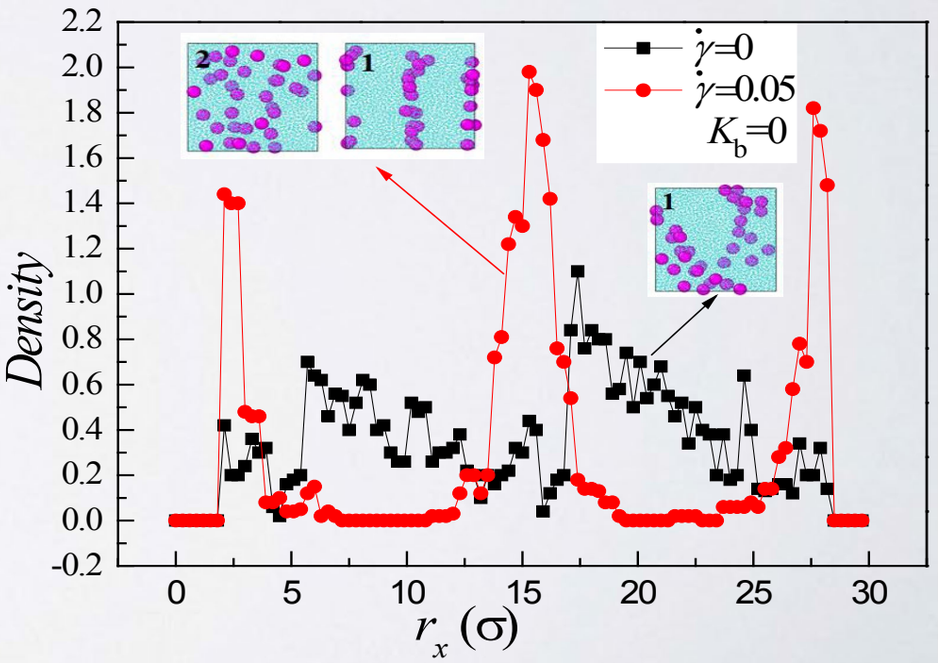




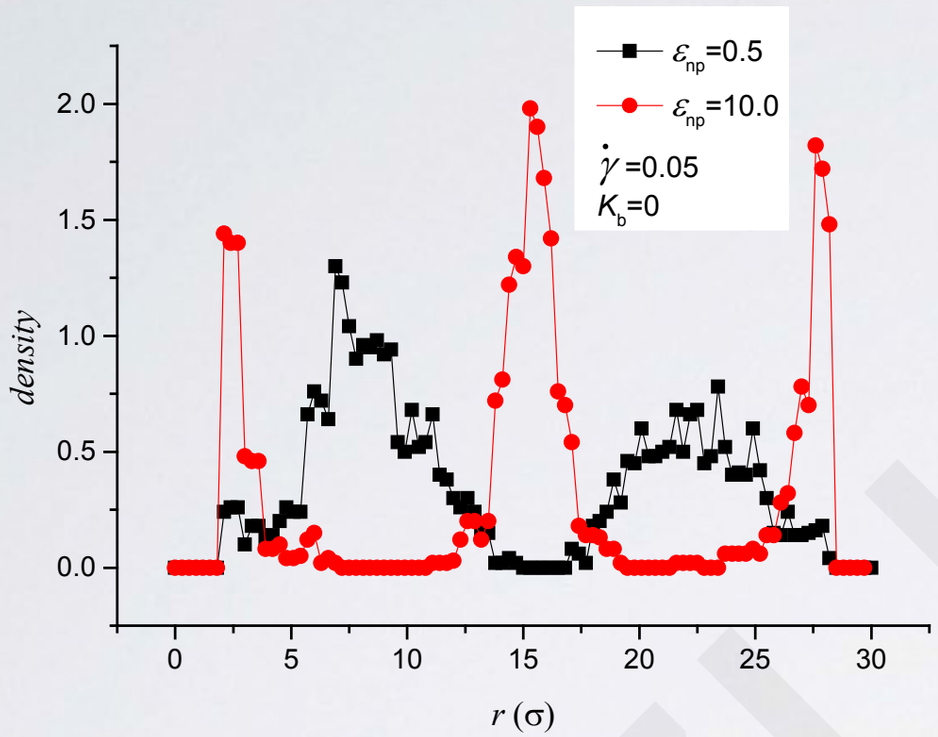


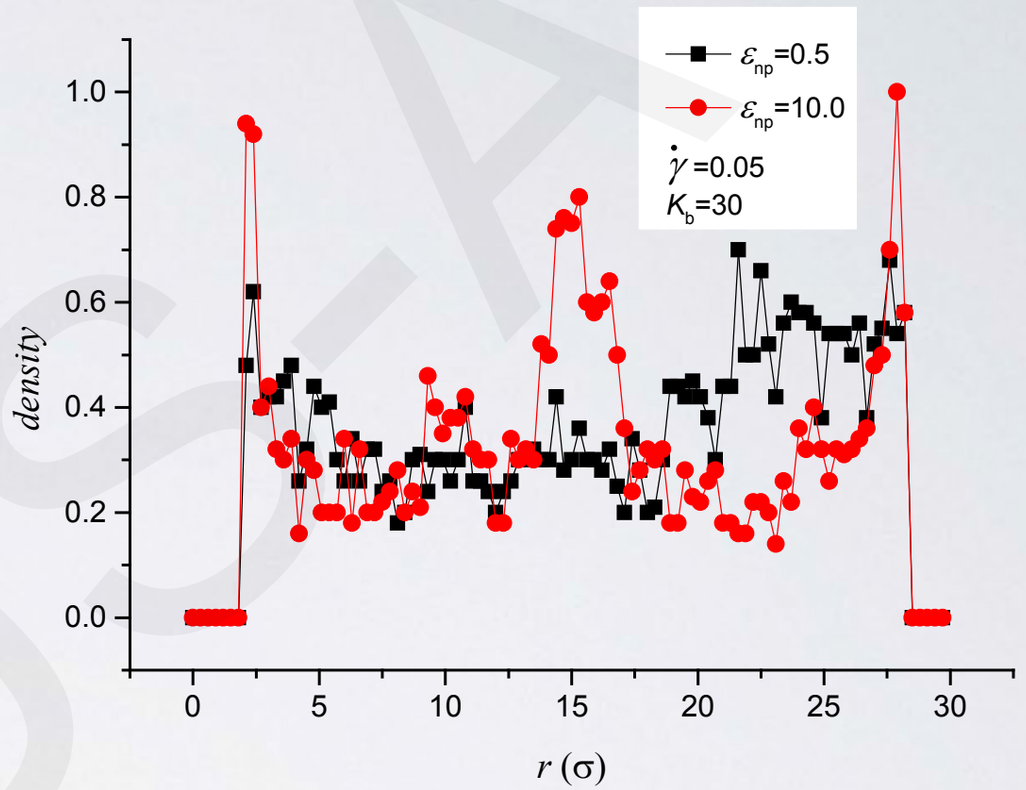


ε_{np}=10.0 $\dot{\gamma}$ ↑



Shear flow and chain stiffness are considered at the same time





The NPs in the simulated box are oriented and layered under shear flow.

Perspectives and Research Priorities

Research Priorities:

- A transition from NPs aggregated state to dispersed state can be induced by increasing the ring chain stiffness
- With increasing shear strength, aggregated NPs tend to be dispersed. When polymer–NP interaction is strong, the spatial distribution of NPs is well–ordered and well dispersed.
- The well–ordered structure is gradually disturbed by the increase of chain stiffness when shear flow and chain stiffness are considered at the same time in polymer chains.

The mechanical, optical, and electrical properties of polymer nanocomposites (PNCs) can be significantly enhanced by adding NPs. We combine some internal factors with external factors to achieve good dispersion of NPs. Moreover, the distribution of NPs in the desired direction can be realized by changing the external conditions. This research provides ideas for improving the mechanical properties of PNCs to a certain extent.