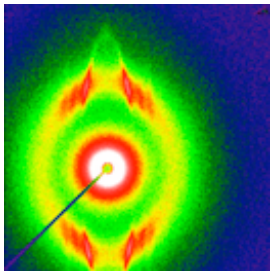

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Keynote 7 - Molecular Rheology of Entangled Polymeric Fluids: New Discoveries and Remaining Challenges

Tuesday, 11 December 2018 11:50 (40)

Quantitative understanding of the influence of environmental variables on the dynamic evolution of microstructure in polymeric fluids plays a central role in soft matter physics as well as the processing of a wide variety of soft materials. Atomistic simulation via non-equilibrium molecular dynamics (NEMD) offer a viable alternative to experiment wherein the dynamics of individual macromolecules can be tracked independently, thus allowing for relevant calculations of their single-chain configurational properties as well as the individual chain contributions to bulk-average properties. Specifically, large scale NEMD simulation results of entangled polymeric fluids allow examination of the fundamental tenants of reputation/ tube based theories including calculation of essential variables such as the tube orientation tensor, tube stretch, and disengagement and Rouse times.

In this presentation, I will briefly review the progress made in fundamental understanding of non-equilibrium dynamics of polymeric melts as well as the remaining challenges in development of a unified approach for quantitative prediction of dynamics of this class of fluids in processing flows commonly used to produce structural and functional soft materials. Specifically, I will discuss, Non-Equilibrium Molecular Dynamics Simulations (NEMD) results of linear monodisperse entangled macromolecular melts in shear and extensional flows that depict existence of new phenomena that challenges the fundamental tenants of reputation/tube based theories and models used to describe fast flow of entangled polymeric fluids. In turn, the intricate connection between single chain dynamics and the macroscopic response of this class of fluids including the intriguing phenomena of shear banding and configurational microphase separation in planar extensional flows will be discussed.

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