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Molecular Simulations of Particle Nanorheology MIR KARIM, RAJESH KHARE — Over the past few years, experimental and theoretical developments in the field of microrheology have enabled determination of the local mechanical properties of complex materials. In this presentation, we will extend this approach to determine the local viscoelastic properties of polymeric materials using molecular dynamics (MD) simulations. Molecular simulations provide the unique ability to explicitly account for the intermolecular interactions in the system. Thus an approach based on molecular simulations allows for the determination of the viscoelastic properties at the nanoscale. The specific system that is studied in this work consists of a polymeric melt in which the polymers are modeled as bead-spring chains. We will present a comparison of the results obtained from the passive and the active nanorheology approaches. A discussion of the parameter (e.g. amplitude and frequency) ranges that allow usage of these techniques will also be presented.

Mir Karim

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