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Molecular Dynamics Simulations of Nanoparticle-Based Rheology TING GE, University of North Carolina, GARY GREST, Sandia National Laboratories, MICHAEL RUBINSTEIN, University of North Carolina — We perform molecular dynamics simulations of nanoparticles (NPs) in entangled melts of linear polymers and non-concatenated ring polymers to explore NP-based rheology. As in conventional micro-bead rheology, the generalized Stokes-Einstein relation (GSER) is employed to extract an effective stress relaxation function $G_{GSE}(t)$ from the mean square displacement of NPs. $G_{GSE}(t)$ for different NP diameters d are compared with the stress relaxation function $G_{GK}(t)$ obtained from applying the Green-Kubo formula to a pure polymer melt. By comparing $G_{GSE}(t)$ and $G_{GK}(t)$, we demonstrate the slip NP-polymer boundary conditions in simulations. For NPs in linear polymers, a plateau in $G_{GSE}(t)$ emerges as d exceeds the tube diameter a and approaches the entanglement plateau in $G_{GK}(t)$ with increasing d. A complete overlap of $G_{GSE}(t)$ and $G_{GK}(t)$ is not observed for the largest $d \approx 3a$, but is anticipated to occur for $d > 4a$. The progressive coupling of NPs to the bulk viscoelasticity reflects the intriguing interplay between NPs with d moderately larger than a and the entanglement network. For NPs in ring polymers, as d increases towards the spanning size R of ring polymers, $G_{GSE}(t)$ approaches $G_{GK}(t)$ that exhibits no entanglement plateau. The d-dependence of the local viscoelasticity probed by NPs indicates the coupling between NPs and the relaxation of ring polymers at larger length and time scales with increasing d. Finally, $G_{GSE}(t)$ and $G_{GK}(t)$ are anticipated to overlap for $d > 3R$, corresponding to the coupling of NPs to the bulk viscoelasticity.

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