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Multiscale Modeling of Viscoelastic Properties of Polymer Nanocomposites OLEG BORODIN, JOHN NAIRN, DMITRY BEDROV, GRANT SMITH, University of Utah — A methodology for a simple multiscale modeling of polymer nanocomposites has been developed and applied to simulations of random polymer nanocomposites. This methodology consisted of three steps: a) obtaining viscoelastic properties of bulk-like polymer and approximating behavior of the interfacial polymer from molecular dynamics (MD) simulations; b) using bulk and interfacial polymer properties obtained from MD simulations, performing stress-relaxation simulations of nanocomposites with material point method (MPM) simulations in order to extract nanocomposite viscoelastic properties; c) performing direct validation of viscoelastic properties obtained from MPM simulations with those obtained from MD simulations for relatively small nanocomposites consisting of one nanoparticle in polymer matrix. MPM calculation of random nanocomposites with attractive and neutral interfaces indicated that turning on attraction between polymer and cylinder could increase time dependent shear modulus by multiple orders of magnitude with the increase being more substantial at longer times.

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