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Nonlinear viscoelastic behavior of polymer nanocomposites: Coarse-grained-based predictions and experimental validation

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The nonlinear viscoelasticity characterizes the mechanical behavior of polymer nanocomposites. The present work bridges the inherently different time scales of coarse-grained (CG) models and experiments by assessing viscoelastic theories. The predictive capability of physically motivated Eyring and Argon models [1, 2, 3] is evaluated to characterize the viscous behavior of pure epoxy and nanoparticle/epoxy nanocomposites over a broad range of temperatures and strain rates. For this, the effect of strain rate and temperature on the yield stress is examined by performing the tensile simulations using CG simulations at different strain rates and temperatures in the glassy regime.

In this study, it is demonstrated that viscoelastic theories can be successfully calibrated using CG simulation results. In experiments, tensile tests are also perfomed at different strain rates and different temperatures in the glassy regime. Experimental validation confirms the predictive capability of the Argon model for the pure epoxy and nanoparticle/epoxy nanocomposites at different temperatures. It is shown that the viscosity of the nanocomposites depends on the weight fraction and distribution of nanoparticles. The proposed CG model offers a suitable numerical tool for the characterization of the viscoelastic material behavior of nanoparticle/epoxy nanocomposites.

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