Abstract Submitted
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A hybrid Brownian Dynamics model for yielding, aging, and rejuvenation in deforming polymeric glasses[1] WEIZHONG ZOU, RONALD LARSON, Department of Chemical Engineering, University of Michigan, Ann Arbor — We describe the rheology of polymeric glasses by combining a simple constitutive equation for the fast segmental modes, borrowed from Fielding, et al.[1], with Brownian dynamics (BD) simulations of the slow polymer modes. The BD simulations determine the polymeric stress from ensembles of finitely extensible bead-spring chains, where the bead drag coefficient is governed by solutions to the equation for segmental relaxation. Thus the model treats the short glassy segmental mode as "solvent" for the polymer modes. With rubbery modulus for the slow-relaxing polymer modes as one of our model parameters, stress-dependent relaxation, physical aging, flow rejuvenation as well as strain-hardening and recovery can be successfully accounted for in uniaxial extension and steady shear, without the use of an artificial "crinkle factor" used to account for recoil dynamics in previous work [1]. Our simulation results remarkably agree with the experimental data from Lee et al.[2] A comparison between our model and the barrier-hopping theory [3] is also made.
[1] Fielding, S.M.; Larson, R.G.; Cates, M. E. Simple model for the deformation-induced relaxation of glassy polymers. Physical Review Letters, 2012, 108, 048301. [2] Lee, H-N.; Paeng, K.; Swallen, S.F.; Ediger, M.D. Direct measurement of molecular mobility in actively deformed polymer glasses. Science, 2009, 323, 231-234. [3] Chen, K.; Schweizer, K.S. Theory of relaxation and elasticity in polymer glasses. The Journal of Chemical Physics, 2007, 126, 014904.

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