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Nonequilibrium Atomistic Polymer Simulations Under Shear
STEVEN VALONE, Materials Science and Technology Division, Los Alamos National Laboratory, VIVEK KAPILA, Dept of Materials Science Engineering, University of Arizona — The present effort is intended to provide insights into acceleration-driven instabilities in complex fluids. The vast majority of studies into Rayleigh-Taylor (steady acceleration), Richtmyer-Meshkov (impulsive acceleration or shock loading), and Kelvin-Helmholtz (shear) instabilities have been limited to simple fluids with relatively simple constitutive properties. Some fluids of interest originate from polymeric materials that will behave like complex fluids under sufficiently strong shock or shear loading. The resulting fluids possess very complicated shear-rate dependent viscous behavior. This shear-rate dependence is explored through nonequilibrium molecular dynamics simulations using shear boundary conditions [1] applied to an atomistic model of polyethylene. The shear-rate dependence is determined over a range of rates, not just for low shear rates. The viscosity data are fit to a generalized Lorentzian and rate-theory models. The low shear-rate results are compared to experimental data for the two models.
[1] B.L. Holian, J. Chem. Phys., 117, 1173 (2002).

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