PSF20-2020-000062

Abstract for an Invited Paper
for the PSF20 Meeting of
the American Physical Society

Discrete Slip-Link Theory[1]

JAY SCHIEBER, Illinois Institute of Technology

The discrete slip-link theory is a hierarchy of strongly connected models that have demonstrated great success in predicting the linear and nonlinear rheology of high-molecular weight polymers. Three of the four parameters of the most detailed model can be extracted from primitive path analysis, which give quantitative experimental agreement for all examined chemistries (PS, PI, PBd and PE). Here we show that the remaining friction parameter can also be extracted from atomistic simulations. In particular, an available quantum chemistry-based force field for polyethylene oxide (PEO) was used to perform molecular dynamics simulations of a 12kDa melt. Once the four parameters are determined for any chemistry, all parameters for all members of the slip-link hierarchy are determined. Then, using a coarser member of the hierarchy the dynamic modulus and nonlinear rheology of a 256kDa PEO melt was predicted. The predictions are compared to experimental measurements performed at the same temperature. Unfortunately, the extracted friction differs by a factor of two from experiment, which presumably arises from insufficient accuracy in the force field. Nonetheless, the work demonstrates that theory predictions without adjustable parameters should be possible.

In Collaboration With: Diego Becerra, Universidad de Concepcion; Andres Cordoba, Universidad de Concepcion; Maria Katzarova, University of Delaware; Marat Andreev, MIT; David Christopher Venerus, New Jersey Institute of Technology.

[1]Funded by FONDECYT grant 11170056 and NLHPC, ECM-02, Chile