

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Tube diameter of oriented polymer melts JIAN QIN, University of Chicago, SCOTT MILNER, Pennsylvania State University — The tube diameter is a key material parameter controlling the flow behavior of polymer melts. The Lin-Noolandi ansatz successfully accounts for the dependence of the tube diameter on polymer density, chain stiffness and diluent concentration. We extend the Lin-Noolandi ansatz to polymer melts under uniform tension. We find that the tube diameter a decreases as $F^{-1/2}$ when the pulling force F exceeds the thermal tension $k_B T/a$, and approaches a limiting value for typical flexible polymers near full extension of about half the unperturbed value. Our prediction is compatible with assumptions made in the GLaMM model [1] for polymer rheology. We have directly verified the predicted force-dependence of tube diameter by using isoconfigurational ensemble averaging [2] to measure the tube diameter in simulations of oriented polymer melts. In the simulations, the chains are oriented by pulling on the ends of the chains, and topologically equilibrated by allowing the chains to occasionally cross.

[1] R. Graham, A. Likhtman, T. McLeish, and S. Milner, *J. Rheo.*, 47(2003):1171;

[2] W. Bisbee, J. Qin, and S. Milner, *Macromolecules*, 44(2011):8972)

Jian Qin
University of Chicago

Date submitted: 27 Nov 2012

Electronic form version 1.4