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Rheology of linear monodisperse polyethylene melts from atomistic Molecular Dynamics simulations<sup>1</sup> NIKOS KARAYIANNIS, Institute of Optoelectronics and Microsystems (ISOM) and ETSII, Polytecnic University of Madrid (UPM), Spain, JORGE RAMIREZ, Department of Chemical Engineering, ETSI Industriales, Polytecnic University of Madrid (UPM), Spain, ALEXEI LIKHTMAN, Department of Mathematics, University of Reading, United Kingdom — In our contribution we present results from very long, Molecular Dynamics simulations of linear monodisperse polyethylene (PE) chains with lengths ranging from 0.5 to 18 entanglements. We adopt a hierarchical modeling approach: in the first step we employ Monte Carlo simulations consisting of chain-connectivity altering algorithms to ensure full scale equilibration. Secondly, massive parallel MD simulations are conducted in the canonical ensemble. Besides the standard dynamical information, the stress relaxation curves are calculated for all PE systems. By bridging present atomistic results with the tube theory through the newly-introduced slip-spring model [Likhtman, Macromolecules 38, 6128 (2005)] we are able to calculate the plateau modulus and viscosity for well entangled, industrially relevant PE melts. In all cases, comparison between available experimental data and present simulation findings reveals a very good to excellent agreement. The proposed multi-scale methodology is generally applicable and can be extended to polymers of different molecular architecture and chemical constitution, as well as blends and more complex interfacial systems. Nikos Karayiannis

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