

Abstract Submitted  
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**Molecular dynamics simulations of layers of linear and branched alkanes under shear**<sup>1</sup> P. SOZA, P.U. Catolica Chile, F.Y. HANSEN, Tech. Univ. of Denmark, H. TAUB, U. Mo.-Columbia, U.G. VOLKMANN, P.U. Catolica Chile — We have previously studied the equilibrium structure and dynamical excitations in films of the linear alkane tetracosane ( $n\text{-C}_{24}\text{H}_{50}$ ) and the branched alkane squalane ( $\text{C}_{30}\text{H}_{62}$ ) in great detail<sup>2</sup>. Here we report the results of nonequilibrium molecular dynamics simulations of these systems in order to compare the rheological properties of alkanes of the same length but with different architecture. The simulations were done in the NVT ensemble using the reverse nonequilibrium algorithm proposed by F. Müller-Plathe et al.<sup>3</sup>. The viscosity was calculated for different shear rates and compared with experimental values. Different structural parameters such as the mean end-to-end distance, the radius of gyration, and the angle of alignment of the molecules with the flow were studied as a function of the shear rate. <sup>2</sup>A.D. Enevoldsen et al., J. Chem. Phys. 126, 104703-10 (2007); 126, 104704-17 (2007). <sup>3</sup>F. Müller-Plathe et al., Phys. Rev. E, **59**, 4894 (1998)

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