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ACCEPTED MANUSCRIPT

Shear thinning behavior of nanometer-thick perfluoropolyether films confined between corrugated solid surfaces: a coarse-grained molecular dynamics study

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Abstract: Using a coarse-grained model that accurately reproduces the structures and pressures of the parent all-atom simulations, we performed molecular dynamics simulations to gain insight into the high-speed shear behavior of nanometer-thick perfluoropolyether (PFPE) films confined between two corrugated solid surfaces. The PFPE films exhibit shear thinning behavior (i.e., decrease of viscosity with increasing shear rate) following a power law. The degree of shear thinning (i.e., the exponent of the power law) is largely determined by the degree of geometric confinement rather than layering and molecular orientation of the confined films. Severe geometric confinement at a small solid–solid spacing gives a large degree of shear thinning.

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