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Multiscale simulation of polymer melt flows between parallel plates SHUGO YASUDA, RYOICHI YAMAMOTO, Dept. of Chemical Engineering, Kyoto University — The behaviors of polymer melt composed of short chains with ten beads in parallel plates are simulated by using a hybrid method of molecular dynamics and computational fluid dynamics. The creep motion under a constant shear stress and recovery after removing the stress, the pressure driven flows and the flows in rapidly oscillating plates are simulated. The flow profiles of polymer melt are quite different from those of the Newtonian fluid due to the elasticity or the shear thinning. The delayed elastic deformation and plug-like velocity profile are reproduced, respectively, in the creep and pressure driven flow. In the rapidly oscillating plates the viscous boundary layer of the melt is much thinner than that of the Newtonian fluid due to the shear thinning of the melt. Three different rheological regimes, i.e., the viscous fluid, viscoelastic liquid, and viscoelastic solid regimes, form over the oscillating plate according to the local Deborah numbers. The melt behaves as a viscous fluid in a region for $\omega\tau^R \lesssim 1$, and the crossover between the liquid-like and solid-like regime takes place around $\omega\tau^\alpha \simeq 1$ (where ω is the angular frequency of the plate and τ^R and τ^α are Rouse and α relaxation time, respectively).

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