CYCLIC MOTION OF GRATED POLYMERS UNDER SHEAR FLOW

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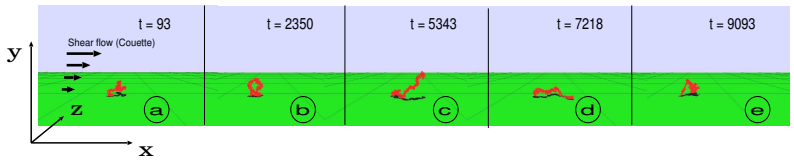
The long-time dynamics of a single end-tethered chain under shear flow were studied using molecular and Brownian dynamics simulations of a flexible polymer. As observed in previous experiments with tethered DNA [1] when a shear flow is applied the chain performs a cyclic, wagging, motion illustrated in the figure below. Contrary to what it has been suggested [1], the present work shows that the chain motion has a well defined characteristic period [2]. This fact is clearly revealed in the cross-spectra of the chain extension along flow and gradient directions. This resonant mechanism involves the coupling of the drag force by the solvent, the entropic restoring force of the chain and the transport of normal-to-wall momentum fluctuations along flow direction due to the presence of a shear flow. Interestingly enough this mechanism is quite general: it does not depends on the presence of hydrodynamic interactions or on the length of the chain. The resonant frequency scales like the reciprocal of the time needed to stretch the polymer by convection and it is quite low: the cyclic time is more than ten times the natural relaxation time of the chain in flow. For instance, the sequence illustrated by the figure covers about $10^4\tau$ and the relaxation time is 1250τ. This coherent recursive motion introduces long memory in the fluid and suggests resonance effects under periodic external forcing, such as those observed in polymer brushes [3], ligand-receptor binding [4] or the drag reduction by polymeric fluids .



[1] P. Doyle et al. Phys. Rev. Lett. **84**, 4769 (2000)

[2] R. Delgado-Buscalioni, Phys. Rev. Lett. **96**, 088303 (2006)

[3] Warburg et al. Nature, **352**, 143 (1991)

[4] B. Xue and W. Wang, J. Chem. Phys. **122**, 194912 (2005).