Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information

Force-Driven Active Dynamics of Thin Nanorods in Unentangled Polymer Melts

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Decomposition of mean squared displacement

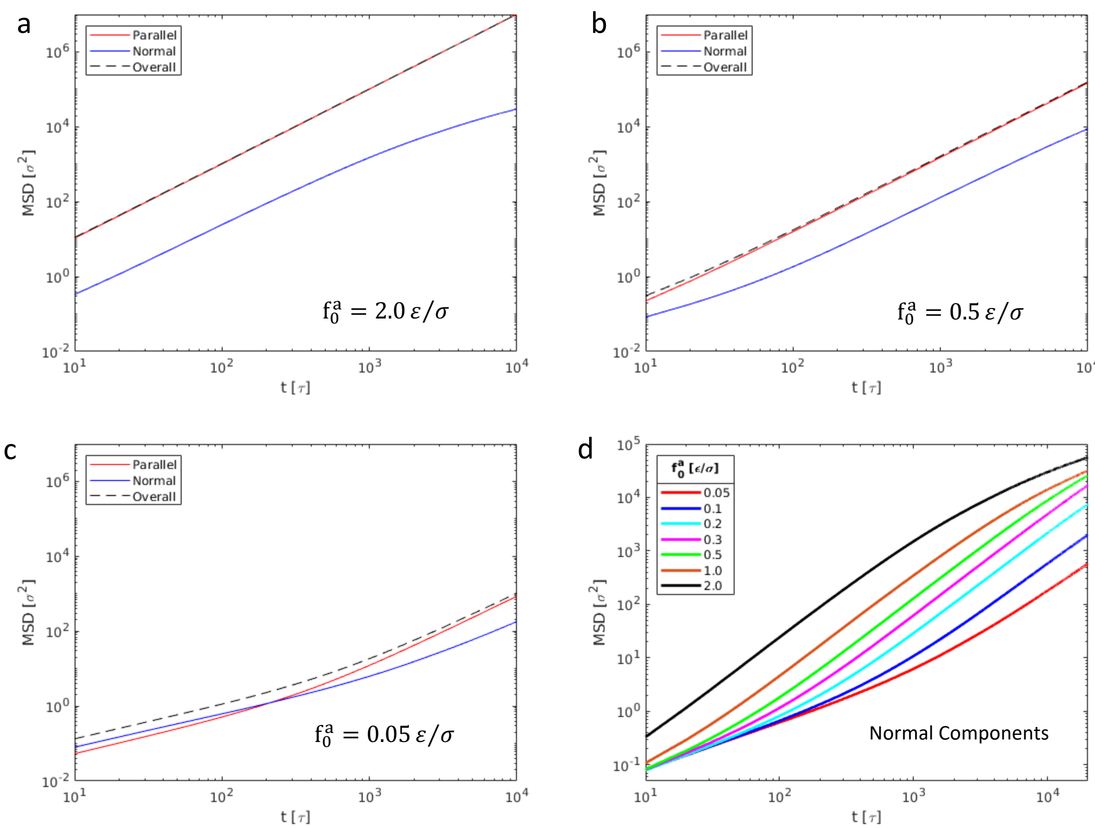

Figure S1 Decomposition of the overall mean square displacement (black dashed lines) of thin nanorods of $l = 32\sigma$ in the polymer melt of $N = 16$ to two components that are parallel (red solid lines) and normal (blue solid lines) to the direction of the applied force, respectively. The strength of the force per monomer length is (a) $f_0^a = 2.0\,\varepsilon/\sigma$, (b)$0.5\,\varepsilon/\sigma$, and (c) $0.05\,\varepsilon/\sigma$. The normal components for all different values of f_0^a are shown in (d).

For the strongest force with $f_0^a = 2.0\,\varepsilon/\sigma$, the overall mean square displacement (MSD) for $10\tau < t < 10^4\tau$ is in the force-driven ballistic regime and dominated by the parallel component, as shown in Fig. S1a. The normal component exhibits a non-trivial crossover from super-diffusive motion to the terminal diffusive motion with increasing time but remains a minor contribution to the overall MSD. Because of the intermediate super-diffusive regime, the terminal diffusive motion is enhanced with respect to that of the same nanorod with no active force. This enhanced terminal diffusion corresponds to the reduction of friction coefficient due to the applied force.

For the weakest force with $f_0^a = 0.05\,\varepsilon/\sigma$, there is a crossover from the passive thermal diffusion, which is not affected by the applied force, to the force-driven ballistic regime with increasing time for $10\tau < t < 10^4\tau$, as shown in Fig. S1c. In the regime of passive thermal diffusion prior to the terminal ballistic motion, the overall MSD has more contribution from the normal component. Since the normal component involves two directions whereas the parallel component involves only one direction, the normal component of MSD (blue solid line) surpasses the parallel component (red solid line) for the passive thermal diffusion. In the terminal ballistic regime, the overall MSD (black dashed line) is dominated by the parallel component. Meanwhile, the normal component, as a minor contribution to the overall MSD, is in the regime of super-diffusive motion and has not reached the terminal diffusive regime by $t = 10^4\tau$.

For the intermediate force with $f_0^a = 0.5\,\varepsilon/\sigma$, the overall MSD is almost all in the terminal ballistic regime and dominated by the parallel component for $10\tau < t < 10^4\tau$, as shown in Fig. S1b. The normal component exhibits first a crossover from the passive thermal diffusion to the intermediate super-diffusive motion and then a crossover to the terminal diffusion regime, which is not fully developed at $t = 10^4\tau$.

Fig. S1d shows the normal components of the MSD in the time range $10\tau < t < 2 \times 10^4\tau$ for different values of f_0^a in the simulations. With increasing f_0^a, it takes a shorter time to accumulate sufficient work to compete with the thermal energy k_BT. As a result, the normal component of MSD is raised above that for the passive thermal diffusion at a smaller time scale. Likewise, as f_0^a increases, the time to go through an intermediate super-diffusive regime and reach the terminal diffusive regime is reduced as well. Additionally, as the applied force becomes stronger, the normal component of MSD in the terminal diffusive regime is higher, although in most cases the terminal diffusion has not been well developed by $t = 2 \times 10^4\tau$.