Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information for Stretching Self-Entangled DNA Molecules in Elongational Fields

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Channel Schematic

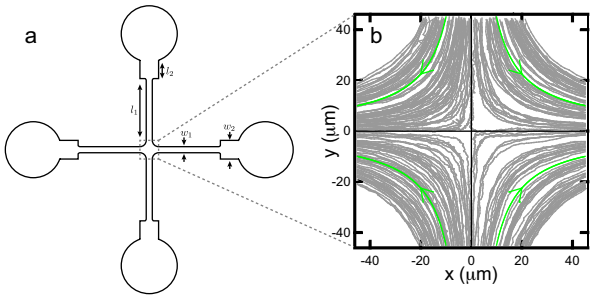

Figure S1: (a) 2-D illustration of the cross-slot channel geometry with the following dimensions: $l_1 = 3000$ μm, $l_2 = 1000$ μm, $l_H = 100$ μm, $w_1 = 40$ μm, and $w_2 = 100$ μm. DC power supplies are used to establish electric potentials (Φ_+) at the left and right reservoirs and ground ($\Phi_\circ$) the top and bottom reservoirs, generating a planar elongational electric field at the center of the device. (b) Streamlines (gray) of λ-DNA electrophoresing through the center of the device with 30 V applied potentials. The direction and shape ($y \propto 1/x$) of the field is indicated by the field lines (green).

Relaxation Time of DNA

The relaxation time of DNA, λ, is affected by the contour length length of the molecule as well as several experimental variables such as the slit height,[1] buffer ionic strength,[2] and buffer viscosity, to name a few. Accordingly, the calculated value of the relaxation time is specific to the experimental setup.

We calculated the rotational relaxation time of T4 DNA by fitting a single exponential decay to the angular autocorrelation function, $C_r(\delta t)$, of an ensemble of molecules, seen in Figure 2a. This procedure has been frequently employed in past work from this research group.[1–4]

For a given snapshot of a molecule, $\theta(t)$ is defined as the angle between the principle eigenvector of the radius of gyration tensor and the x-axis. This signal is used to construct an autocorrleation function, $C_r(\delta t)$, by

$$C_r(\delta t) = \frac{\langle(\theta(t) - \theta_{avg})(\theta(t+\delta t) - \theta_{avg})\rangle}{\langle(\theta(t) - \theta_{avg})(\theta(t) - \theta_{avg})\rangle} = \frac{\langle\theta(t)\theta(t+\delta t)\rangle}{\langle\theta(t)^2\rangle} \tag{1}$$

with $\langle\rangle$ denoting both temporal and ensemble averages and $\theta_{avg} = 0$. The fitting region is $0.3 < C_r(\delta t) <$statistical noise. The upper bound for the fitting region acts to exclude the influence of higher order decay modes on the fit for the longest relaxation time. The lower bound, the statistical noise, is defined as $1/n^{1/2}$ where n is the total number of statistical samples in the data set. Here, $n \approx \frac{t_{\text{total}}}{3\tau}$ where t_{total} is the total amount of video time analyzed for all molecules.

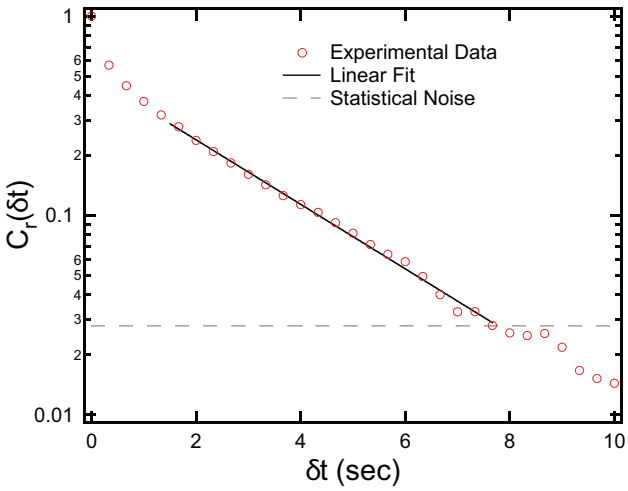

Figure S2: Measurement of the rotational relaxation time of T4 DNA in the buffer and channel described in the manuscript. In the fitting region, the slope of the exponential yields a relaxation time of $\lambda = 2.6\ s$.

Strain Rate Calibration

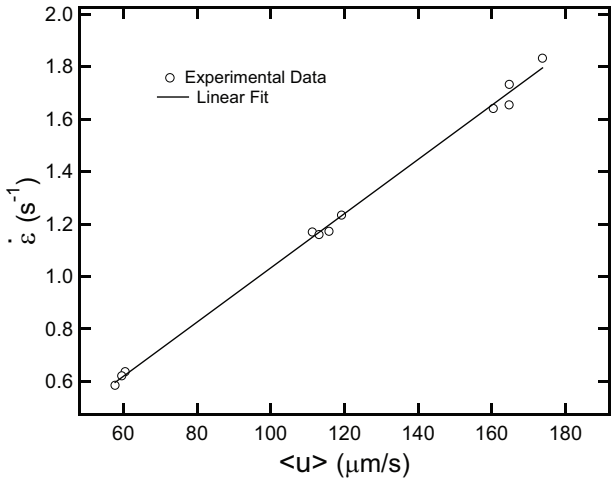

Figure S3: Strain rate calibrated against the average electrophoretic velocity in the cross-slot channel arms. The linear best fit to the experimental data is given by $\dot{\varepsilon} = (0.0103 \pm 0.002)\mu m^{-1}\langle u \rangle - (0.0016 \pm 0.02)s^{-1}$.

Effect of Extension Thresholds

Upper and lower extension thresholds were required in order to decompose the trajectories of unentangled and self-entangled molecules into their composite stages: arrested, stretching, and extended. In Figure 4, we show the effect that changing these cutoffs has on the results shown in Figure 7b.

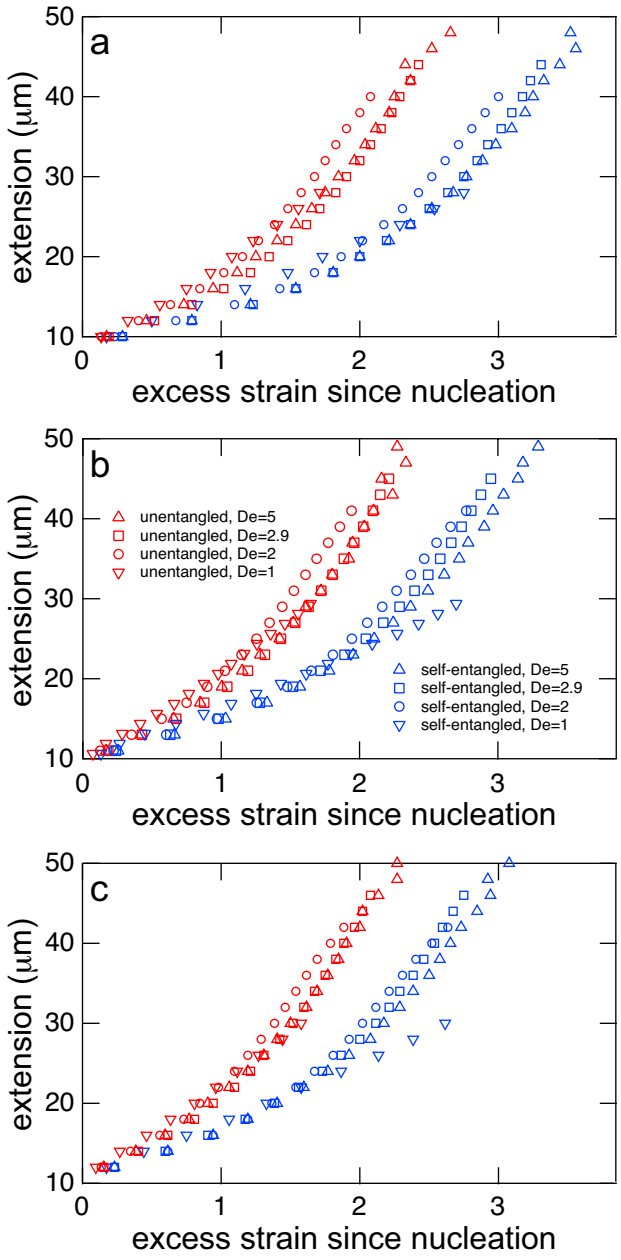

Figure S4: Effect of varying upper and lower extension thresholds on mean stretching curves. The binning and averaging conditions are identical to those employed in Figure 7 of the main text. (a) The mean stretching curves with a lower extension threshold of 9 μm and upper extension thresholds of 29 μm, 41 μm, 45 μm, and 49 μm. (b) The mean stretching curves with a lower extension threshold of 10 μm and upper extension thresholds of 30 μm, 42 μm, 46 μm, and 50 μm. This is simply a copy of Figure 7b. (c) The mean stretching curves with a lower extension threshold of 9 μm and upper extension thresholds of 31 μm, 43 μm, 47 μm, and 51 μm.

References

(1) Tang, J.; Levy, S.; Trahan, D.; Jones, J.; Craighead, H.; Doyle, P. *Macromolecules* **2010**, *39*, 7368–737.

(2) Hsieh, C.; Balducci, A.; Doyle, P. *Nano Lett.* **2008**, *8*, 1683–1688.

(3) Jones, J. J.; van der Maarel, J. R. C.; Doyle, P. S. *Nano Lett.* **2011**, *11*, 5047–5053.

(4) Hsieh, C.; Balducci, A.; Doyle, P. *Macromolecules* **2007**, *40*, 5196–5205.