Bottlebrush polymer melts with variable molecular architecture exhibit shear thinning and align parallel to flow direction under shear deformation

Shear Thinning of Bottlebrush Polymer Melts

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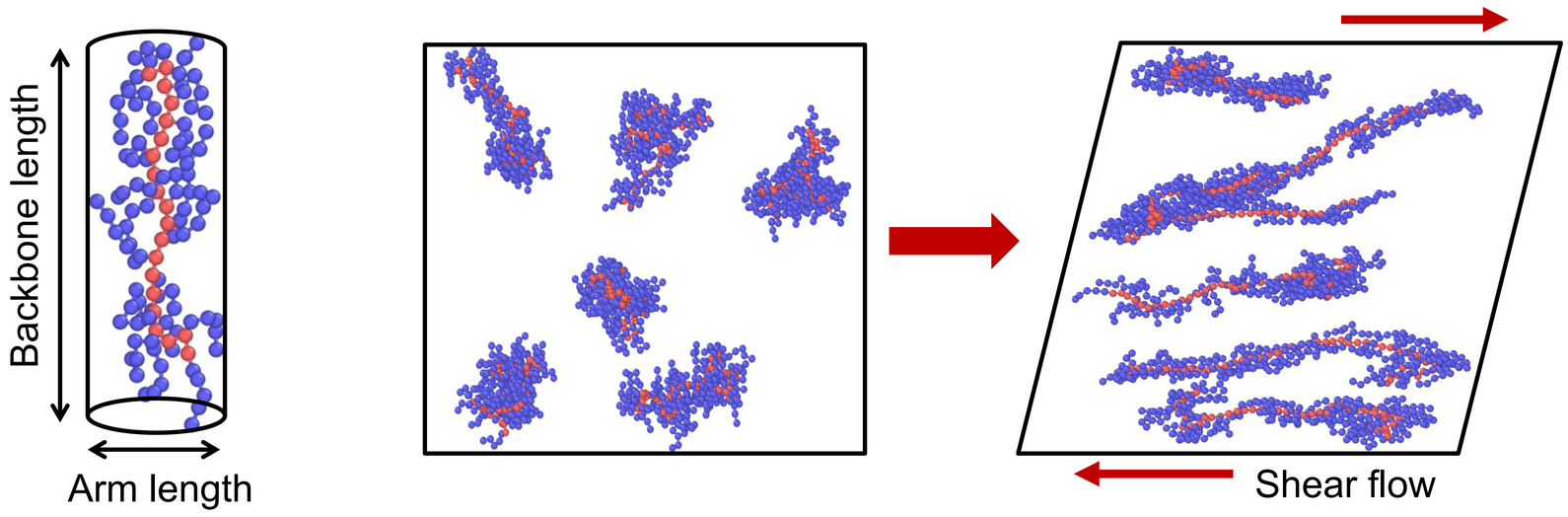

INTRODUCTION

- Bottlebrush polymers have various applications ranging from biomimetic tissues to 3D printing

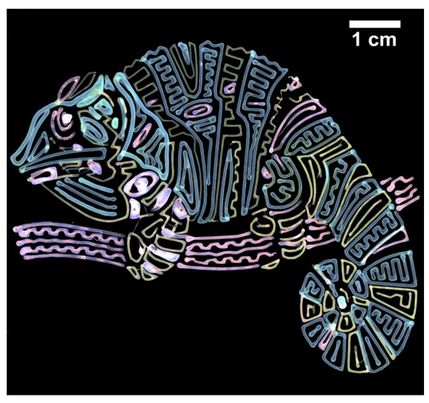

Fig.1 3D printed bottlebrush photonic crystals with tunable domain size and colour. This can be achieved by modulating polymer conformation [1]

- We simulate bottlebrush polymer melts for various molecular topologies under shear flow

RESULTS

Fig.2 Backbone chains of bottlebrush-like polymers align parallel to flow direction more than that of star-like and sphere-like polymers

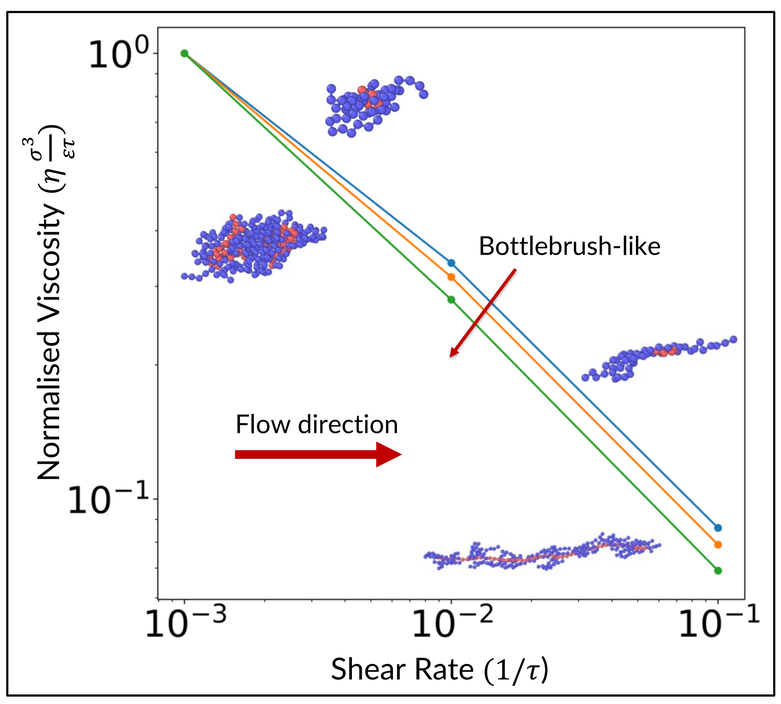

Fig.3 All three topological polymer regimes exhibit shear thinning behaviour

DISCUSSION

- Our first observations suggest that the viscosity and the orientation parameter are linked to the polymer topology.
- We are currently testing this hypothesis with systems at lower shear rates and different molecular architectures of the same molecular weight.

METHODS

Fig.4 Illustration of coarse-graining with the bead-spring model often used in molecular dynamics (MD) simulations

Scan to see this poster and related animations

Supplementary Information

Non-bonded interactions

$$U^{\mathrm{LJ}}(r) = \varepsilon \left[\left(\frac{\sigma^*}{r} \right)^{12} - 2 \left(\frac{\sigma^*}{r} \right)^{6} \right] + U_{\mathrm{cut}}$$

Bonded interactions

$$U^{\mathrm{b}}(r) = k(r - r_0)^2$$

Orientation parameter

$$\chi = \frac{|\vec{r} \cdot \hat{x}|}{||\vec{r}||}$$

Applied shear

$$\vec{v}_{shear} = \dot{\gamma} y \hat{x}$$

Reduced Lennard-Jones (LJ) units

$$\varepsilon = \sigma = 1$$

Mapping from LJ units to physical units can be made by taking the MD time (τ), length (σ), and energy (ε) units roughly about 2 *ps*, 0.5 *nm*, and 3.7 *kJ/mol*

Polymer topologies in the figures

Star-like: $N_b = 5, M = 10$
Sphere-like: $N_b = 20, M = 10$
Bottlebrush-like: $N_b = 50, M = 5$

Fig.5 Three polymer regimes based on the shape of a single chain where N_b is the backbone length and *M* is the side chain length. We simulated a total number of 1818, 454, and 333 chains in a melt, respectively. Adapted from [3]

REFERENCES

[1] B.B. Patel, *et al.* Sci. Adv. **6**, 24 (2020)
[2] A. Giuntoli, *et al.* Sci Adv. **6**, 17 (2020)
[3] A. Chremos *et al.* J. Chem. Phys. **149**, 044904 (2018)

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