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# THE RESPONSE OF SEMI-FLEXIBLE DENS POLYMER BRUSHES ON SHEAR FLOW.

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The response of dense brushes of semi-flexible polymers to flow is of great interest in both technological and biological contexts. Examples include the glycocalyx or the endothelial surface layer in blood vessels [1] and mucus-like layers in lungs [2] or the interior of nuclear pores [3].

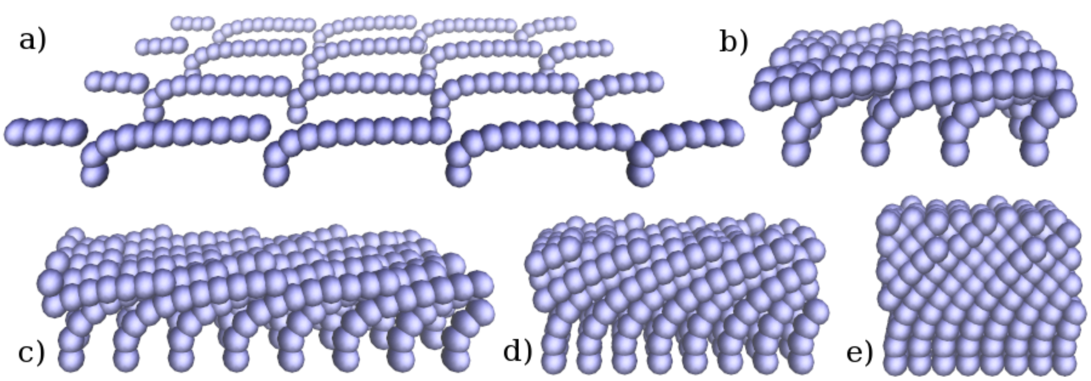


Figure 1: Semi-flexible polymer brushes in comparable shear flow at a grafting density $\sigma = 0.01$ (a), 0.0625 (b), 0.111 (c), 0.25 (d) and 0.51 (e).

In contrast to full-flexible end-tethered polymers the literature about semi-flexible is quite narrow. Kim *et al.* [4] studied grafted semi-flexible polymer in shear flow, but they focused on low grafting densities where the interaction between the polymer beams are negligible. At high grafting densities not only the effect on the flow profile [5] is of importance, also the excluded volume interaction between the polymer beams become more dominant and non negligible, as in Figure  shown.

We employ smoothed dissipative particle dynamics (SDPD) [6] simulations to study semi-flexible polymer brushes for a wide range of conditions including grafting density, polymer elasticity, and shear stress due to flow. Our simulation results are in good agreement with previous studies [4]. For proper representation of the excluded volume interaction we add a short-ranged soft-repulsive potential between the polymer beads.

We also propose a theoretical model which describes the deformation of dense semi-exible polymer brushes in shear flow for a wide parameter range. Beside excluded volume interaction we consider a shape dependent local friction coefficient derived from *slender body theory* [7] to cover high densities respectively strong deformations. The model allows us to predict effective deformation (height), inner density profile and hydrodynamic penetration depth (solvent velocity profile). Therefore, it is suitable to predict the effect of grafted surfaces on the flow profile in a slit or tube.

## REFERENCES


[1] S. Weinbaum, J. M. Tarbell, E. R. Damiano, *Annu. Rev. Biomed. Eng.* **9**, 121–167, 2007

[2] H. Matsui, *Proc. Natl. Acad. Sci. U.S.A.* **103**, 18131–18136, 2006

[3] K. Ribbeck, D. Gorlich, *EMBOL J.* **20**, 1320–1330, 2001

[4] Y. W. Kim, V. Lobaskin, C. Gutsche, F. Kremer, P. Pincus, R. R. Netz, *Macromolecules* **42**, 3650–3655, 2009

[5] S. T. Milner, *Macromolecules* **24**, 3704–3705, 1991

[6] P. Español and M. Revenga, *Phys. Rev. E* **67**, 026705, 2003

[7] R. G. Cox, *J. Fluid Mech.* **44**, 791–810, 1970