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THE RESPONSE OF SEMI-FLEXIBLE DENS POLYMER BRUSHES TO 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].

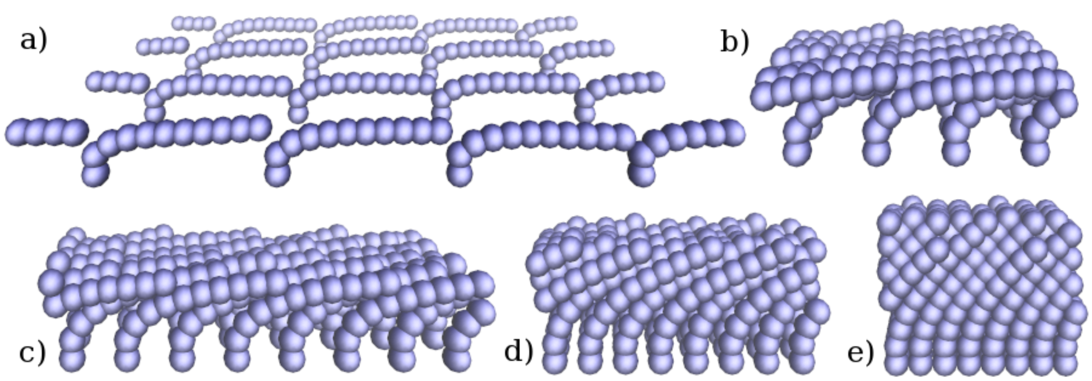

Figure 1: Semi-flexible polymer brushes at comparable shear flow, and a grafting density $\sigma = 0.01$ (a), 0.0625 (b), 0.111 (c), 0.25 (d) and 0.51 (e).

In contrast to fully-flexible end-tethered polymers, the literature on semi-flexible polymer brushes is quite limited. Kim *et al.* [4] studied grafted semi-flexible polymer in shear flow, but they focused on low grafting densities where the interactions between the polymer beams are negligible. At high grafting densities, not only the effect of the flow [5] is of importance, but also the excluded volume interactions between the polymer beams become more dominant and non negligible, as shown in Figure 1.

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-flexible polymer brushes in shear flow for a wide parameter range. Beside excluded volume interaction we consider a shape dependent local friction coefficient derived from the *slender body theory* [7]. 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.

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