End-Tethered Polymers on Periodically Nanopatterned Substrates: Towards Tunable Soft Templates

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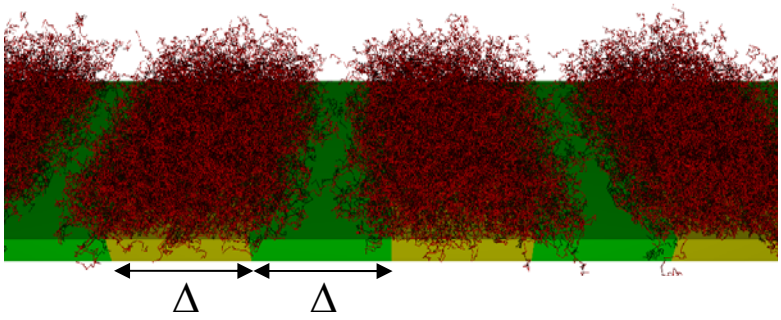
In this work we study by means of Monte Carlo computer simulations the equilibrium morphology of monodisperse linear-homopolymers end-tethered on certain domains of a periodically patterned substrate (*1*). We study a specific class of grafting substrates that consist of two different types of equal-width parallel stripes with alternating capability, due to appropriate surface treatment, to tether the polymer chains (see figure). The stripes are assumed infinitely long and their width, Δ, is the only parameter needed to describe this specific motif. We have examined in detail the equilibrium morphology of the patterned polymer brush as a function of the molecular weight N, the surface coverage (grafting density) of the grafting stripes, σ_S and the width of the stripes Δ. The main body of our results concerns good solvent conditions although preliminary results of the same system under poor solvent conditions are also presented.



Three distinct morphologies of the nanopatterned brush have been identified and their range of stability has been determined in terms of a single universal parameter $\xi = \Delta / N\sigma_s^{1/3}$ that combines the grafting density, the polymer length and the stripe width. Under good solvent

conditions, when $\xi < \xi_1 \approx 1$ the polymer film has similar properties with a homogenously grafted brush with grafting density $\sigma_s / 2$. For $\xi > \xi_2 \approx 4$ the tethered polymers form a sequence of isolated sub-brushes initiated from the grafting stripes. Finally for $\xi_1 < \xi < \xi_2$ the polymer layer exhibits a wavy outer surface and elongated parallel pores above the non-grafting stripes.

We propose two scaling relations for the average brush height and the architectural properties of the outer surface of the nanopaterned brush under good solvent conditions. Our analysis provides guidelines for fabricating well defined and tunable soft templates with applications that may include manipulation and ordering of nanoparticles of various sizes or mechanical control on liquid crystalline alignment.

References

(1) Koutsioubas A. G., Vanakaras A. G., *Langmuir*, **2008**, *24*, 13717.