Adsorption of Polymers on a Brush: Tuning the Order of the Wetting Phase Transition

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We have recently employed a self consistent field theory for inhomogeneous polymer fluids, in order to study the wetting properties of a polymer fluid on a brush [1]. We have found that in the absence of long range interactions, grafting chains at the substrate has the effect of bounding a liquid film, eventually leading to a first order wetting transition. Further increase of the grafting density leads to autophobicity: the dewetting of a polymer on a brush made of like polymers. Including the effect of long range forces leads to a rich phase diagram, including a new wetting state, which is wet in the sense that a small droplet will spread, but frustrated-wet, in the sense that the film cannot grow indefinitely [2]. On decreasing the intensity of the repulsion, the system shows a second order phase transition. This behavior is a result of the competition between short range attractions, originating from the grafted chains, which tend to stabilize a thick layer, and long range repulsions between the wall and the monomers, which limit the growth of a macroscopically thick layer [3]. The theoretical predictions have been tested by a general simulation methodology for the explicit calculation of the interface potential [4]. This allows us to determine directly whether the system is wet, to infer the order of the wetting transition, and to evaluate contact angles and adsorption isotherms. Our results fully confirm theoretical predictions, and allow us to determine a detailed wetting phase diagram in the space of the grafting density and the Hamaker constant.

[1] M. Mueller and L.G. MacDowell, *Europhys. Lett.* **55**, 221 (2001).
[2] N. Shahidzadeh, D. Bonn, K. Ragil, D. Broseta, and J. Meunier, *Phys. Rev. Let.* **80**, 3992 (1998).
[3] E. Bertrand, H. Dobbs, D. Broseta, J. Indekeu, D. Bonn, and J. Meunier, *Phys. Rev. Let.* **85**, 1282 (2000).
[4] L.G. MacDowell and M. Mueller, J. *Phys.: Condens. Matter* **17**, S3523 (2005).