

MAR11-2010-005037

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Polymer Physics Prize Talk: Polymer Brushes: Why do we still care?¹

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Polymer molecules have been widely used to modify the properties of surfaces including its adhesion. Among the most studied have been polymer brushes, in which polymer chains are grafted at one end to a surface and immersed in a small molecule solvents. Experiments and simulations have shown that the conformation of the chains grafted onto a flat surface depends on the grafting density and the interaction of the polymer with the solvent. As the molecular weight of the solvent increases, the structure of the brush changes. Consequently the brush chains are expelled from the solvent due to entropic loss that originate from the fact that the melt chains penetrating the brush cannot overcome the translational, or mixing, entropy. This crossover from wetted to non-wetted brushes, has important implications for polymer adhesion, where the phase separation of melt and brush chains reduces entanglements at the interface. As polymers are grafted to nanoparticles, the curvature of the surface offers the polymer brush chains a significantly larger space to explore compared to a flat surface, reducing the tendency for autophobic dewetting. Using large scale molecular dynamics simulations we have studied the interface between brush coated nanoparticles and a polymer melt. Effects of chain length of the brush, and that of the polymer melt, the coverage of the nanoparticle and its curvature on the brush/melt interface will be discussed. The role of individual entanglements, between the brush chains and the melt, as identified by primitive path analysis will be introduced. These simulations provide insight into the structure of the brush/polymer interface which is not accessible through other theoretical or experimental means.

¹Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.