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Stress in a Polymer Brush

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A brush-like structure emerges from the stretching of long polymer chains, densely grafted on to the surface of an impermeable substrate. This structure arises from a competition between the entropic elasticity of grafted polymer chains, and the intra and interchain excluded volume repulsion. Classical studies on polymer brushes focus on the structure of a brush, monomer density, end-distributions etc. but not on the stress. Recent advances in polymer-brush based soft active materials required us to understand the nature of stresses and forces in these material systems. In this talk two strong stretching theories (SST), based on Gaussian and Langevin elasticity of chains, are compared and contrasted with Molecular Dynamics calculations. Continuum mechanics plays a fundamental role in providing the analytical and semi-analytical theoretical methods to evaluate stress and its distribution within polymer brushes. For Gaussian chains, our theory predicts that the normal stress, parallel to the substrate, is a quartic function of the distance from the grafting surface with a maximum at the grafting surface. Idealizing the brush as a continuum elastic surface layer with a residual stress, closed form expressions for resultant surface stress and surface elasticity as a function of molecular weight and graft density are obtained. For higher graft density brushes, a (semi) analytical SST with Langevin chain elasticity will be discussed. Theoretical predictions are assessed by molecular dynamics simulation of a brush using bead-spring model. Experimental estimation of resultant stress due to a polymer brush will also be discussed. We conclude that classical scaling theories as well as the SST theories can be coupled with continuum mechanics to understand stress in a polymer brush.

Primary authors: MANAV, M. (University of British Columbia); PONGA, M. (University of British Columbia); PAHANI, A.S. (University of British Columbia)

Presenter: MANAV, M. (University of British Columbia)

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