Polymer brushes in weakly interpenetrating regimes

PARTH RAKESH DESAI, SHAYANDEV SINHA, SIDDHARTHA DAS, Univ of Maryland-College Park — We employ Molecular Dynamics (MD) simulations and develop new scaling laws to probe the behavior of semi-dilute polymer brushes in the weakly interpenetrating regime. This particular regime is characterized by the condition $d_g$ being more than $d_0$ but less than $2d_0$, where $d_g$ is the gap between two opposing surfaces with grafted polymer brushes and $d_0$ is the unperturbed brush height. Our results, showing excellent match between the MD simulation and scaling theory predictions, establish (a) unlike the classically studied case of strongly interpenetrating polymer brushes with $d_g$ less than $d_0$, here the brush height ($d$), instead of being solely dictated by the interpenetration length, can be expressed in a power law form where $d$ scales as $N^{\chi}$ (where $N$ is the polymer size), (b) the exponent $\chi$ shows a monotonic increase with a decrease in the degree of interpenetration, (c) the interpenetration length shows a different scaling behavior as compared to the strongly interpenetrated case, and (d) the scaling behavior of the experimentally-witnessed variation of the compressive energy between the brushes can be reproduced.

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