

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Tension Amplification and Structural Rearrangement in Tethered Bottle-Brush Layers via Molecular Dynamics Simulation**<sup>1</sup> GARY LEUTY, MESFIN TSIGE, University of Akron, MICHAEL RUBINSTEIN, University of North Carolina, GARY S. GREEST, Sandia National Laboratories — Bottle-brush polymers are a subgroup of comb polymers – linear polymer backbones to which linear polymer side chains are grafted. What sets bottle-brushes apart is the density of side chains grafted to the backbone; in bottle-brushes, that density is high enough that neighboring side chains experience significant mutual steric repulsion. This repulsion restricts the conformations available to the backbones and forces them to stretch, generating considerable tension that is controlled primarily by the density of side chains and their length. When bottle-brush polymers are end-tethered to a solid substrate, however, intermolecular interactions can augment the generation of tension as the number of side chains per unit area increases, leading to crowding. Using coarse-grained molecular dynamics simulations of homopolymer bottle-brush layers tethered to a flat wall, we have examined the effects of varying the chain length of both the backbone and side chains and the number of chains per unit surface area. We then show that the side chains are compressed and reorient during the transition from isolated macromolecules to dense but unentangled layers.

<sup>1</sup>This work is supported by NSF grant DMR0847580.

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Date submitted: 13 Nov 2013

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