

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Synthesis of polymer brushes by surface-initiated controlled radical polymerization in the presence of free initiators. A Monte Carlo investigation SALOMON TURGMAN-COHEN, JAN GENZER, North Carolina State University — Simultaneous controlled radical polymerization from free and surface-grafted initiators is studied by means of computer simulations. We model “truly living” reactions by neglecting chain termination and chain transfer. We study the competition between bulk- (i=b) and surface-initiated (i=s) polymers by monitoring the rates of polymerization ($d\langle N \rangle_i/dt$), the average molecular weight ($\langle N \rangle_i$), and the polydispersity index (PDI_i) while varying the initiator grafting density (σ), the fraction of surface based polymers (η), and the initial number of free monomers (I_o). We find that $d\langle N \rangle_B/dt > d\langle N \rangle_S/dt$ and that $d\langle N \rangle_S/dt$ decreases with increasing σ . The difference in polymerization rates between the bulk and surface polymerizations results in polymer populations with different $\langle N \rangle$; this has implications for the experimental determination of σ and $\langle N \rangle_S$. Although η affects $\langle N \rangle_S$ and $\langle N \rangle_B$, it does not influence the PDI. At a specific $\langle N \rangle_i$, the PDI_i has a value independent of η . In addition, $PDI_S > PDI_B$; this difference increases with increasing σ . We therefore conclude that polymerization conditions that yield bulk polymers with low PDI do not guarantee the same PDI for the surface-initiated polymers.

Salomon Turgman-Cohen
North Carolina State University

Date submitted: 21 Nov 2010

Electronic form version 1.4