

Abstract Submitted
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Understanding “grafting through” polymerization reactions involving surface-bound monomers PREETA DATTA, JAN GENZER, North Carolina State Univ — “Grafting through” polymerization is based on a bulk radical polymerization reaction utilizing a self-assembled monolayer that contain polymerizable units. Free polymer chains formed in solution can incorporate the surface-bound monomers, and thereby, get covalently bonded to the surface. As more growing chains attach to the surface-bound monomers, an immobilized polymer layer is formed on the surface. We use a combination of computer simulation and experiments to comprehend this process. Specifically, we report on the effect of spatial density of the surface-monomers on the formation of the surface-bound polymers. We use a lattice-based bond fluctuation model with periodic boundary conditions to simulate such systems. For experimental validation, we create gradients of density of methacrylate units on flat Si wafers using silane chemistry. The proximity of the surface-bound polymerizable units promotes the “grafting through” process but prevents more free growing chains to “graft to” the polymerizable units. Our studies indicate that these two counter-active effects balance each other and do not affect the overall density of the surface-bound polymer layer, except in case of the highest theoretical packing density of surface-bound monomers.

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