Abstract Submitted
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In silico polymerization: Computer simulation of controlled radical polymerization in bulk and on surfaces[1] JAN GENZER, NCSU — We use Monte Carlo computer simulation to study the effect of several molecular parameters on controlled/"living" radical polymerization in bulk and on substrates. Specifically, we investigate how the molecular weight and molecular weight distribution of grown polymers depend on the geometry of the substrate, the initial number of initiators, the initial number of monomers, the initiator activation probability, the initial probability of addition of a new monomer to a growing chain, the probability of terminating two "living" polymers, and the numbers of "living" polymers and their lifetime. We demonstrate that increasing the termination probability and/or decreasing the initial probability of addition of a new monomer to a growing chain broadens the molecular weight distribution. Our results further reveal that the confinement experienced by the surface-initiated polymers leads to an increased number of early terminations, relative to the bulk-initiated polymerization, which in turn, broadens the molecular weight distribution. This effect is enhanced by increasing the grafting density of the initiators on the surface and the concave nature of the substrate.

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