

Abstract Submitted
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Template Polymerization using a controlled reaction scheme

PREETA DATTA, JAN GENZER, North Carolina State University — We employ a Monte Carlo simulation scheme based on the bond fluctuation model to simulate template polymerization via controlled scheme (*i.e.*, termination and chain transfer reactions are neglected) involving co-polymerization of free monomers and monomers bound to a planar template with equidistant sites occupied by bound monomers. A new macromolecule is initiated in bulk by activation of an initiator; any monomer (free or bound) that is within the reaction distance (nearest neighbors) of the initiator can be incorporated into the growing chain. As the chain propagates, it adds new monomers to the macromolecule. Those monomers can either be bulk (*i.e.* free) monomers or those that are placed on the predefined template. We analyze the effect of the number and the density of monomers bound on the substrate on the composition and monomer distribution in the resultant co-polymers. Our results reveal that a greater number of bound monomers on the planar template promotes polymerization of most/all of the bound monomers to form an array attached to the template. In addition, there exists an optimum density of spacing of bound monomers on the template, at which the likelihood of the bound monomers getting incorporated in the growing chains is maximum. This is in contrast to our earlier findings for linear templates, where a higher density of spacing favors the incorporation of bound monomers in the growing chains.

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