Abstract Submitted
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Template polymerization using a controlled reaction scheme JAN GENZER, PREETA DATTA, NC 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 template that consists of four linear substrates with equispaced sites occupied by bound monomers. A new macromolecule is initiated 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 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 of spacing of the bound monomers on the composition and monomer distribution in the resultant co-polymer. Our results reveal that the larger the total number of bound monomers in the system and the more dense spacing, the greater is the likelihood of those getting incorporated in the growing chains. In addition, a greater number of bound monomers on the linear template promotes polymerization of most/all of the bound monomers to form a linear array attached to the template.

Jan Genzer
NC State University

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