

Abstract Submitted
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Computer-Aided Design of Photocured Polymer Networks SWARNAVO SARKAR, SHENG LIN-GIBSON, MARTIN CHIANG, NIST - Natl Inst of Stds Tech — Light-initiated free radical polymerization is widely used for manufacturing biomaterials, scaffolds for micromolding, and is being developed as a method for fast 3D fabrication. This process has a large set of control parameters in the composition of the photocurable matrix and the photocuring conditions. But a quantitative map between the choice of parameters and the properties of the resultant polymer is currently unavailable. We present a computational approach to simulate the growth of a polymer network using the stochastic differential equations of reactions and diffusion for a photocuring system. This method allows us to sample trajectories of a growing polymer network *in silico*. Thus, we provide a computational alternative to synthesize and probe a polymer network for properties like the degree of conversion, structure factor, density of states, and viscosity. We present simulation results that agree with the universal features observed in photopolymerization. Our proposed method enables a thorough and systematic search over the entire parameter space to discover interesting combinations for synthesis.

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