

Abstract Submitted
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Role of Inhomogeneity in Mechanochemically Active Polymers

MEREDITH SILBERSTEIN, Cornell University — Mechanically-induced reactivity is a promising means for designing self sensing and autonomous materials. Mechanically sensitive chemical groups termed mechanophores can be covalently linked into polymers in order to trigger specific chemical reactions upon mechanical loading. The mechanophore reaction kinetics, as determined by *ab initio* steered molecular dynamics, are exponential in force. As such the mechanochemical behavior of a solid-state polymer is highly sensitive to stress carried by that polymer, including local spatial and temporal fluctuations. Previously we developed microstructurally-based continuum models for fluorescence response in spiropyran-linked rubbery (poly methacrylate) and glassy (poly methylmethacrylate) polymers. The homogenization scheme in each relied on assigning mean effective forces acting on the mechanophores. Here we explore the theoretical influence of nanoscale spatial force distributions and fast temporal force fluctuations on the mechanochromic response of these systems. The effect of each is found to be significant and highly dependent on the intrinsic polymer mechanical behavior.

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