Mechanochemical Triggers for Self-Reinforcing Polymers

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Mechanical stress causes failure of polymeric materials, resulting from bond scission that generates macroradicals. We seek to design and synthesize mechanochemical triggers capable of diverting the mechanical energy stored in a stressed polymer to promote useful chemical reactions. Polymers containing mechanochemical triggers would undergo self-assessment through generation of new chromophores and self-reinforcement through the generation of new crosslinks or new polymeric material.

A computational method was developed to model mechanochemical activation in small molecules. It was found that when the stress-induced motions of molecules are congruent with the intended thermal reaction pathway, the energy barrier for the reaction is reduced by the amount of work that stress performs on the molecule. One such example of a congruent reaction is the degradation of azo compounds. High-intensity ultrasound was used to apply stress to linear macromolecules containing a single azo unit. Mechanical stress was found to bring about nitrogen extrusion below ambient temperatures. Progress toward other stress-induced chemical reactions, such as electrocyclic ring opening, will also be discussed.