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Kunhao Yu , An Xin , Qiming Wang

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Kunhao Yu, An Xin, Qiming Wang*
Sonny Astani Department of Civil and Environmental Engineering, University of Southern California, Los Angeles, CA 90089, USA.
*Email: qimingw@usc.edu

Abstract

Dynamic polymer networks (DPNs) crosslinked by dynamic bonds have received intensive attention because of their special crack-healing capability. Diverse DPNs have been synthesized using a number of dynamic bonds, including dynamic covalent bond, hydrogen bond, ionic bond, metal-ligand coordination, hydrophobic interaction, and others. Despite the promising success in the polymer synthesis, the fundamental understanding of their self-healing mechanics is still at the very beginning. Especially, a general analytical model to understand the interfacial self-healing behaviors of DPNs has not been established. Here, we develop polymer-network based analytical theories that can mechanistically model the constitutive behaviors and interfacial self-healing behaviors of DPNs. We consider that the DPN is composed of interpenetrating networks crosslinked by dynamic bonds. The network chains follow inhomogeneous chain-length distributions and the dynamic bonds obey a force-dependent chemical kinetics. During the self-healing process, we consider the polymer chains diffuse across the interface to reform the dynamic bonds, being modeled by a diffusion-reaction theory. The theories can predict the stress-stretch behaviors of original and self-healed DPNs, as well as the healing strength in a function of healing time. We show that the theoretically predicted healing behaviors can consistently match the documented experimental results of DPNs with various dynamic bonds, including dynamic covalent bonds (diarylbibenzofuranone and olefin metathesis), hydrogen bonds, and ionic bonds. We expect our model to be a powerful tool for the self-healing community to invent, design, understand, and optimize self-healing DPNs with various dynamic bonds.

Keyword: Self-healing | Dynamic bond | Mechanochemistry | Interpenetrating network model | diffusion-reaction model.