

Abstract Submitted
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Theory of self-healing polymer networks with reversible bonding

EVGENY STUKALIN, ARUN KUMAR N, Department of Chemistry, The University of North Carolina at Chapel Hill, NC 27599-3290, LUDWIK LEIBLER, Matière Molle et Chimie, CNRS-ESPCI, 75005 Paris, France, MICHAEL RUBINSTEIN, Department of Chemistry, The University of North Carolina at Chapel Hill, NC 27599-3290 — The polymer networks formed by reversible bonds, e.g., hydrogen bonds, feature the striking ability to restore their structural integrity after damage. This self-healing effect is sustainable following an appreciable waiting time after the fracture. The ability of these polymers to self-repair is attributed to very slow decay of non-equilibrium concentration of broken bonds during the waiting time followed by an efficient re-formation of bonds across the interface after two fractured surfaces are brought into contact. This process is distinct from self-adhesion which proceeds at equilibrium (very low) density of broken bonds. By means of analytical theories and scaling arguments we study the reaction kinetics of polymer chain systems that can form reversible bonds. The importance of anomalous diffusive motions of “stickers” as portions of dangling chains and reaction kinetics of bonding events including renormalization of bond lifetime and sticker partner exchange have been established for the self-healing process. Theoretical modeling that maps the results of MD/MC simulations onto kinetic models are used to capture the self-healing mechanism and its dynamics.

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