Continuum and Molecular-Level Modeling of Fatigue Crack Retardation in Self-Healing Polymers

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A numerical model to study the fatigue crack retardation in a self-healing material (White et al., 2001, Nature, **409**, pp. 794–797) is presented. The approach relies on a combination of cohesive modeling for fatigue crack propagation and a contact algorithm to enforce crack closure due to an artificial wedge in the wake of the crack. The healing kinetics of the self-healing material is captured by introducing along the fracture plane a state variable representing the evolving degree of cure of the healing agent. The atomic scale processes during the cure of the healing agent are modeled using a coarse-grain molecular dynamics model specifically developed for this purpose. This approach yields the cure kinetics and the mechanical properties as a function of the degree of cure, information that is transmitted to the continuum-scale models. The incorporation of healing kinetics in the model enables us to study the competition between fatigue crack growth and crack retardation mechanisms in this new class of materials. A systematic study of the effect of different loading and healing parameters shows a good qualitative agreement between experimental observations and simulation results.