Dissolution of Covalent Adaptable Network Polymers in Organic Solvent

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Dissolution of Covalent Adaptable Network Polymers in Organic Solvent

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Abstract: It was recently reported that thermosetting polymers can be fully dissolved in a proper organic solvent utilizing a bond-exchange reaction (BER), where small molecules diffuse into the polymer, break the long polymer chains into short segments, and eventually dissolve the network when sufficient solvent is provided. The solvent-assisted dissolution approach was applied to fully recycle thermosets and their fiber composites. This paper presents the first multi-scale modeling framework to predict the dissolution kinetics and mechanics of thermosets in organic solvent. The model connects the micro-scale network dynamics with macro-scale material properties: in the micro-scale, a model is developed based on the kinetics of BERs to describe the cleavage rate of polymer chains and evolution of chain segment length during the dissolution. The micro-scale model is then fed into a continuum-level model with considerations of the transportation of solvent molecules and chain segments in the system. The model shows good prediction on conversion rate of functional groups, degradation of network mechanical properties, and dissolution rate of thermosets during the dissolution. It identifies the underlying