Multifunctional Thermoset Polymer Matrix with Self-Sensing and Self-Healing Capabilities

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Objectives:
- Identification of damage precursors in polymer matrix composite structures
- Synthesis and characterization of mechanophore embedded thermoset polymer (self-sensing/self-healing)
- Development of a novel modeling framework to simulate mechanochemical reaction of mechanophores
- Validation of the modeling framework with experimentally observed responses

Motivation for Research:
- Urgent need for novel materials for damage precursor detection in polymer matrix composites

Mechanophores:
- Spiropyran-based
- Dioxetane-based
- Dimeric Anthracene

Employment of Dimeric Anthracene (Di-AC)-based Mechanophore Polymers

Modeling of Di-AC based Mechanophore Thermoset Polymers
- Develop a new method to generate epoxy network (epoxy curing) and simulate mechanophore activation (covalent bond breakage)
- Physico-based modeling approach provides information to mechanophore design enhancement

Hybrid MD Simulation Framework
- Key elements
  - Epoxy network
  - Perform covalent bond generation method
  - Covalent bond dissociation
  - Implement bond-order based force field
  - Mechanical loading test in MD
  - Develop a quasi-continuum deformation method
  - Characterization of Di-AC (mechanophore)
    - Calculate bond dissociation energy

Epoxy Curing Simulation
- Simulation of Curing Process
- Nitrogen
- Cure Process
- Carbon

Mechanophore Activation using Virtual Loading Test
- Virtual loading test with ReaxFF capture damage initiation and plastic deformation
- During virtual loading test, covalent bonds of Di-AC break and Di-AC (red) changes to anthracene groups (green)

Characterization of Di-AC
- Bond dissociation energy of Di-AC >> 58.5 kcal/mol
- Critical bond length >> 2.16 Å
- QM 6.52 nN
- Bond rupture force of Di-AC (6.7 nN)
- BDE : 58.5 kcal/mol
- BFR : 6.7 nN

Mechanophore activation can represent intensity curve
- Proportional increase in intensity as specimen deforms; good correlation between modeling and experiments
- Critical strain values representing the onset of mechanophore activation are estimated

Early Signal Detection
- Early signal detection of Di-AC was observed in experiments
- Early signal detection is captured computationally through the comparison of stress-strain curve and mechanophore activation

Yield Strength Comparison
- Neat Epoxy vs. 5 wt% Di-AC
- Comparability difference in yield strength between simulations and experiments
- Captures experimentally observed responses

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