Damage Precursor Identification in Polymer Matrix Composites Using Novel Smart Composite Particles

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Objectives:
• Identification of damage precursors in polymer matrix composite structures
• Synthesis, characterization, modeling and validation of smart particles as a multifunctional sensor
• Investigation of the interactions between the smart particles and the polymeric matrix (experiments/simulation)
• Verification of the interfacial effects between carbon fiber and the host polymer matrix (experiments/simulation)

Fluorescence Generation from Cleavage of Cyclobutane
Mechanism
• Cyclobutane has highly strained structure, cleavage of the C-C bonds of cyclobutane was relatively easy.
• Cyclobutane-containing cross-linked polymers of trimers generated fluorescence upon the cleavage of cyclobutane.

Fluorescence Observation for Coating on Polystyrene
• Cracks on polystyrene coated with cross-linked TCE or PVC polymer.

Fluorescence Observation for Different Concentration of TCE Polymer
• Crack generated on epoxy with different concentration of TCE polymer

Multiscale modeling for smart material embedded epoxy composite
Key issues:
• Simulation of epoxy network considering realistic curing process
• Extraction of mechanical property from MD simulation
• Investigation of interfacial effect between smart material & polymer matrix
• Transfer of relevant information across length scales

Simulation of curing process
Configuration of molecular model of epoxy system

Validation of MD simulation: Glass transition temperature

Prediction of mechanical properties of epoxy polymer

Mechanical properties: MD simulations