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

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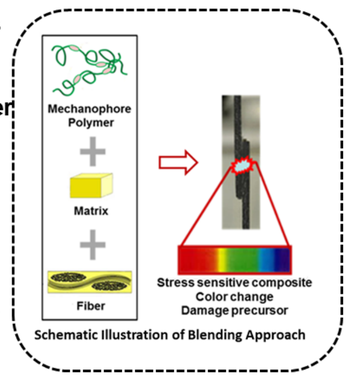
Objectives:

- **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)**

Motivations/Objectives

- ***Synthesis and Characterization*** **of stress sensitive mechanophore**
- ***Incorporation*** **smart material and polymer matrix composite (PMC)**
- ***Development of multiscale modeling framework*** **for smart material embedded PMC**
- ***Validation of the modeling framework*** **by comparing with experimental results**

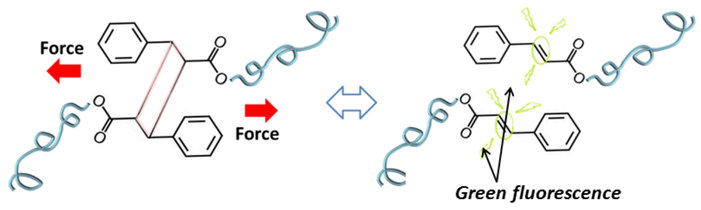


Schematic Illustration of Blending Approach

Fluorescence Generation from Cleavage of Cyclobutane

Mechanism

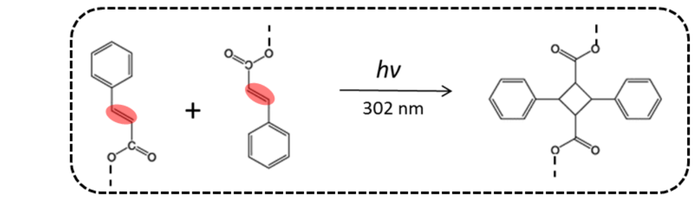
- **Cyclobutane has highly strained structure, cleavage of the C-C bonds of cyclobutane was relatively easy.**
- **Cyclobutane-containing cross-linked polymers of *tricinnamates generated fluorescence* upon the cleavage of cyclobutane*.**

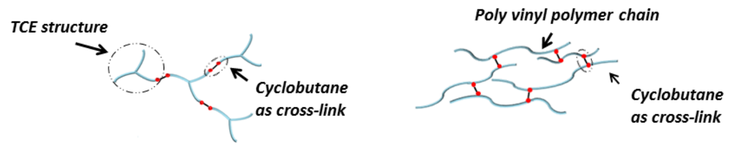


*Davis, Douglas A., et al. "Force-induced activation of covalent bonds in mechanoresponsive polymeric materials." *Nature* 459.7243 (2009): 68-72.

Synthesis of Cyclobutane Polymer

- **Synthesis cyclobutane-containing polymer by [2+2] cycloaddition through photoirradiation**

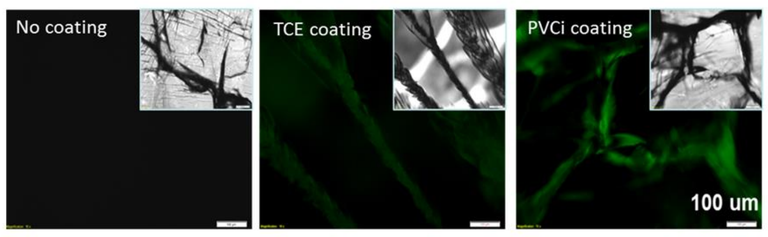




Structure of cross-linked TCE polymer ***Structure of cross-linked PVCi polymer***

Fluorescence Observation for Coating on Polystyrene

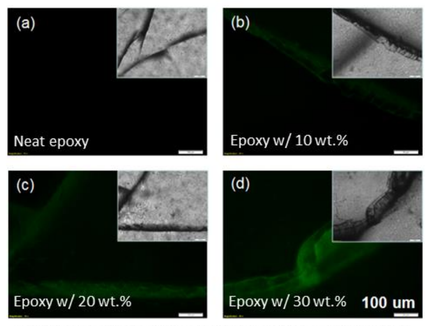
- **Cracks on polystyrene *coated with cross-linked TCE or PVCi polymer*.**



Microscopic images of fluorescence emission along cracks

Fluorescence Observation for Different Concentration of TCE Polymer

- **Crack generated on epoxy with different concentration of TCE polymer**

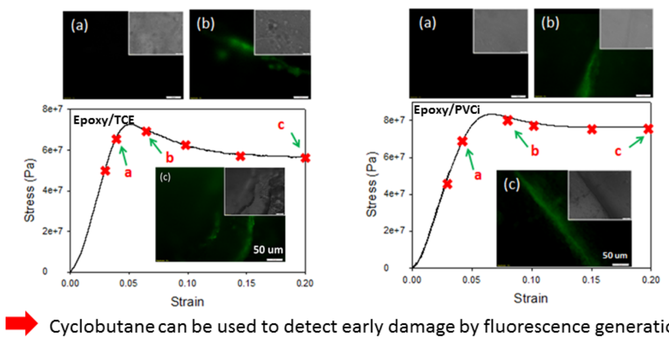


Microscopic images of fluorescence emission along cracks

Either TCE polymer coated on polystyrene or blended with epoxy, fluorescence can be observed along crack under UV.

Fluorescence Observation under Compression Test

- **The visual fluorescence was not observed before the yield point.**
- **The visual fluorescence was observed under UV; The cracks were not clearly detected under white light.**
- **The fluorescence intensified with strain accumulation.**

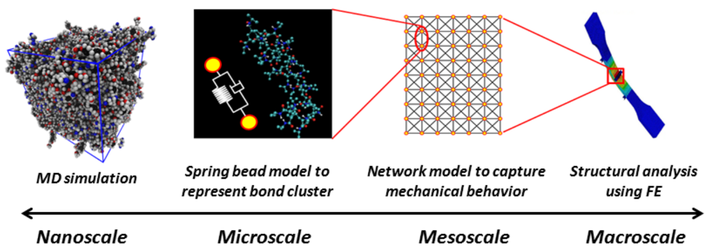


Cyclobutane can be used to detect early damage by fluorescence generation.

Multiscale modeling for smart material embedded epoxy composite

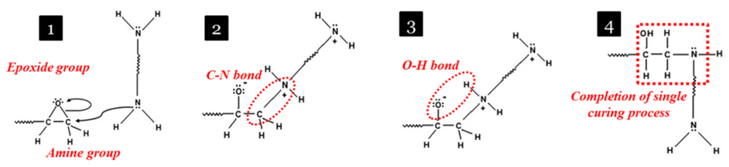
Key Issues:

- **Simulation of epoxy network considering *realistic curing process***
- **Extraction of *mechanical properties* from MD simulation**
- **Investigation of *interfacial effect* between smart material & polymer matrix**
- **Transfer of relevant information *across length scales***

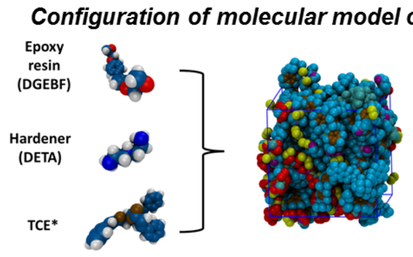


Simulation of curing process

Chemical curing process



Configuration of molecular model of epoxy system

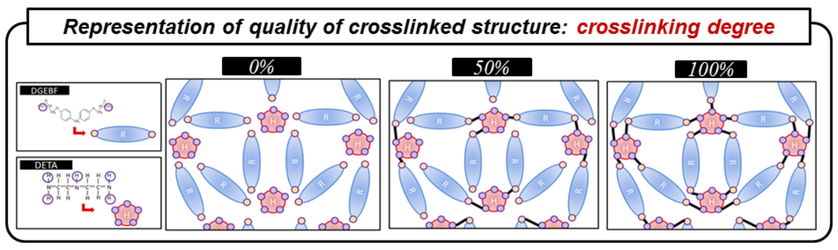


	Weight	molecules
Epoxy resin	313g/mol	650
Hardener	103g/mol	550
Smart material*	510g/mol	50

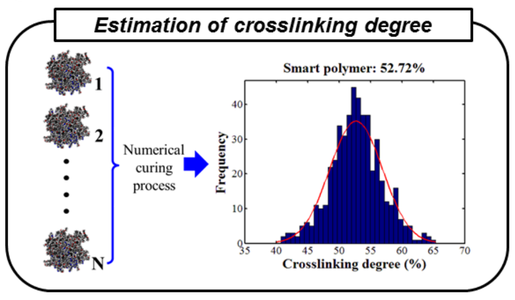
*TCE : Tris-(Cinnamoyloxymethyl)-Ethane

Epoxy cross-linked structure

Representation of quality of crosslinked structure: crosslinking degree



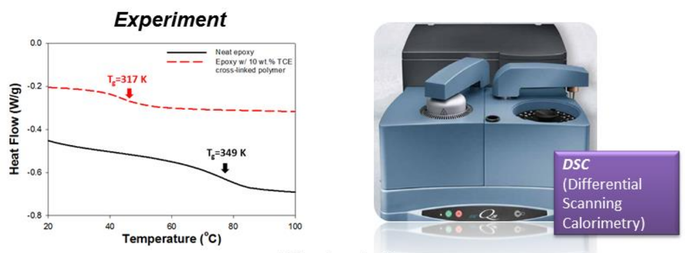
Estimation of crosslinking degree



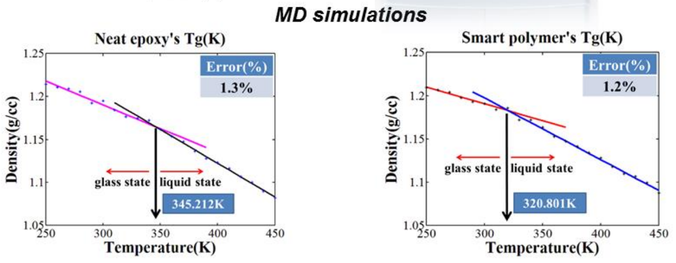
- ***Probability density of crosslinking degree*** **based on a decent number of unit cells with random initial positions of molecules (N=500)**
- **Development of *realistic thermoset matrix model* including strong stochastic curing phenomena**

Validation of MD simulation: Glass transition temperature

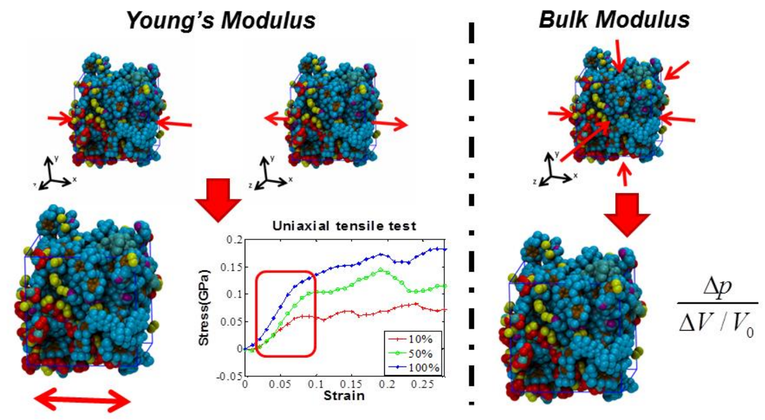
Experiment



MD simulations

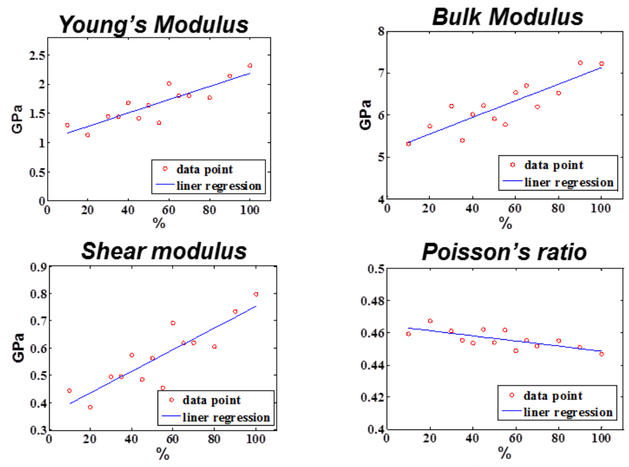


Prediction of mechanical properties of epoxy polymer



- **Uniaxial deformation test => Young's modulus**
- **Triaxial deformation test => Bulk modulus**

Mechanical properties: MD simulations



- **High crosslinking degree means high Young's modulus/bulk modulus/shear modulus.**
- **Poisson's ratio are *inversely proportional* to stiffness of materials**

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