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Advanced Mechanical Performances of Polymer Composites

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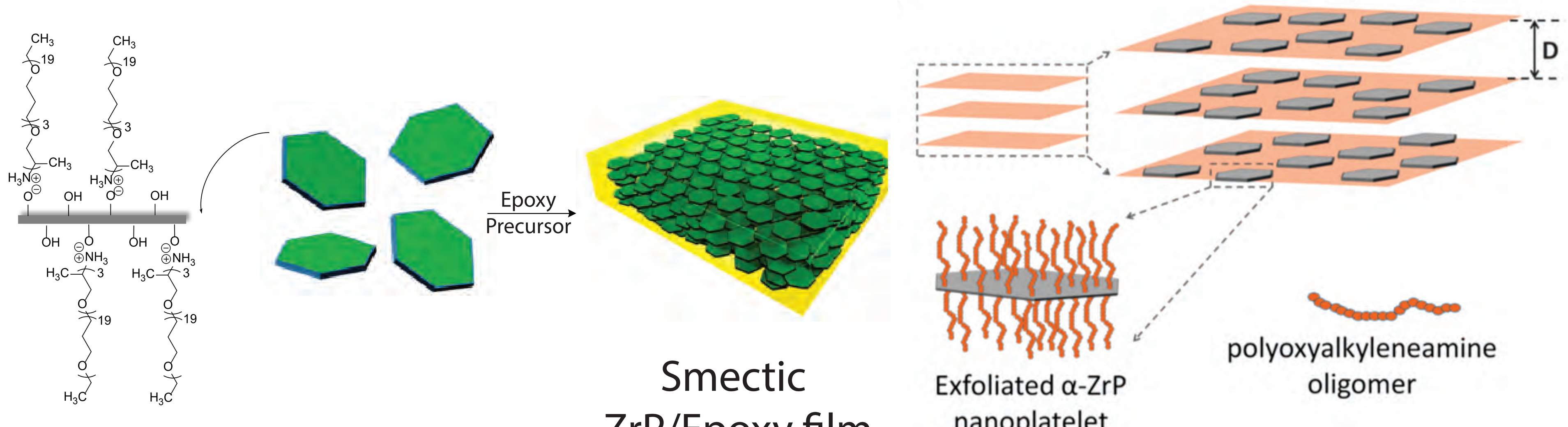
Epoxy/ZrP Nanocomposites

Motivation



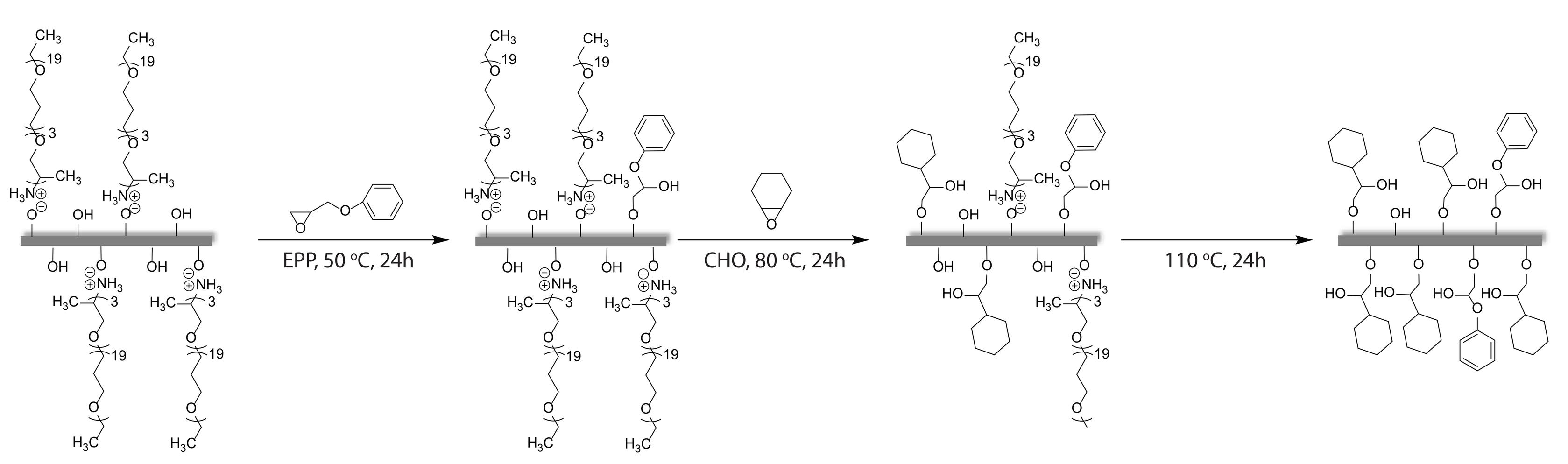
Applications:

- Gas barrier
- Anti-corrosion

Drawbacks:

- Low T_g
- High CTE (at 35-100 °C)

ZrP Epoxide Modification

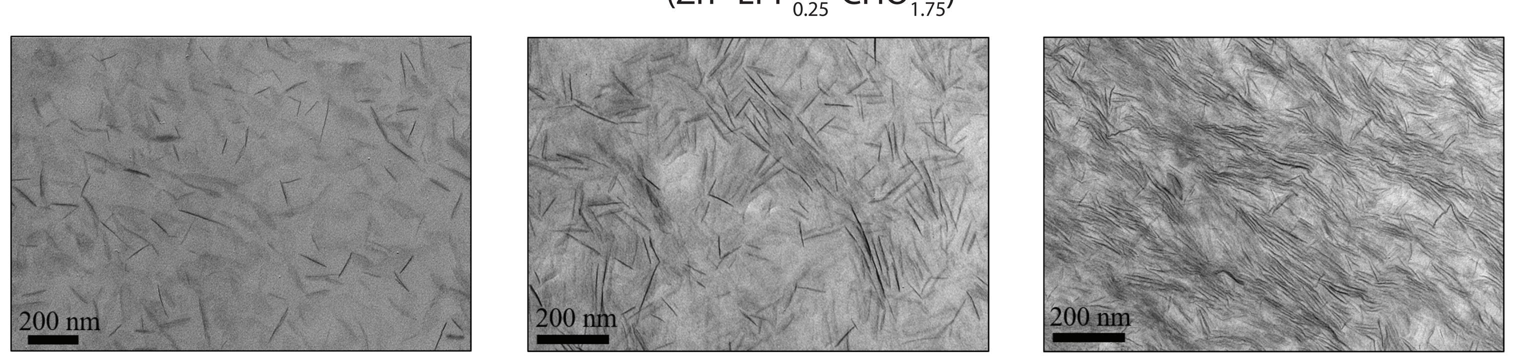


Advantages:

- Stronger covalent bonds, more stable when heated
- π-π interaction between modified ZrP and polymer, better dispersion

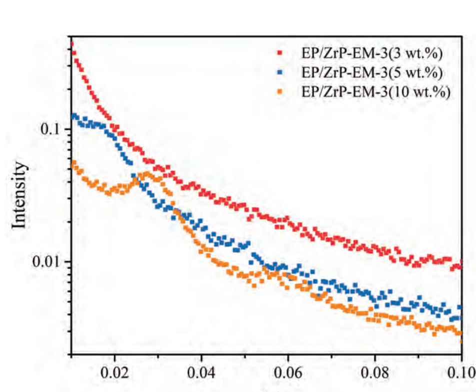
Morphology

Epoxy/ZrP-EM-3 ($ZrP\text{-}EPP_{0.25}\text{-}CHO_{1.75}$)



3 wt% 5 wt% 10 wt%

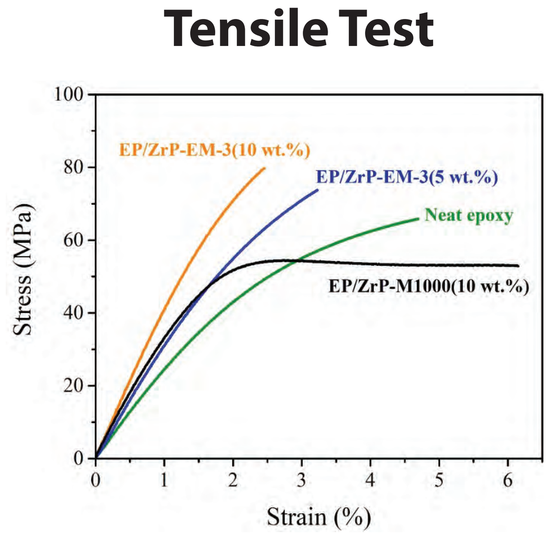
SAXS



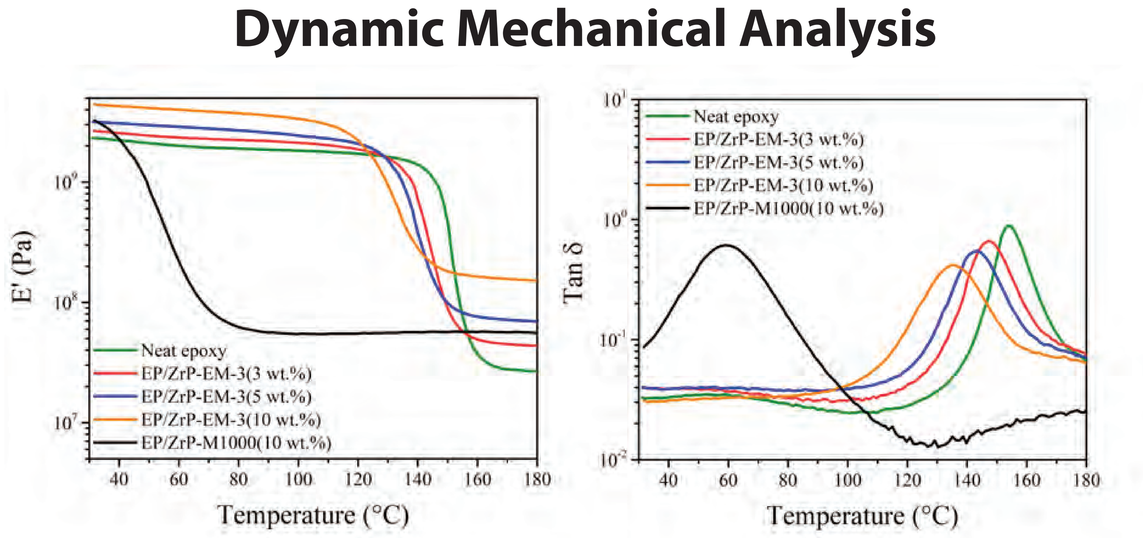
- Good dispersion at high ZrP loading
- Self-assembly of ZrP-EM-3

Mechanical Properties

Tensile Test



Dynamic Mechanical Analysis



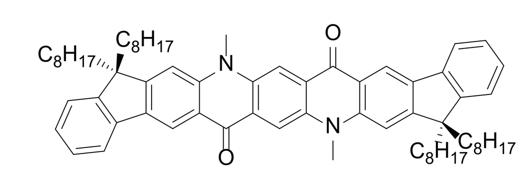
Sample	T_g (°C)	Young's modulus (GPa)	Tensile strength (MPa)	Elongation at break (%)	CTE (ppm /°C) (30-50 °C)	E′ (MPa) at 40 °C	E′ (MPa) at 180 °C
Neat epoxy	153	2.8±0.2	64±6	4.6±1.0	71.7	2.22	2.68
Epoxy/ZrP-EM -3(5 wt.%)	143	3.3±0.2	70±4	3.2±0.5	67.5	3.07	69.29
Epoxy/ZrP-EM -3(10 wt.%)	136	4.3±0.2	75±5	2.3±0.1	47.0	4.28	151.92
Epoxy/ZrP-M1000(10 wt.%)	59	3.9±0.1	54±2	6.3±1.1	3269.1	--	--

Advantages:

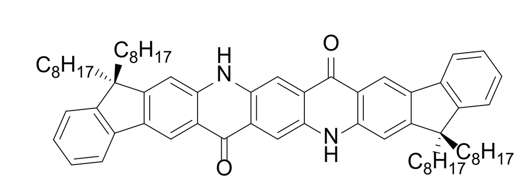
- Increased Young's modulus
- Improved tensile strength
- Higher storage modulus at both room and high T
- High T_g maintained
- Significantly reduced thermal expansion coefficient

Epoxy/Quinacridone composites

Additives



$C8IQA\text{-}CH_3$



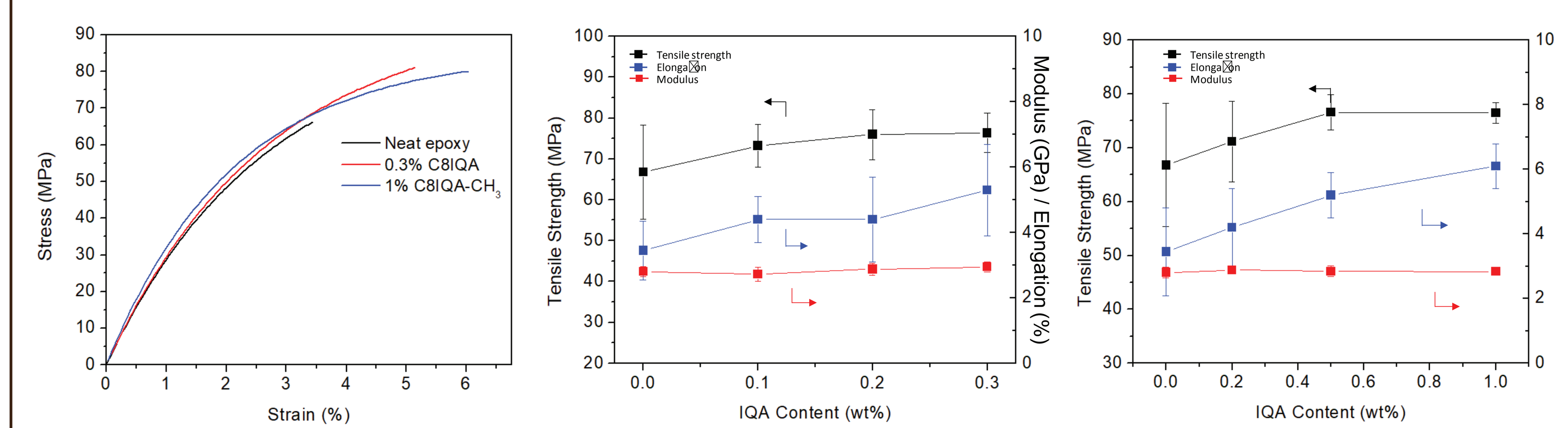
C8IQA

Features:

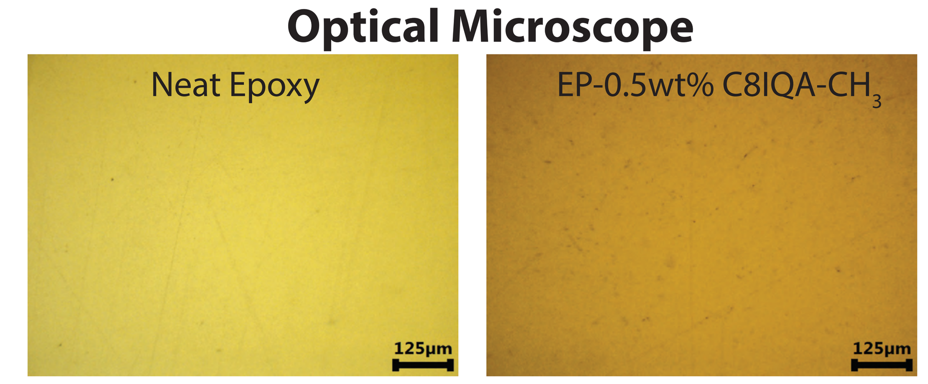
- Fused-aromatic rigid backbone
- Long alkyl chains
- Solvent free processing

Characterization

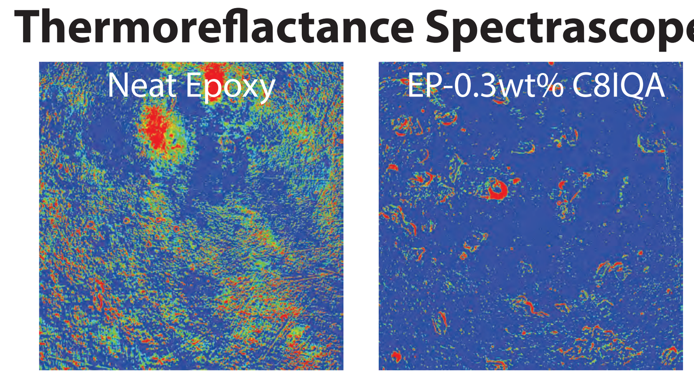
Tensile Test



Optical Microscope



Thermoreflactance Spectrascope

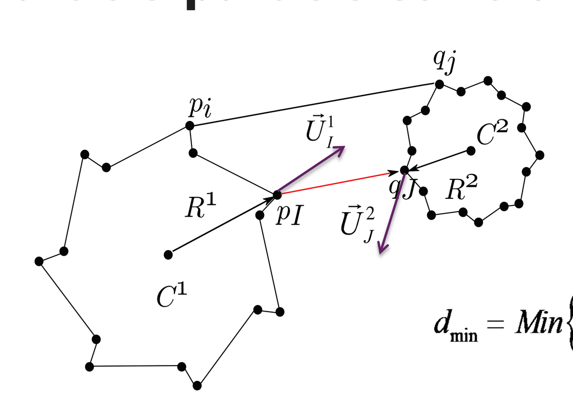


Advantages:

- Both tensile strength and elongation at break increased with IQA content
- No observable aggregation of IQA additives at 0.3 wt% for C8IQA and 1 wt% for $C8IQA\text{-}CH_3$
- Better dispersion for IQA without hydrogen bonding

Numerical Rheology Simulation

Particle-particle Collision Detection Model



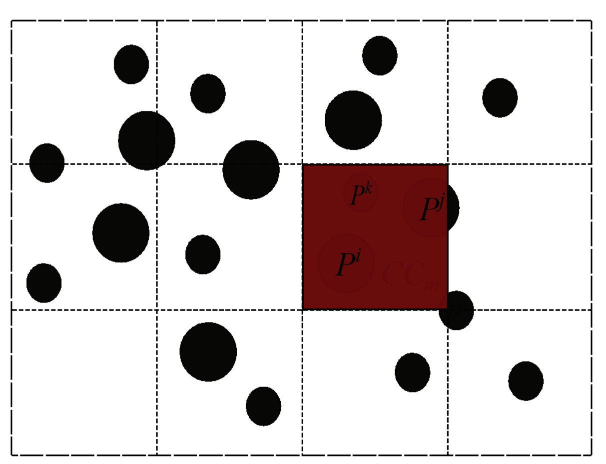
$\vec{e}_d = \frac{\vec{p}_i - \vec{q}_j}{|d_{min}|}$

$d_{min} = Min\{|p_i - q_j|, i = 1,\ldots,N^1, j = 1,\ldots,N^2\}$

$d_{min} < d_{critical}$ ⟹ Modify distance ⟹ $d'_{min} = d_{critical}$

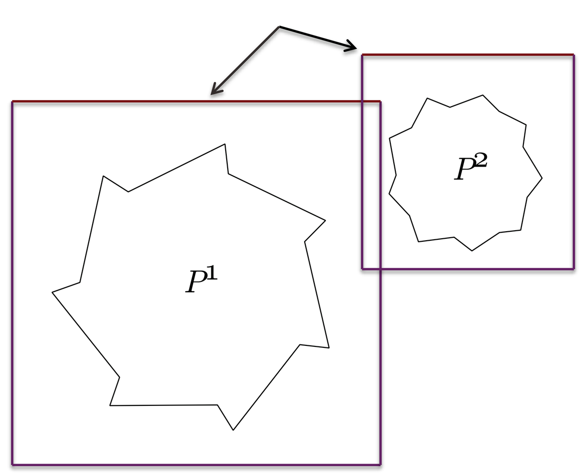
$(\vec{U}_i^1 - \vec{U}_j^2)\vec{e}_d > 0$ ⟹ Modify velocity ⟹ $(\vec{U}_i'^1 - \vec{U}_j'^2)\vec{e}_d = 0$

Control Cell



Only particles within each control box is considered for possible collision

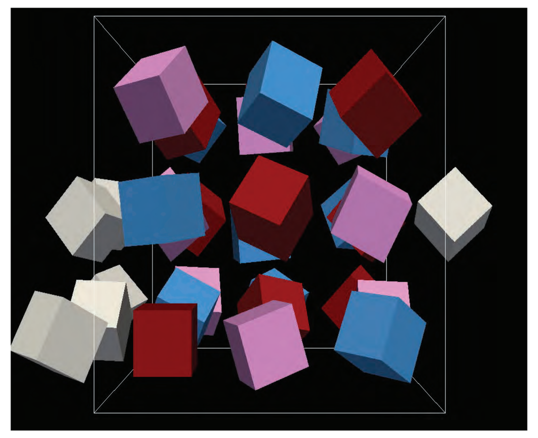
Bounding Box



If bounding boxes overlap, particles are tested for possible collision

Influential Geometric Factors

A_p / V_p Surface to volume ratio $\bar{\Sigma}^p_{yz}$ Shear particle stress

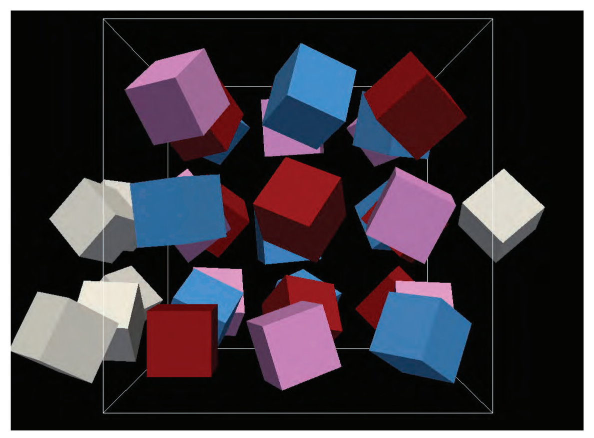


Prolate sheroids Volume fraction 15%

$S_p / V_p = 4.58$

$\bar{\Sigma}^p_{yz} = 0.573$

$\eta_r = 1.573$



Cubes Volume fraction 15%

$S_p / V_p = 10.39$

$\bar{\Sigma}^p_{yz} = 0.573$

$\eta_r = 1.573$

Advantages:

- Efficient numerical framework
- Works for suspensions of irregular-shaped particles
- Particle geometry is verified

Acknowledgement

PRESIDENT'S EXCELLENCE FUND

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