Atomistic scale simulation for the inter-diffusion of Epoxy-Amine (Interphase modeling)

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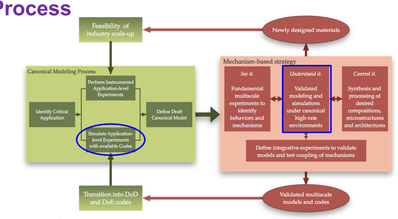
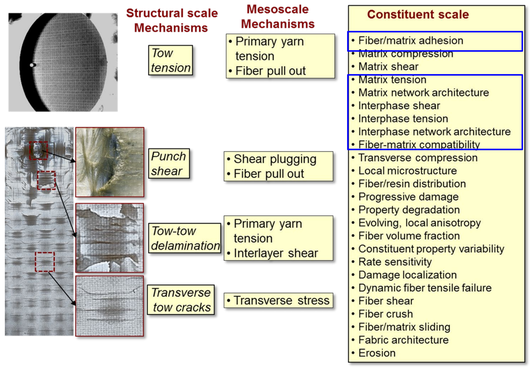
Enterprise for Multi-scale Research of Materials

How We Fit

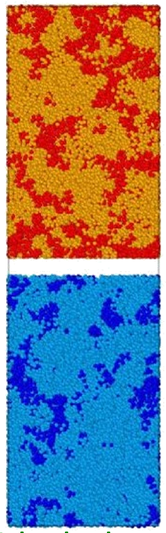
Materials-by-Design Process



Mechanism-based Approach



Technical Approach



Molecular dynamic simulation between epoxy and amine molecules

MD model of Fickian diffusion based on different temperature: predict the diffusion characteristic at short time frame

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Predict the concentration profiles of epoxy and amine across the interphase thickness as a function of time.

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Model validation through correlate with diffusion experiments

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Determine whether the final interphase is diffusion or reaction controlled

Key Accomplishments

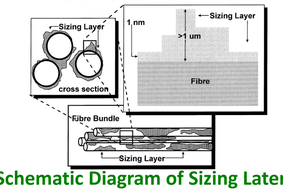
Properties	Epon828-Jeffamine	Epon1001F-PACM20
E_a, Activation Energy (kJ/mol)	25.6	28.9
D_0, maximum diffusivity (cm^2/s)	2.4e-4	1.132e-4
Estimated diffusivity at 300K (cm^2/s)	1.9530e-9 ~ 4.4091e-8 (8.3759e-9)	3.7211e-10 ~ 3.1527e-9 (1.0641e-9)
Diffusivity from experiment (cm^2/s)	3e-9 (From Drexel Univ)	2.5e-10 (Skourlis et al.)

❖ MD simulation from diffusivity is comparable with experiment, slightly higher.

System thickness	100nm	500nm	1μm	10μm
Epon1001F-PACM20	75s	1869.4s	7477.6s (~2hr)	~33.2 hr
Epon828 – Jeffamine	10s	237.5s	950s	~4.2 hr

❖ Based on diffusivity from MD simulation, it is estimated to cost hours to days order of time to reach equilibrium state for different system thickness condition.

❖ Typical sizing layer thickness is ranging from 1nm to 1μm. Time to reach diffusion equilibrium state between two species is faster than known gelation time, order of hours under room temperature condition.



Schematic Diagram of Sizing Later (Ref: Thomason et al.)

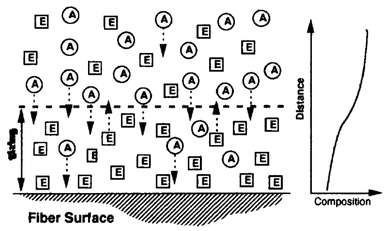
Impact / Transition

❖ **MD based materials-by-design framework will guide ARL/CMRG experimentalists to design optimum interphase structure**

❖ **MD based diffusion modeling will identify pattern of epoxide-amine stoichiometric gradient in the interphase**

❖ **Estimated long-term diffusivity from MD simulation will be used as a guideline for future simulations, and would be a reference for experiments**

Key Goals



Diffusion of amine molecules into sizing (Ref. Palmese et al)

❖ Diffusion governs the concentration gradients, interphase thickness and the resulting atomic structure and properties of the interphase.

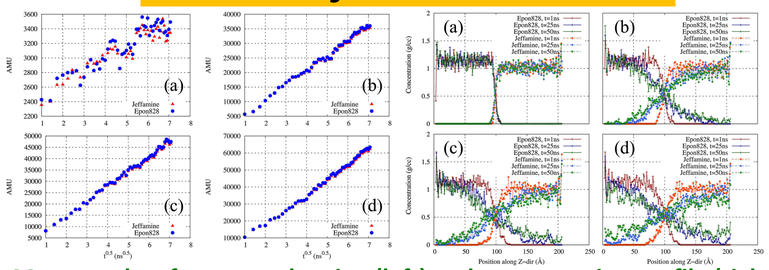
➔ Well developed interphase will bring better composite strength, toughness, and damage modes.

❖ Design of interphase requires optimization of species involved in mixing and control of chemical reaction.

➔ Atomistic scale point of view is essential.

Theoretical modeling of diffusion and mixing ➡ Achieve long term prediction based on estimation from simulation

Major Results



Mass uptake of epoxy and amine (left) and concentration profile (right)

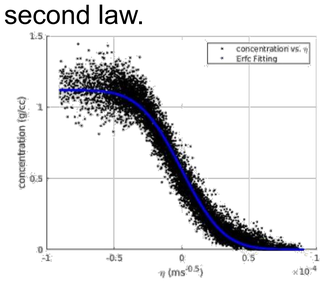
❖ Diffusion simulation showed that the mixing between Epon828-Jeffamine and Epon1001F-PACM20 is typical Fickian diffusion. This allow us to analyze diffusion using Fick's second law.

$$c(z,t) = c_0\left(1 - \mathrm{erf}\left(\frac{z}{2\sqrt{Dt}}\right)\right)$$

❖ Diffusivity is estimated from curve-fitting data of eta ($\eta = z/\sqrt{t}$) and concentration profile data

Diffusivity	600K	750K	900K
Epon 828	1.79e-6	3.01e-6	6.96e-6
Jeffamine	1.67e-6	3.16e-6	6.91e-6
Average	1.73e-6	3.08e-6	6.93e-6

Diffusivity (cm^2/s) of Epon828 and Jeffamine

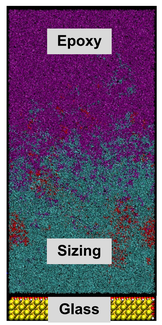


Estimation of diffusion coefficient

Future plan

❖ **MD simulation for interdiffusion under more "realistic" conditions (i.e., diffusion of epoxy-amine into sizing layer in the presence of glass surface)**

❖ **Reactive force field (ReaxFF) parametrization for S-Glass and its interaction with sizing and epoxy resin**



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UNIVERSITY OF DELAWARE