Effect of Microstructural Damage on the Thermomechanical Properties of Composite Electrodes in Proton Exchange Membrane Fuel Cells

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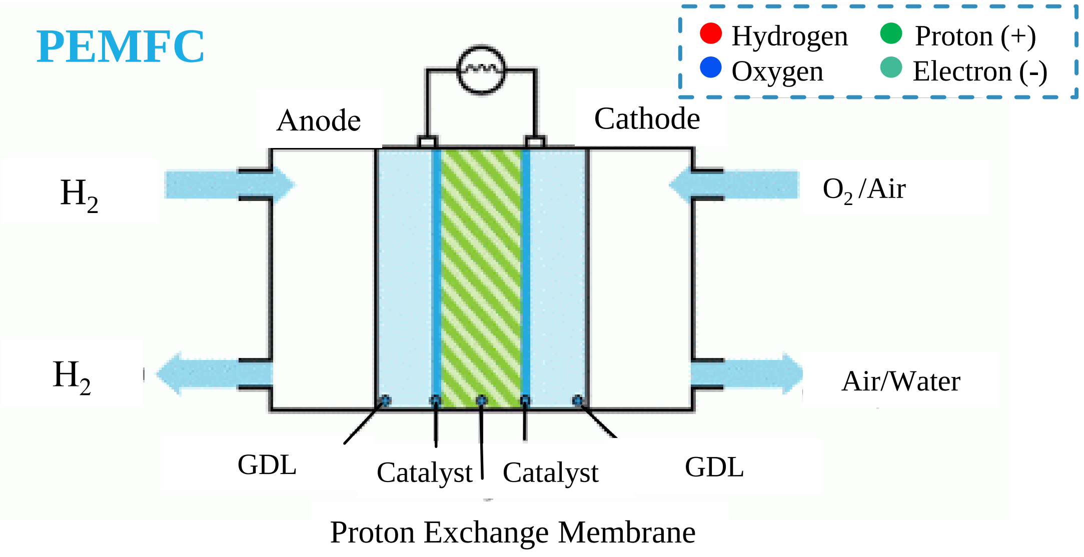
Proton exchange membrane fuel cells (PEMFC)

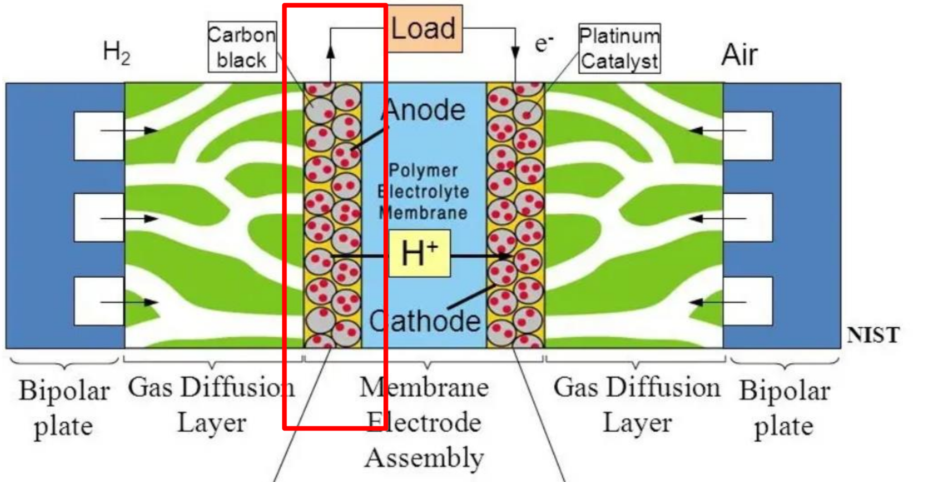


Chemical energy → Electrical energy

Transportation & Stationary power plants

Damage Failure Affects PEMFC Durability

- ➢ Electrode component: most likely to suffer damage

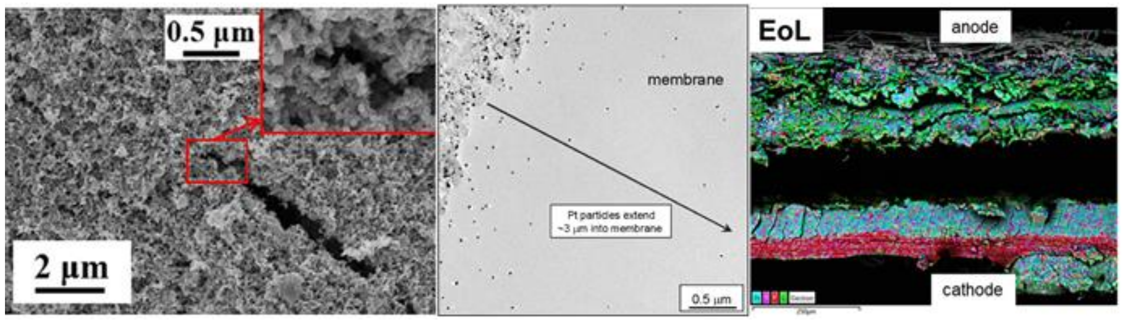


Anode Reaction

$2H_2 \rightarrow 4H^+ + 4e^-$

Cathode Reaction

$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$



Crack | Pt migration | Delamination

Chemical degradation

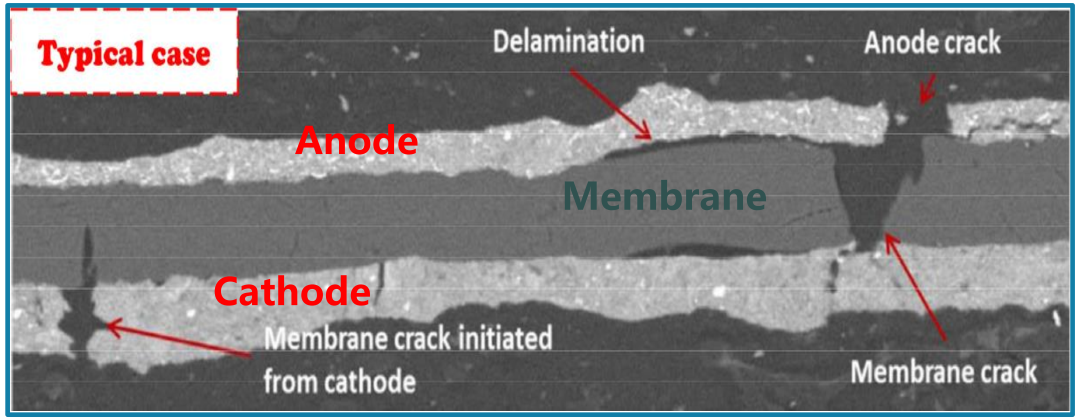
Thermomechanical degradation

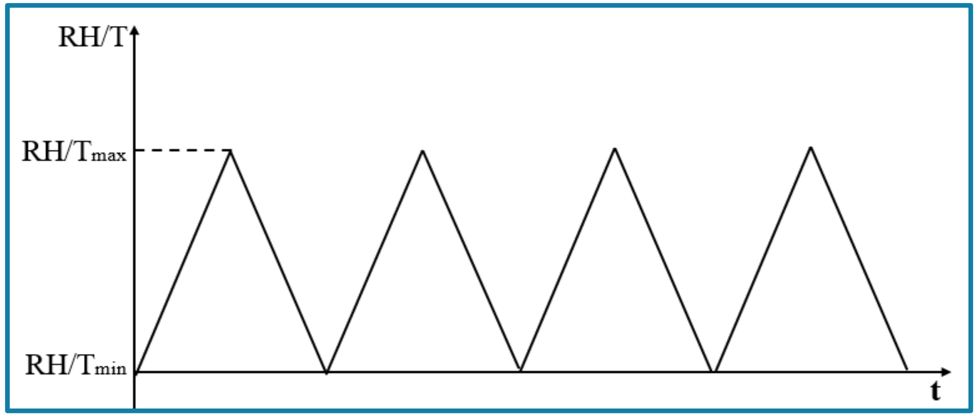
Electrode reactive site

Damaged electrode

Thermomechanical Degradation

➢ Damage due to mechanical and thermal actions



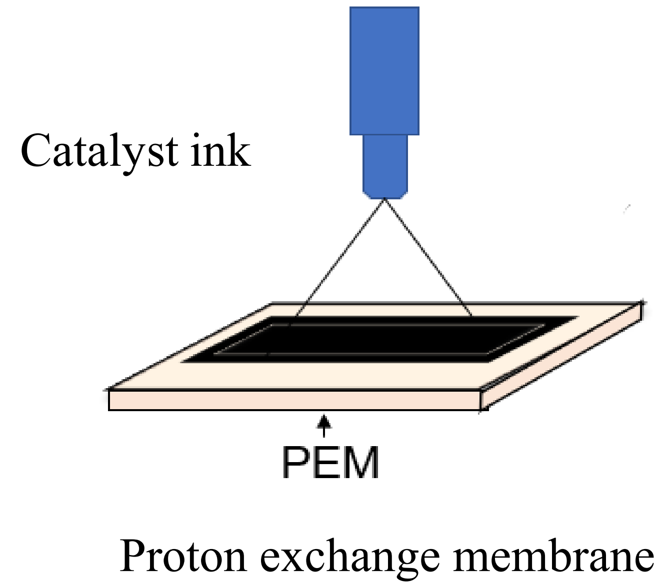


Start-up and shutdown condition

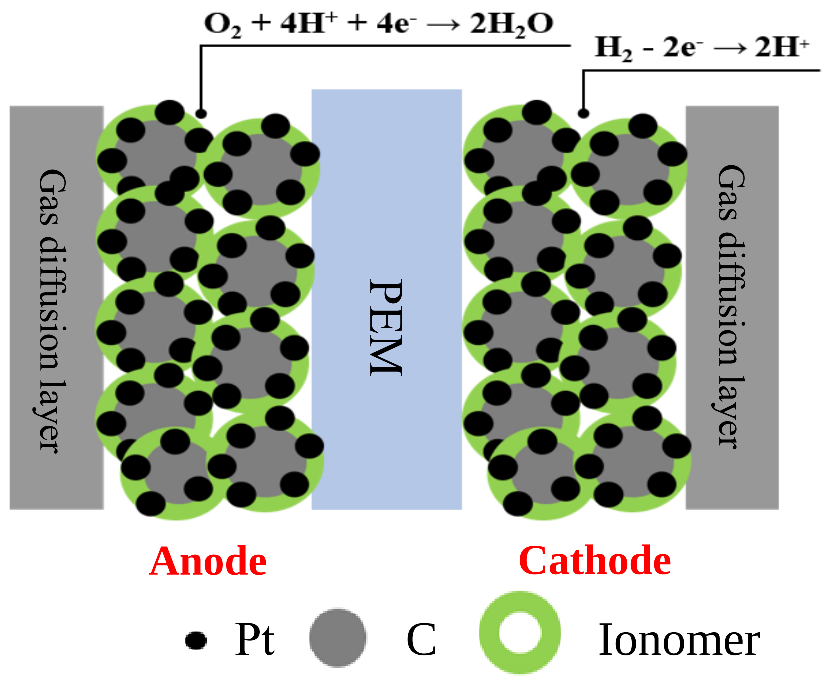
Hydrothermal loading cycles

Multiscale Simulation

- Microstructural changes and macroscopic properties



Preparation



Schematic

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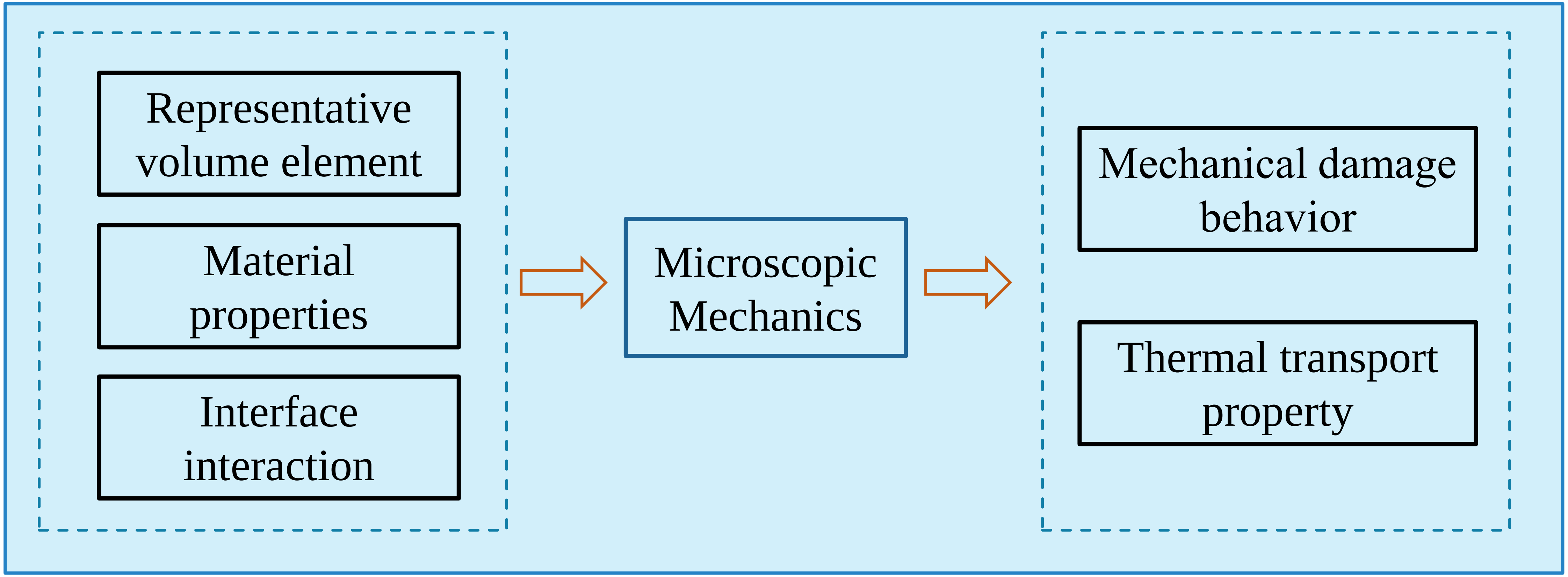
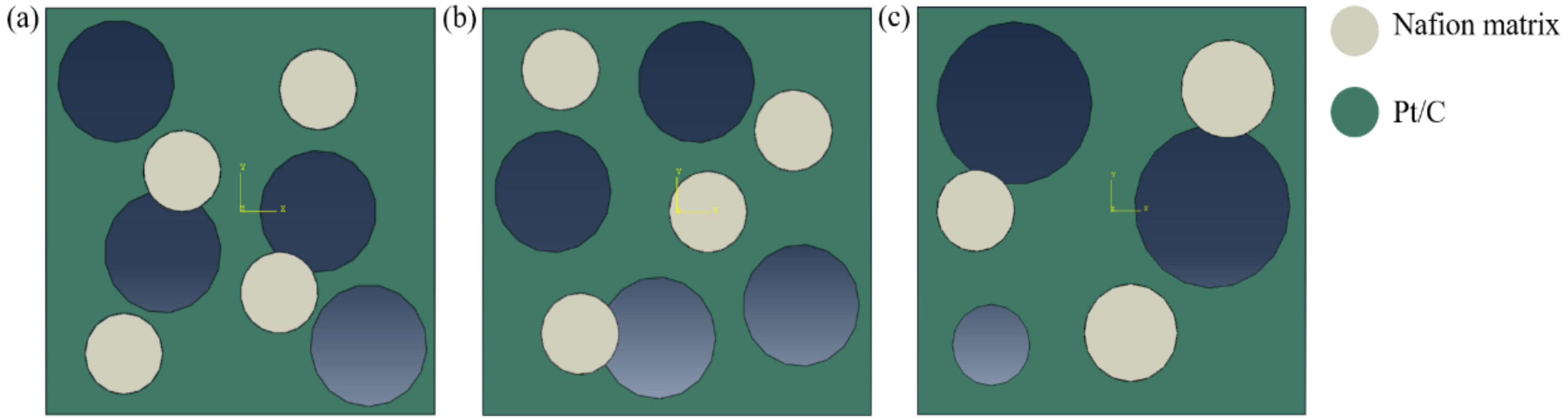
Research Methods and Framework

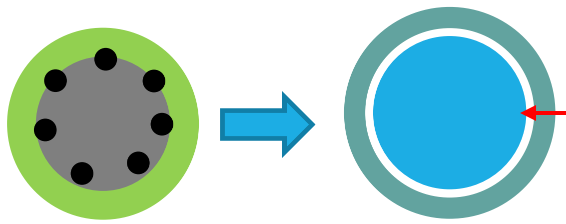


Representative Volume Element (RVE)

Characteristic	Matrix	Pt/C	Pore
Size (nm)	100	20-50	20-100
Volume fraction	30-55	15-40	30-40



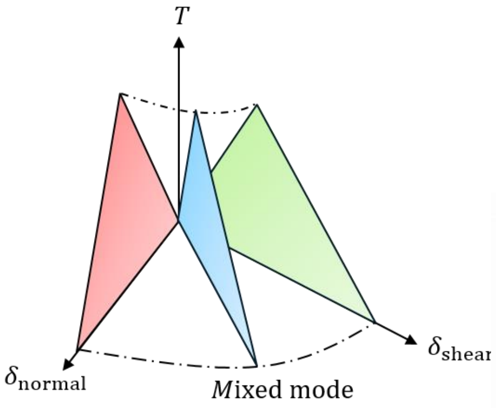
➢ Interface interaction

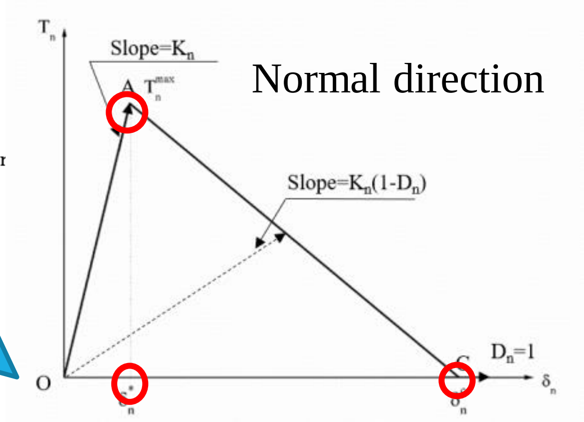


- Friction $\boxed{\tau = \mu P + P_0}$

- Delamination $\boxed{T = K\delta(1 - D_m)}$

➢ Interface delamination model: mixed cohesive zone model



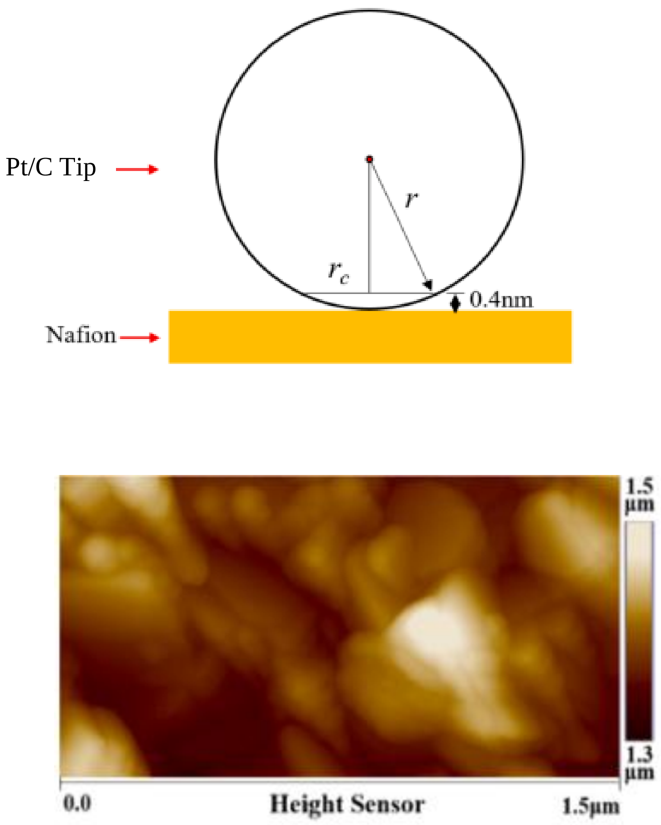


$$\boxed{T = K\delta(1 - D)}$$

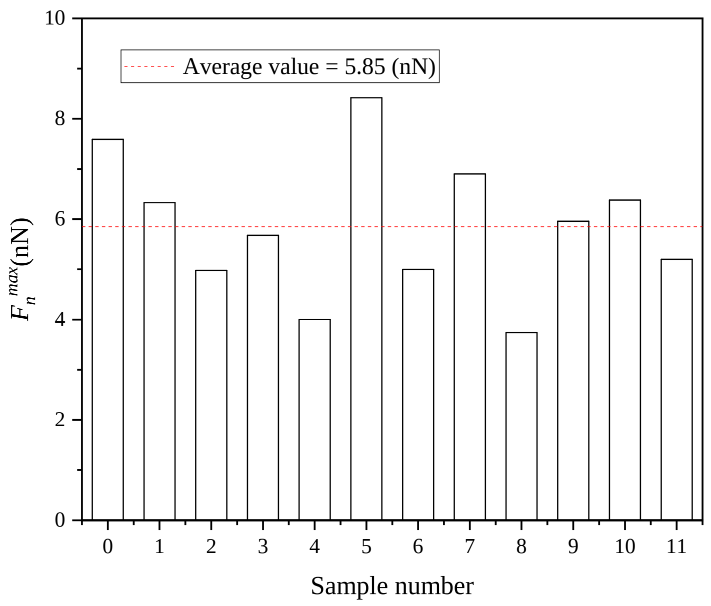
$$D = \begin{cases} 0 & ,\delta \le \delta^* \\ \left(\frac{\delta - \delta^*}{\delta}\right)\left(\frac{\delta^c}{\delta^c - \delta^*}\right) & ,\delta^* < \delta < \delta^c \\ 1 & ,\delta > \delta^c \end{cases}$$

Mechanical parameters ⇨ ? Diversity and sizes

➤ Interface adhesive force (AFM Experiment)



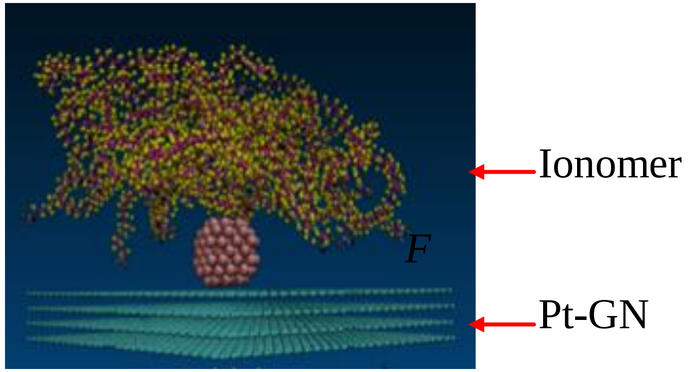
Measurement



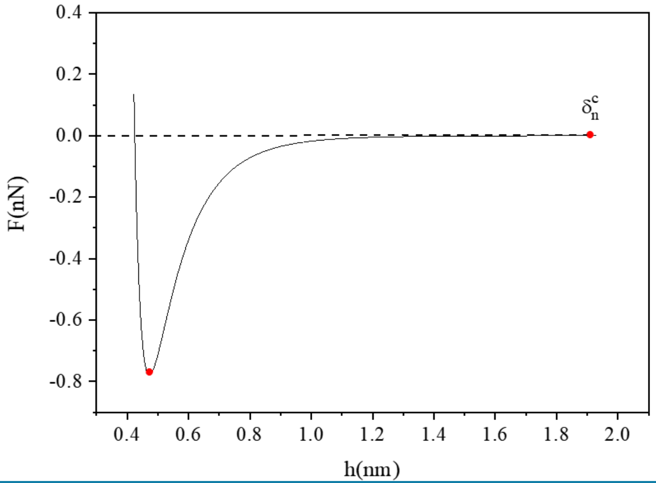
- Maximum force： 3.74~8.42 nN
- Adhesive strength： 47.4~106.7 MPa

Results (11 samples)

➢ Interface adhesive force (MD simulation)

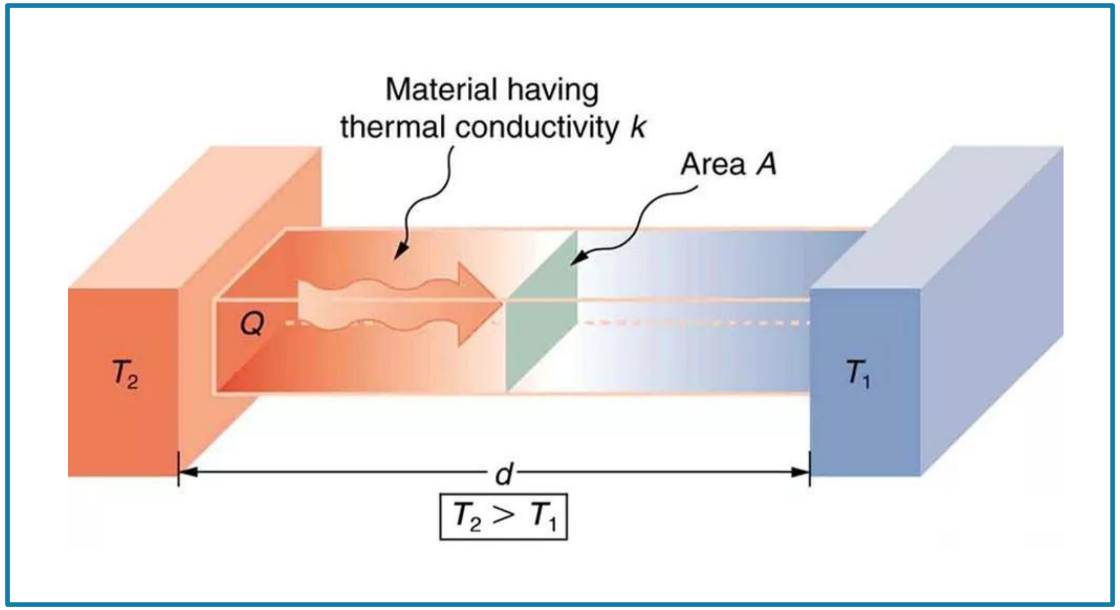


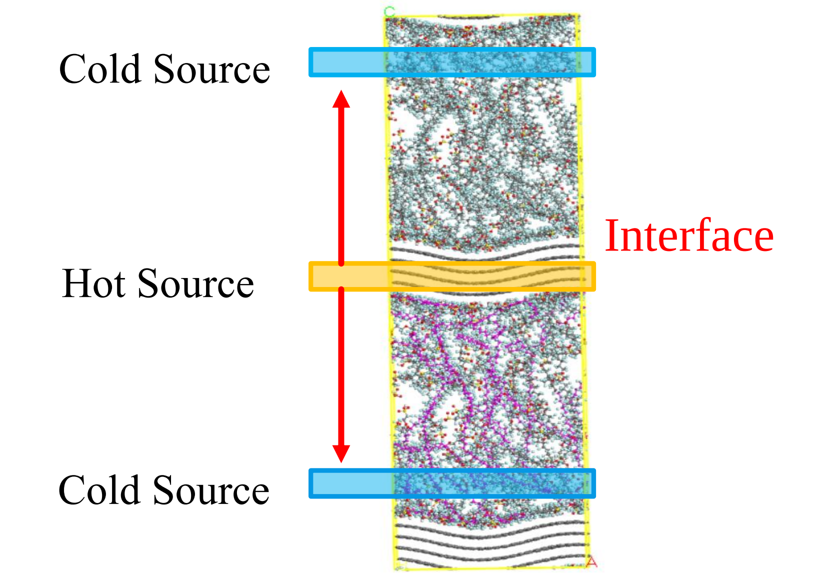
Molecular model



Force-displacement curve

➢ Interfacial thermal conductivity





$$Q = \frac{\kappa A t \Delta T}{x} \qquad J = -\kappa \frac{dT}{dx}$$

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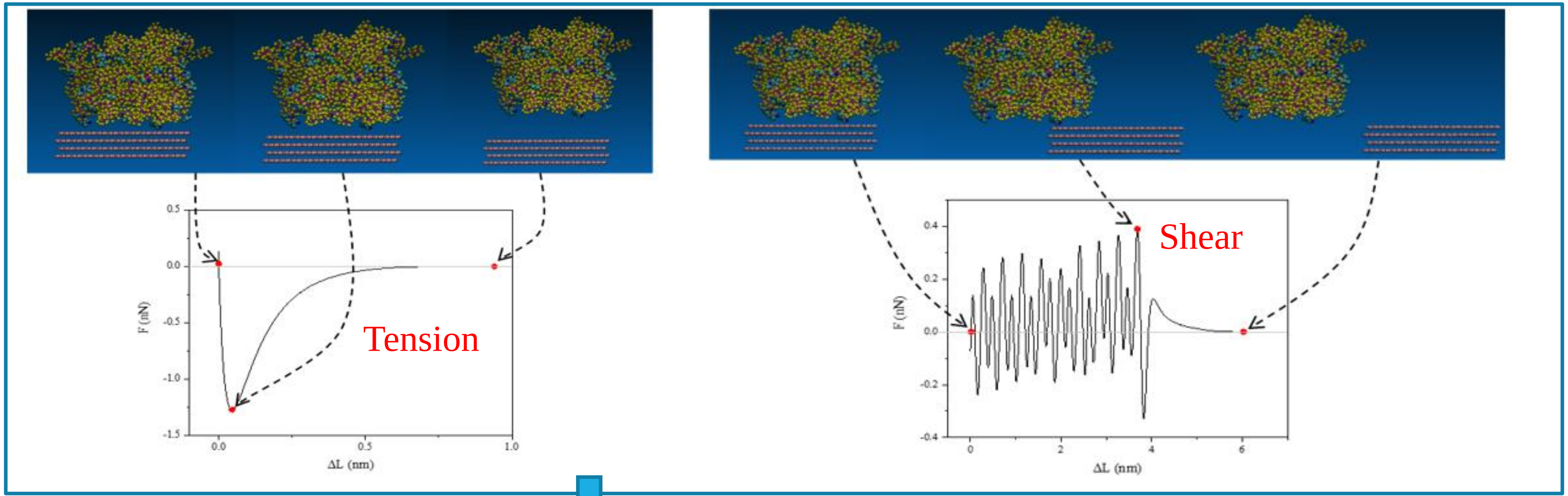
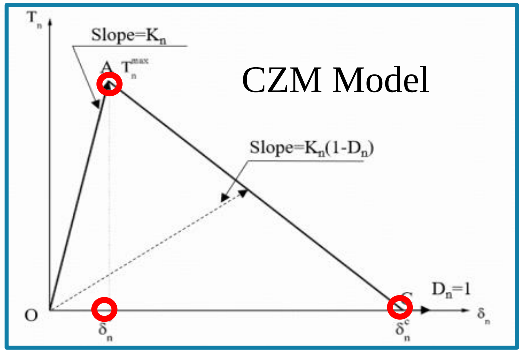
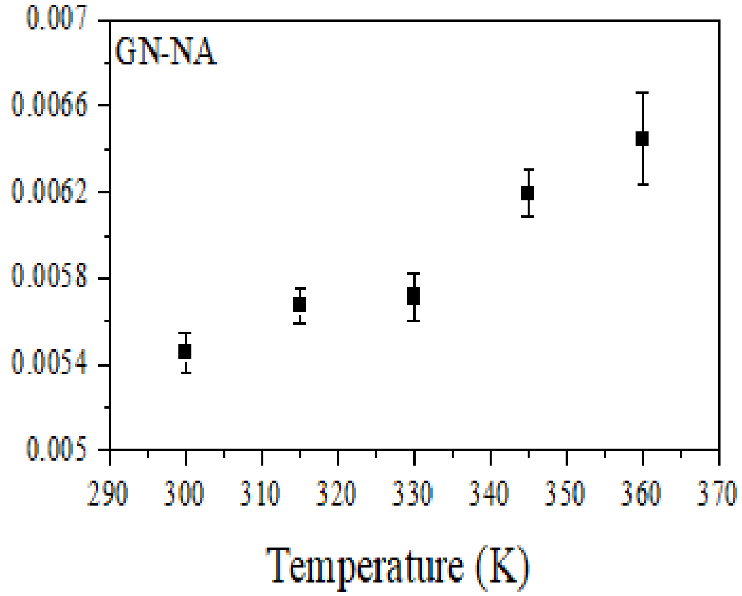
Interface type & mechanical parameters



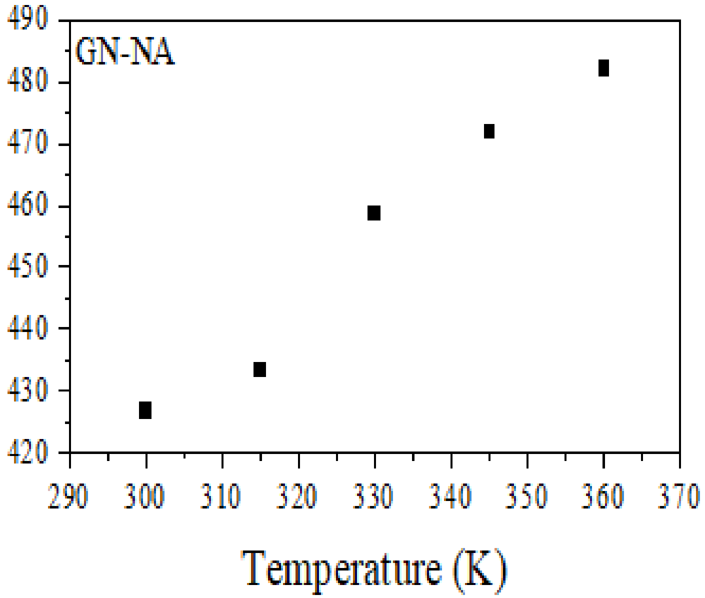
Model	Binding energy (kcal/mol)	T_t^{max} (MPa)	T_s^{max} (MPa)	$\delta_t{}^*$ (nm)	$\delta_s{}^*$ (nm)	$\delta_t{}^c$ (nm)	$\delta_s{}^c$ (nm)
Type I	11.12	13.58	5.44	0.044	2.356	0.925	5.826
Type II	21.47	24.73	6.81	0.046	3.544	0.927	5.657
Type III	38.73	43.57	16.87	0.046	3.689	0.940	6.029



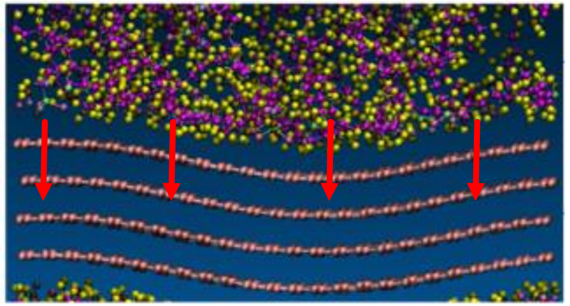
➢ Interfacial thermal conductivity

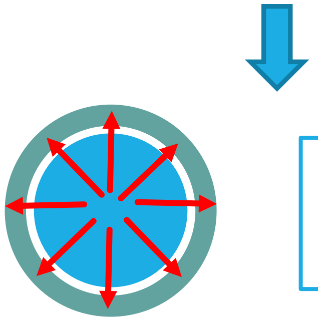


Interfacial thermal conductivity



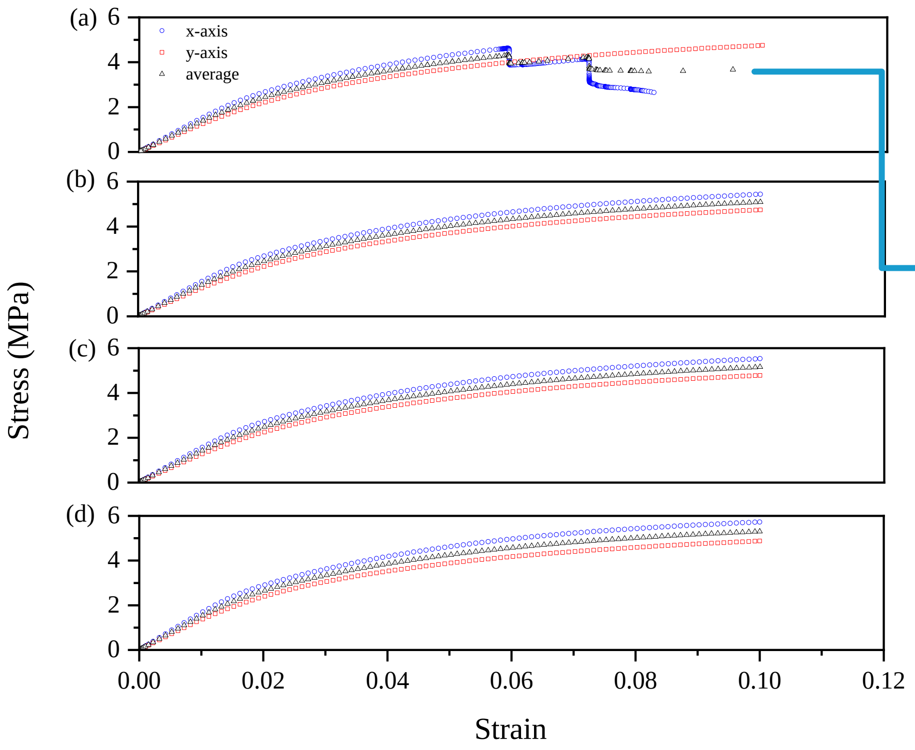
Interfacial binding energy





$$J = -\kappa \frac{dT}{dx}$$

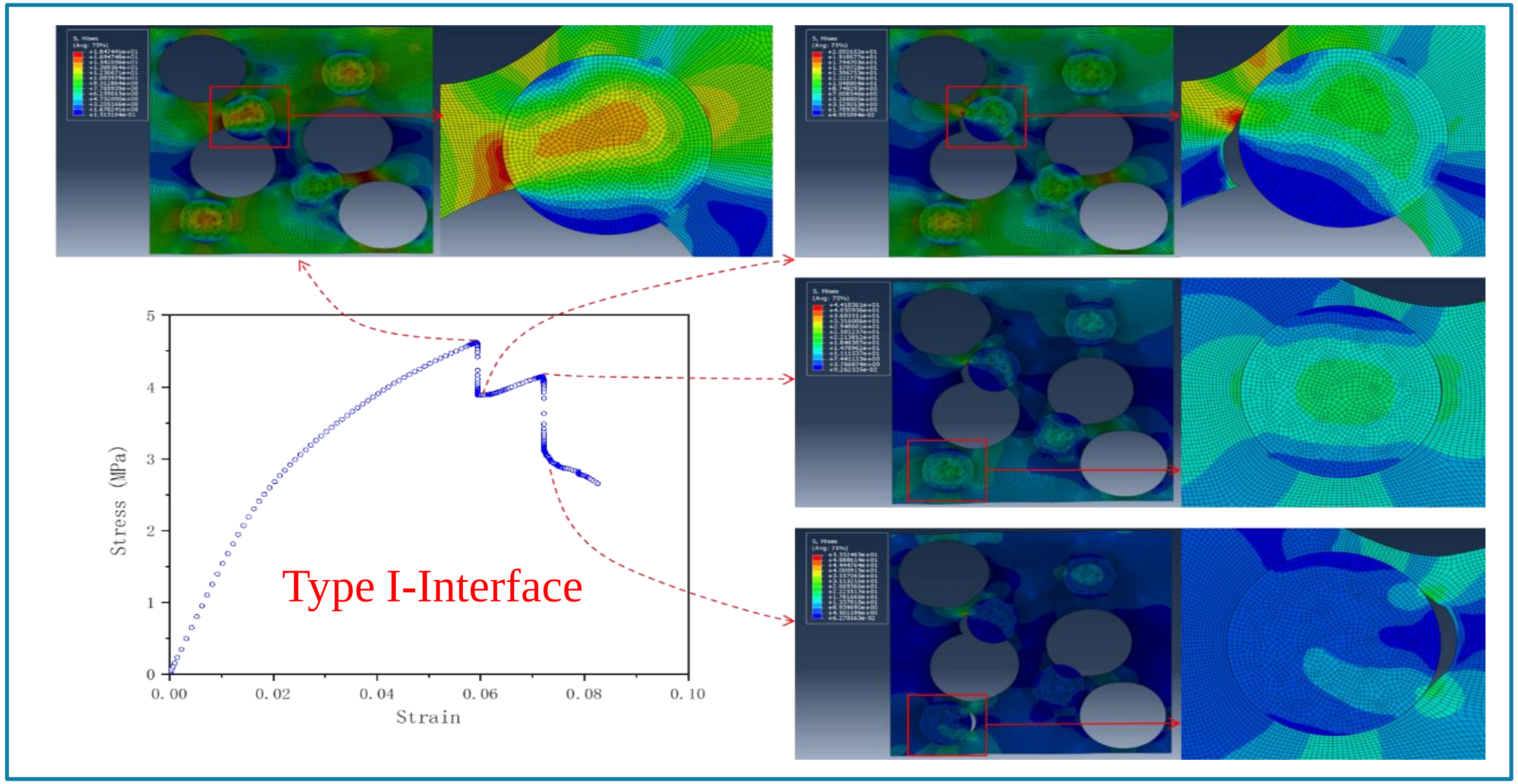
➢ Electrode's mechanical property

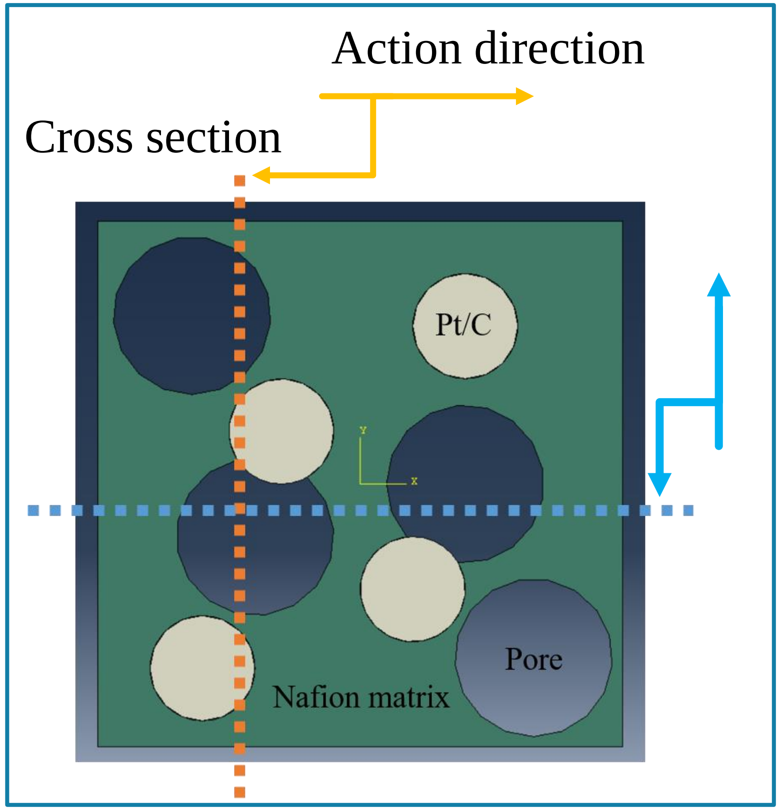


Interfacial strength $\propto$ Elastic modulus

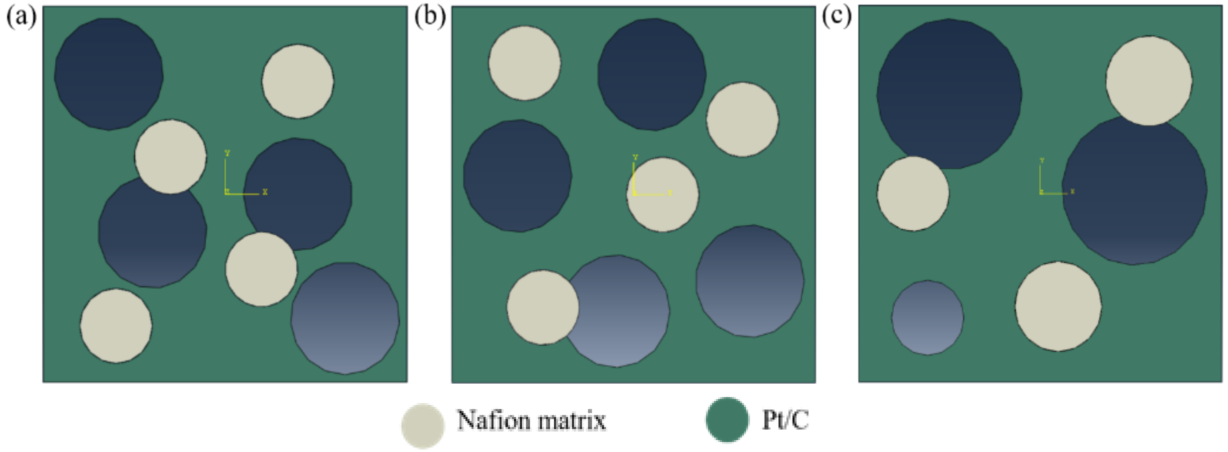
Interface	E_b(kcal/mol)	E_0/MPa	σ_y/MPa	ε_y/%	ν
Type I	11.12	138.38	1.40	1.018	0.291
Type II	21.47	139.02	1.41	1.014	0.290
Type III	38.73	141.16	1.44	1.021	0.284
Type IV	∞	153.30	1.53	0.934	0.262

Delamination evolution ⇄ Sudden stop in stress





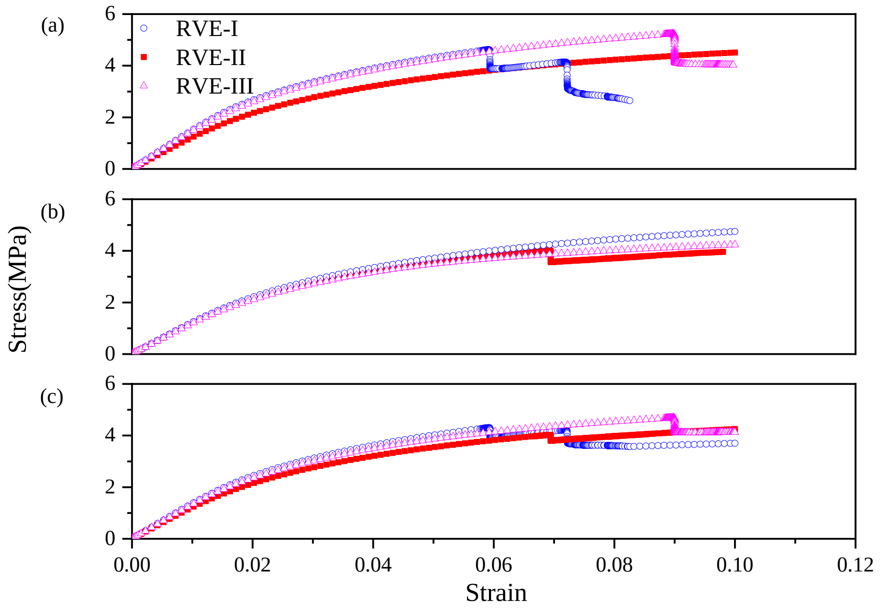
➢ **Electrode's** mechanical properties



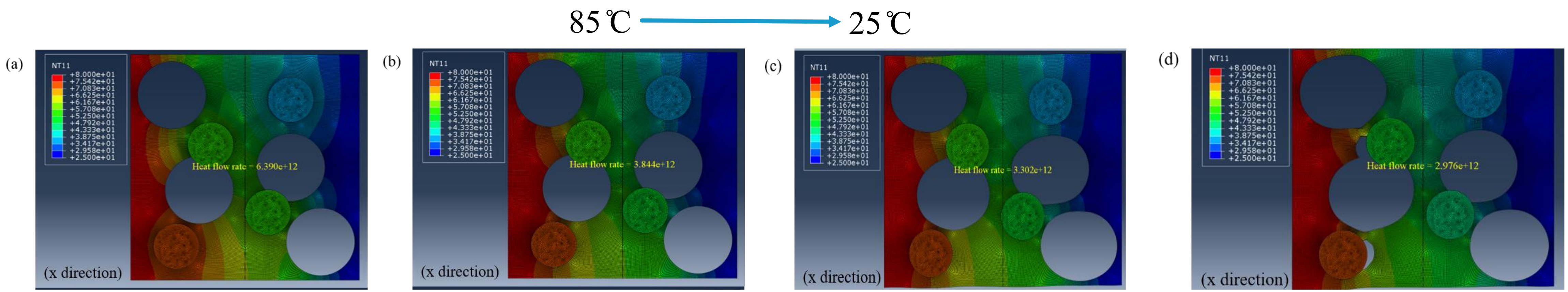
RVE I   RVE II   RVE III

Model	**E_0/MPa**	**σ_y/MPa**	**ε_y/%**	**ν**
RVE I	138.38	1.40	1.02	0.291
RVE II	123.77	1.25	1.01	0.303
RVE III	134.27	1.38	1.03	0.239

Three RVE models with Type I-Interface



➢ **Electrode's** thermal conductivity



Type IV   Type II   Type II & 1% strain   Type I

Interface	ITC ($W \cdot m^{-1} \cdot K^{-1}$)	Strain	Porosity (%)	k_c($W \cdot m^{-1} \cdot K^{-1}$)
Type IV	0	0	28	0.1121
Type II	MD results	0	28	0.0735
Type II	MD results	0.1	30	0.0632
Type I	MD results	0.085	31	0.0541

MD results

Temperature (°C)	ITC ($W \cdot m^{-1} \cdot k^{-1}$)
25	0.0054
45	0.0056
65	0.0057
80	0.0064

➢ Electrode's thermal conductivity

- Effective medium theory

$$\sum_{i=1}^{s} f_i \frac{k_c - k_i}{k_i + (z/2 - 1)k_c} = 0$$

- f_i volume fraction (ith phase)
- k_i thermal conductivity (ith phase)
- k_c thermal conductivity (composite)

Comparison

Interface	**Porosity (%)**	**k_c(W·m^{-1}·K^{-1}) (Present)**	**k_c(W·m^{-1}·K^{-1}) (EMT)**
Type II	28	0.0735	0.093
Type II	30	0.0632	0.085
Type I	31	0.0541	0.081

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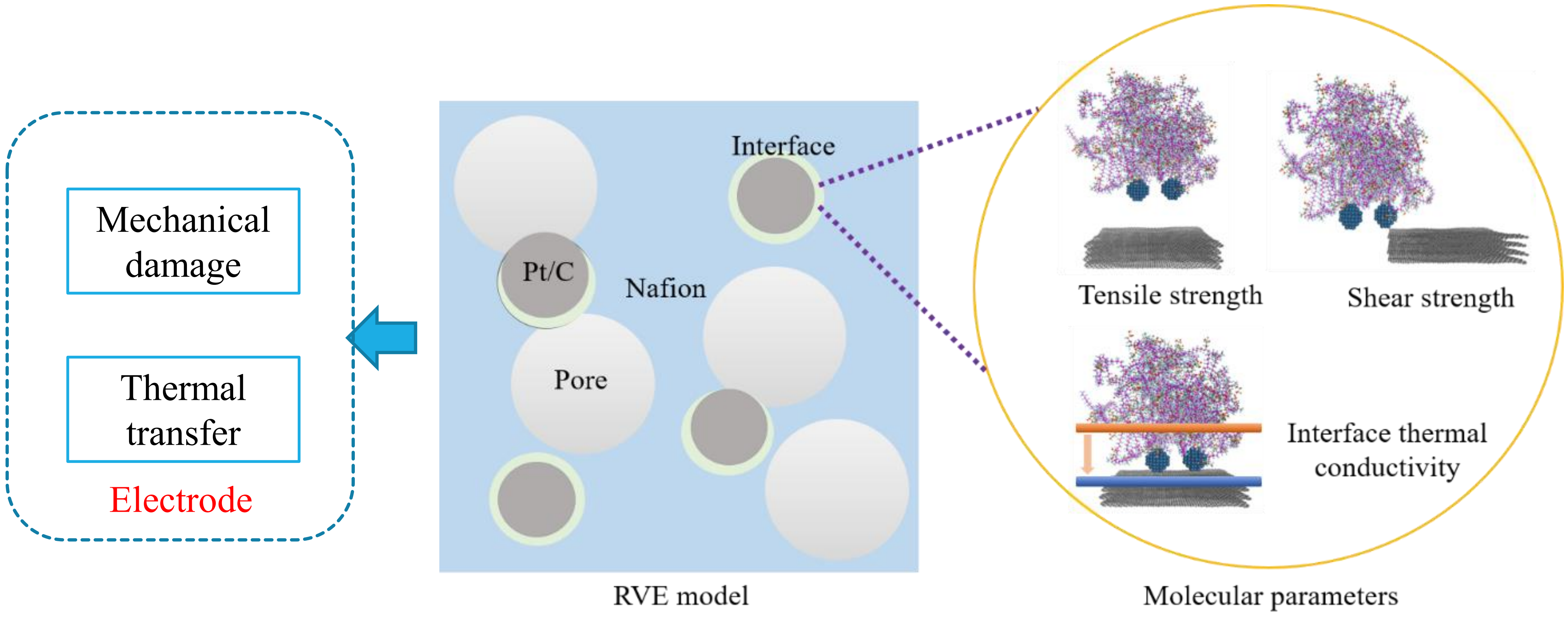
Thermomechanical Properties of Damaged Electrode



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Thank You For Your Attention!