

PROCEEDINGS

Symmetry-Breaking Guided Formation and Regulation of Interfacial Polymerization for Functional Membrane Green Manufacturing: In-situ Monitoring and Modeling

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ABSTRACT

Interfacial polymerization (IP) is a critical technology for fabricating high-performance functional membranes. IP offers a low-energy, fast-curing alternative to traditional thermal processing. However, achieving precise control over micro-scale topology remains challenging due to the complex reaction kinetics under spatial confinement.

This study presents a solvent engineering-based strategy to regulate the IP process, aligning with the goals of low-emission and energy-efficient fabrication. We investigated the effects of solvent polarity on membrane formation at the confined interface in the model system of tetraethylenepentamine (TEPA) and hexamethylene diisocyanate (HDI). Through the in-situ Raman spectroscopy coupled with molecular dynamics (MD) simulations, our work reveals the hierarchical topology regulation mechanism [1]. At the molecular level, we demonstrate how solvent polarity directs molecular orientation at the interface due to the interfacial symmetry breaking, captured as real-time spectral fingerprints [2,3]. At the mesoscale, the solvent-controlled orientation affects the reaction kinetics collaborating with coupled reaction-diffusion processes significantly modulating the resulting crosslinking microstructure and morphology of the formed membranes. These kinetic factors determine the local concentration gradients and mass transport phenomena that ultimately shape the material properties. Finally, at the macroscopic scale, the self-limiting effect inherent to interfacial polymerization reactions dominates the membrane growth termination mechanism, thereby controlling the final membrane thickness and overall structural integrity. Based on these findings, we establish a quantitative correlation model linking solvent effect to interfacial molecular arrangement and reaction-diffusion processes, achieving precise control over membrane thickness, porosity, and surface morphology of polyurea microcapsules for diverse controlled-release and intelligent sensing applications.

This study provides novel theoretical insights and strategies for rational design and functional fabrication of interfacial polymerization membranes, facilitating the expansion of this technology into frontier fields such as sensor, smart-responsive and biomedical functional materials.

KEYWORDS

Interfacial polymerization; symmetry-breaking; topology regulation; reaction-diffusion

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