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Thesis title: Exploration of mechanical response of polymeric gels via molecular dynamics.

November 28, 2025

Here it goes the abstract. 250 word

Keywords: smart polymers, nanomaterials, responsive materials,

Introduction

Hydrogels are crosslinked polymer networks filled with aqueous solvents, resembling biological tissues and providing adjustable mechanical properties. They have extensive uses in tissue engineering, bioadhesives, tissue repair, and soft robotics. Numerous hydrogels exhibiting exceptional mechanical properties, including double network hydrogels, are synthesized using free radical polymerization. It is generally commenced by the generation of free radicals from initiators such as peroxides, ketones, and azo compounds, activated by heat or light. Nonetheless, these procedures frequently exhibit slow speeds and necessitate extended curing durations in conventional batch synthesis. Efforts to accelerate gelation by augmenting initiator concentrations or applying external energy often undermine the mechanical characteristics of the hydrogels (Cheng et al., 2025).

Ultrasound, a high-frequency acoustic wave, has been extensively employed in chemical engineering domains. Acoustic cavitation techniques have been extensively employed to enhance chemical reaction rates and diminish energy consumption by controlling chemical synthesis in the processing of materials including oil, food, and wastewater. Researchers have proposed techniques for designing useful materials by utilizing particle mobility and flow induced by ultrasound. Ultrasound-mediated streaming flow in a solution can facilitate quick chemical mixing for the creation of functional nanoparticles or homogenize the chemical concentration of an electrolyte to prevent precipitation (Kang et al., 2024).

Recently, an ultrasound technique has emerged as a method for fabricating tissue-like materials for biomedical engineering applications. Reports indicate that spatial patterning of cells via surface sonic waves may facilitate the development of in vitro tissues with therapeutic efficacy for tissue regeneration at defect sites. Replicating both the cellular architecture and the physical qualities of the tissue is essential in tissue engineering (Kang et al., 2024).

Poly(N-isopropylacrylamide) (PNiPAAm) is soluble in water at ambient temperature but transitions from a hydrated coil to a dehydrated globule at its lower critical solution temperature (LCST) of around 32°C, which is near body temperature. Due to their temperature sensitivity and excellent biocompatibility, PNiPAAm-containing materials have been extensively employed in drug delivery systems and temperature-targeted therapeutic applications (Lin et al., 2017).

Problem statement In real context

State of the art A brief introduction

Justification of the proposal.

Proposed material

a. Polímero(s) base b. Nanomaterial(es) (aditivo(s) funcional(es)) c. Mecanismo o mecanismo funcional (si aplica) d. Comportamiento inteligente esperado (si aplica, por ej.: sensible a estímulos, autor-reparable, piezoeléctrico, biodegradable, memoria de forma, electroactivo) e. Explique la base científica del material y su propósito. Cuando corresponda incluya: • Modelo conceptual • Esquema del mecanismo • Principio de activación físico o químico • Figuras adaptadas o correctamente citadas

Fabrication technique

Describa la ruta prevista de manufactura, por ejemplo: • Electrospinning • Extrusión • Impresión 3D • Moldeo por solvente (solvent casting) • Modificación superficial • Polimerización in situ • Otra (especificar) • Incluya una breve justificación de la técnica seleccionada.

Characterization

Identifique las evaluaciones necesarias para confirmar la funcionalidad: • Propiedades mecánicas • Estabilidad o transiciones térmicas • Caracterización morfológica • Propiedades eléctricas/ópticas (si aplica) • Biodegradación o estudios de envejecimiento • Validación de respuesta a estímulos

Validation of vialidad

Discuta: • Viabilidad económica • Escalabilidad y capacidad de manufactura • Consideraciones toxicológicas o de bioseguridad • Restricciones ambientales o regulatorias • Potenciales riesgos y debilidades

Conclusion

samples(Gnan et al., 2017).

References

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