Modelling Dynamics of Pattern Formation in Confined Hydrogel Membranes

*Yao Xiong and Olga Kuksenok

Ph.D. Candidate, Clemson University and Associate Professor, Clemson University

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ABSTRACT: Understanding and controlling dynamics of pattern development within hydrogel membranes is critical for tailoring their permeability and fabricating a range of functional surfaces[1]. Hydrogels undergoing volume phase transition are under compression in the presence of confinements. A compression exceeding a critical value triggers mechanical instability and results in patterns formed in constrained gel membranes.[2] Herein, we focus on simulating dynamics of pattern formation in constrained three-dimensional poly(N-isopropylacrylamide) (PNIPAAm) gels via a 3D gel Lattice Spring Model (gLSM)[3, 4]. PNIPAAm gel is thermo-responsive hydrogel which has a lower critical solution temperature (LCST) at about 32℃.[5] Gel membranes with clamped edges are cooled down to various temperatures. Membranes remain flat until the depth of quenching temperature is significant. The pattern observed in membranes is buckling with sinusoidal profile along the length. We characterize the dynamics of pattern formations for a range of applied quenching temperatures and for the gels with various physical properties. We show that an increase in the depth of quenching results in an increase of the amplitude of the pattern; however, the wavelength remains constant. We focus on the effects of the size of the gel sample and its crosslink density on both the criteria of pattern formation and the characteristic features of the steady patterns. Our simulation results show an agreement with analytical calculations that we perform in the limiting case based on Föppl-von Kármán equations[6]. We demonstrate that the topology and the distribution of polymer volume fraction ϕ , which is related to the permeability of gel membranes, can be controlled by altering temperature, sample size, and crosslink density. Meanwhile, the onset and features of the observed patterns, including wavelength and amplitude, are associated with swelling ratio of free gels, α_a.

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