Assembly of tubes in the stretching-dominated limit

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The self-assembly of tubular structures is a fundamental process in both biological systems and nanotechnology, necessitating theoretical models to understand and control its outcomes. In this study, we investigate tubule assembly using Classical Nucleation Theory (CNT) and an elastic model within the stretching-dominated regime [1]. We identify the conditions under which tubules form from free subunits in solution and explore the potential formation pathways. Our analysis reveals that two dimensionless parameters govern the assembly and polymorphism of tubules: the Föppl-von Karman number, which quantifies the balance between stress and bending, and a parameter which measures the relative importance of bending versus line tension. Tubule formation initiates with the spontaneous emergence of a curved square patch, followed by two distinct mechanisms: (i) curvature fluctuations, dominant in systems with high line tension, and (ii) aspect-ratio fluctuations, prevalent in systems with high bending modulus. Using non-equilibrium thermodynamics, we characterize the kinetics of tubule formation and determine the conditions influencing the final radii distribution of the assembled tubules, which may deviate from thermodynamic equilibrium. This work provides a framework for optimizing tubule assembly efficiency and controlling their structural properties, offering insights for applications in nanotechnology and materials science.

References:

[1] Carlos I. Mendoza and David Reguera, “Assembly of tubes in the stretching-dominated limit” The Journal of Chemical Physics **163** , 034905 (2025).