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Simulation of the effect of confinement in actin ring formation MARAL ADELI KOUDEHI, DIMITRIOS VAVYLONIS, Lehigh University, HAOSU TANG TEAM, DIMITRIOS VAVYLONIS TEAM — Actin filaments are vital for different network structures in living cells. During cytokinesis, they form a contractile ring containing myosin motor proteins and actin filament cross-linkers to separate one cell into two cells. Recent experimental studies have quantified the bundle, ring, and network structures that form when actin filaments polymerize in confined environments in vitro, in the presence of varying concentrations of cross-linkers. In this study, we performed numerical simulations to investigate the effect of actin spherical confinement and cross-linking in ring formation. We used a spring-bead model and Brownian dynamics to simulate semiflexible actin filaments that polymerize in a confining sphere with a rate proportional to the monomer concentration. Applying the model for different size of the confining spheres shows that the probability of ring formation decreases by increasing the radius (at fixed initial monomer concentration), in agreement with prior experimental data. We describe the effect of persistence length, orientation-dependent cross-linking, and initial actin monomer concentration. Simulations show that equilibrium configurations can be reached through zipping and unzipping of actin filaments in bundles and transient ring formation.

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