Nonlinear elastic model for faceting of vesicles with soft grain boundaries

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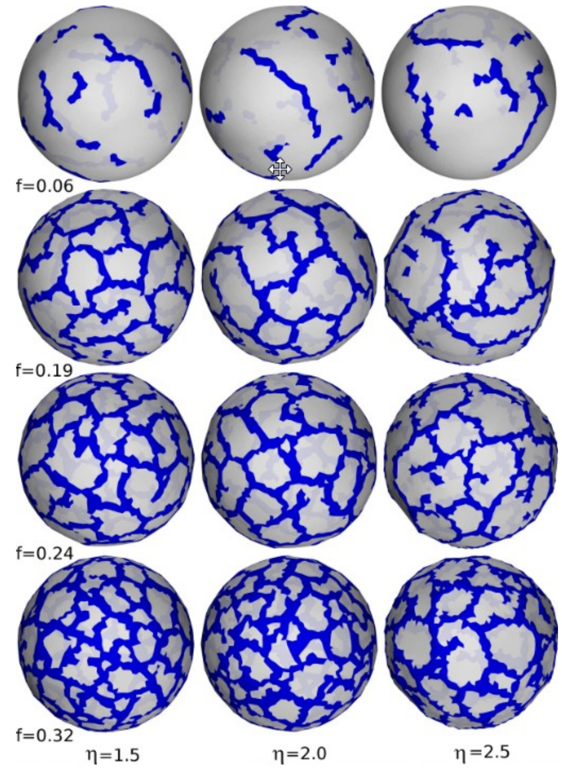
- We developed an elastic model to explore faceting of solid-wall vesicles with elastic heterogeneities. We have implemented a general non-linear elastic model to analyze faceting of solid-wall vesicles with soft domain boundaries into polyhedra other than icosahedra.

- By choosing a suitable reference metric state, we have removed the instability toward buckling into the icosahedron seeded at the twelve five-fold defects. While topological defects are still present as required by the spherical topology, their effects are treated implicitly by assuming that they collect at the boundary between facets making the vesicle wall locally soft.

- We show that faceting occurs in regions where the vesicle wall is softer, such as areas of reduced wall thicknesses or concentrated in crystalline defects.

- The long-range effect of the stress produced by the defects is substantially suppressed resulting in faceting into irregular polyhedra.

- For simplicity, we assumed that the elastic properties of a component are determined by its thickness, with the soft component being thinner. This allows us to explore the phase behavior as a function of only two parameters, relative thickness $\eta = h_{\text{hard}}/h_{\text{soft}}$ and the fraction f of the soft component. The elastic heterogeneities are modeled as a second component with reduced elastic parameters. Using simulated annealing Monte Carlo simulations we obtain the vesicle shape by optimizing the distributions of facets and boundaries. Our model allows us to reduce the effects of the residual stress generated by crystalline defects, and reveals a robust faceting mechanism into polyhedra other than the icosahedron.



Snapshots of typical vesicle shapes as a function of the thickness ratio $\eta = h_{hard}/h_{soft}$ = 1.5, 2.0, 2.5 and the fraction of the soft component f = 0.06, 0.19, 0.24 and 0.32. The soft component is shown in blue (dark) while the hard component is white (light) and slightly transparent. For clarity, width of the soft component region has been enhanced.

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