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Coupled Composition-Deformation Phase-Field Method for Lipid Membranes with Asymmetric Leaflet Compositions

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ABSTRACT

Biological membranes are structures composed of multiple lipid species and proteins. The lipids are bound only through hydrophobic interactions, creating a liquid-like structure. The plasma membrane, a lipid bilayer membrane surrounding all mammalian cells, is not homogeneous, but rather contains domains termed 'rafts,' defined as regions enriched with cholesterol and saturated lipids. These rafts are typically studied in simpler membrane systems such as Giant Unilamellar Vesicles (GUVs). Understanding how and why these rafts form is of great importance to cell biologists and immunologists, since they are involved in many important cell functions and processes including endocytosis, cell adhesion, signalling, protein organization, lipid regulation, and infection by pathogens. These raft structures also show great potential for technological applications, especially in connection with biosensors and drug delivery systems.

We present a continuum-level method for modelling phase separation (raft formation) and morphological evolution of multicomponent lipid membranes. The model applies to binary membranes with planar and spherical background geometries, simulating a nearly planar portion of membrane or entire GUV, respectively. An extension of the nearly planar case models each leaflet of the lipid bilayer separately, accounting for interactions between the leaflets. The local composition and shape of the membrane are coupled through composition-dependent spontaneous curvature in a Helfrich free energy. The composition is modelled using a phase-field method with the evolution described by a Cahn-Hilliard-type equation, while shape changes are described by relaxation dynamics. We use this model to numerically simulate the dynamics of phase separation in spherical systems and planar systems initialized with a variety of compositional and geometrical configurations.

For nearly planar bilayer systems with each leaflet having the same phase fraction, we find that domains align to reduce the interaction energy, as expected. However, when the coupling effect is stronger, this alignment occurs more quickly and more precisely,

showing that the coupling affects the dynamics. For bilayer systems with leaflets having different phase fractions, domains still show a tendency to align, though the phase boundaries on the two leaflets are forced to be offset as a result. The coupling between leaflets is found to influence morphological evolution; in some cases the equilibrium morphological phase observed using this bilayer model is very different from what was observed with our simpler monolayer model using similar parameters and initialization. In nearly spherical systems, spontaneous curvature can influence the compositional evolution, where a phase with positive spontaneous curvature can become the matrix as if it is a majority phase, even when it is in fact a minority phase. This is a result of the intrinsic positive curvature of the spherical surface. Systematic studies of these systems will be presented.

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