Simulation studies of the properties of lung surfactant monolayer-bilayer aggregates

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In the lungs, the gas exchange takes place at the air/water interface of the alveoli. Lung surfactant, a mixture of lipids and proteins, forms a monomolecular film at this air/water interface. The monolayer dramatically lowers the surface tension, which stabilizes the globular alveoli against Laplace pressure and reduces the work of breathing. On interface compression during exhalation, the monolayer surface density increases, and the surface tension decreases. On interface expansion during inhalation, however, the surface tension would increase. The ability of lung surfactant to maintain the surface tension at low values is associated with transfer of lipids between the monolayer at the interface and bilayer reservoirs in water. Surfactant proteins SP-B and SP-C mediate this transfer by providing the monolayer-bilayer connectivity. However, their exact function and the detailed structure of bilayer reservoirs are not known. We use the coarse-grained MARTINI model to perform large scale simulations of lung surfactant monolayer with bilayer reservoirs. We simulate model lipid mixtures of simplified composition with the SP-C peptide and a fragment of SP-B protein (mini-B). We study the effect of the proteins on the structure and topological transformations of the bilayer reservoirs, and characterize the stress distribution in the high curvature intermediates. We also investigate the role of bilayer reservoirs in the mechanical stability of the monolayer at the air/water interface under varying surface tension.