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Shear-induced lamellar to vesicle transition in DDAB lipids.[1]
SUBAS DHAKAL, Department of Biomedical and Chemical Engineering, Syracuse University, RADHAKRISHNA SURESHKUMAR, Department of Biomedical and Chemical Engineering and Department of Physics, Syracuse University — A detailed knowledge of the response of lipid vesicles and lamellar phases to an externally applied stress is essential to understanding many important cellular processes and cell functions. Using molecular dynamics simulations, we study self-assembly and shear flow dynamics of didodecyldimethylammoniumbromide (DDAB) lipids in water. Simulations show various self-assembled structures such as micelles, vesicles and lamellae depending upon the concentration of DDAB. Shear flow simulations show tumbling dynamics of vesicles and shear-induced structure formation resulting from a lamellar to multi-lamellar vesicle transition above a critical shear rate. The role of vesicle shape and imperfections in the lamellar phase on lamellar to vesicle transition will be discussed.

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