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Coarse grained molecular simulations of melting kinetics of DPPC vesicles[1] LARA A. BOLLING-PATEL, JAMES T. KINDT, Emory University — Phase transitions in unilamellar vesicles are of particular interest as the increase in permeability of lipid bilayers around the main phase transition temperature makes them candidates for drug encapsulation and temperature-responsive delivery. We study the transition between the gel and fluid phases of a unilamellar vesicle of MARTINI coarse grain DPPC lipids with a diameter of 40 nm following temperature jumps from 280 K to temperatures near the transition temperature of 295 K. At 290 K and 295 K vesicles show single exponential melting kinetics in qualitative agreement with the early stages of melting measured in IR temperature-jump experiments. These trajectories exhibit partial melting over 500 ns, accompanied by a decrease in the number of gel domains from 8 domains in the initial faceted structure to 5 and 3 respectively. Melting at 295 K results in a shape change to an asymmetric structure that appears to be transforming into an oblate solid. Complete melting is seen for temperature jumps to 300 K and 310 K, in which cases vesicles undergo shape transitions into prolate dumbbell shapes. The shape changes that accompany the phase transition indicate that the phase transition kinetics are correlated to changes in curvature.

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