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Anomalous Freezing Behavior of Nanoscale Liposomes[1] ERIC SPANGLER, MOHAMED LARADJI, University of Memphis, SUNIL KUMAR, IIT Madras, Chennai, India — Experiments have shown that the melting transition of small liposomes is broadened when compared to large vesicles or planar membranes. Despite their significant biological and biomedical importance, theoretical and computational studies of the phase behavior and structural properties of small liposomes have been limited. Presented here is a systematic computational study of the phase behavior and structural properties of liposomes using a recently developed coarse-grained particle-based model. Great assiduity was given on the effect of liposome diameter on their thermal and structural properties. Below the melting transition, liposomes are faceted with the gel facets separated by "grain" boundaries that are in the fluid phase. In agreement with experiments, we found that the melting transition is significantly broadened as the liposome diameter is decreased and that the heat capacity exhibits two distinct peaks for diameters less than 33 nm, an indication of a decoupling of the melting transition of the two leaflets. This decoupling is clearly demonstrated by the chain order parameters of the two leaflets, which show that the upper leaflet undergoes a melting transition before the inner leaflet.

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