

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Simulating Domain Formation and Fusion in Lipid Bilayers MARK

STEVENS, Sandia National Laboratories — The lipid dynamics is the source of the variety of membrane structures and dynamics found in cells. Many of the interesting phenomena of biomembranes involve time scales of at least microseconds, which have been beyond simulations until recently. Coarse-grained models of lipid molecules have been developed to reach these long time scales and maintain the essential physical character of the molecules. Using these models in molecular dynamics simulations, time scales in the μs to ms range are treatable. As examples, simulations of domain formation and membrane fusion will be presented. In mixed lipid systems, the formation of domains is now understood to be an active component in biological processes. Our simulations reveal the dynamics of the lipid molecules that form domains in binary systems. In particular, the correlation between the two monolayers of the bilayer is dependent on the molecular structure of the lipid molecules. Membrane fusion is a fundamental process of cellular transport and infection processes. Understanding the basic principles governing membrane fusion has many important consequences. The coarse-grained molecular dynamics simulations show how lipid molecular structure influences the fusion process.

Mark Stevens
Sandia National Laboratories

Date submitted: 21 Nov 2005

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