Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Application of Small-Angle Neutron and X-ray Scattering in Determining Lipid Bilayer Structure[1] JIANJUN PAN, FREDERICK A. HEBERLE, Neutron Scattering Science Division, Oak Ridge National Laboratory, NORBERT KUCERKA, Canadian Neutron Beam Centre, National Research Council, Chalk River, Ontario, Canada, STEPHANIE TRISTRAM-NAGLE, Department of Physics, Carnegie Mellon University, MICHELLE SZYMANSKI, MARY KOEPFINGER, Douglass Residential College, Rutgers University, JOHN KATSARAS, Neutron Scattering Science Division, Oak Ridge National Laboratory — Accurately determining lipid structure in biologically relevant fluid bilayers is not straightforward. We have recently developed a hybrid experimental/computational technique (i.e., the scattering density profile, or SDP model), which exploits the fact that neutron and X-ray scattering are sensitive to different bilayer thicknesses - the large difference in neutron scattering length density (SLD) between proteated lipid and deuterated water defines the overall bilayer thickness, while X-ray scattering resolves the headgroup-headgroup distance due to the large scattering contrast between the electron-rich phosphate groups and the hydrocarbon/aqueous medium. A key step in the SDP analysis is the use of MD simulations to parse the lipid molecule into fragments whose volume probability distributions follow simple analytical functional forms. Given the appropriate atomic scattering lengths, these volume probabilities can simultaneously predict both the neutron and X-ray SLD profiles, and hence the scattering form factors. Structural results for commonly used phosphatidylcholine and phosphatidylglycerol lipids will be given.

[1]This work acknowledges the support of ORNL, NIST, and Cornell High Energy Synchrotron Source.

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Date submitted: 26 Nov 2011 Electronic form version 1.4