Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Experimental and theoretical studies of collapsed fatty-acids Langmuir monolayers[1] WEI BU, CHRIS LORENZ, ALEX TRAVESSET, Iowa State University and Ames Lab, DAVID VAKNIN, Ames Lab and Iowa State University, SUSHIL K. SATIJA, NIST Center for Neutron Research, National Institute of Standards and Technology — Long-chain Langmuir monolayers collapse by exploring the third dimension after being compressed beyond the point of densely packed chains. Recent experimental investigations using surface sensitive X-ray and neutron techniques have shown that arachidic acid (AA) monolayers, spread on pure water surfaces, collapse by forming a trilayer structure that exhibits a remarkable degree of crystalline order. Similar experiments of AA spread on $CaCl_2$ solutions show that the collapsed film consists of a mixture of hydrophobic bilayer domains (where hydrocarbon chains are in contact with water) and trilayer domains. Under suitable experimental conditions, monolayer collapse on $CaCl_2$ solution can produce an almost pure bilayer phase. We present atomistic simulations that account for the role of water, ion binding, and hydrocarbon chain conformations to better understand these experimental results.

[1]Work at Ames Lab was supported by DOE OBESC under contract # 4-7405-Eng-82, partially funded from NSF, DMR-0426597.

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Date submitted: 21 Nov 2006 Electronic form version 1.4