Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Molecular dynamics of binary and ternary nanodroplets with a miscibility gap[1] GERALD WILEMSKI, FAWAZ HRAHSHEH, Missouri University of Science and Technology — The structure of nanodroplets plays an important role in many natural processes including particle nucleation and aerosol formation in the atmosphere. Among other factors, chemical miscibility and surface tension strongly affect the structure of multicomponent nanodroplets at low temperature. Here, we investigate the structure of water/nonane and water/butanol/nonane nanodroplets using molecular dynamics (MD). Our MD results confirm our theoretical predictions of nonspherical nanodroplet (Russian-Doll) structures at low temperatures using density functional and lattice Monte Carlo techniques. We systematically study the variation of the droplet structure with temperature and with butanol concentration.

[1]Supported by National Science Foundation Grant No. CBET-1033387.

Gerald Wilemski
Missouri University of Science and Technology

Date submitted: 11 Nov 2011 Electronic form version 1.4