Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effects of temperature on structure and mechanical properties of alkanethiol coated gold nanoparticle membranes[1] K. MICHAEL SALERNO, GARY GREST, Sandia National Laboratories — Single-nanoparticle-thick membranes have a variety of potential uses due to unique mechanical properties. While these membranes have been studied experimentally and computationally at 300K, the effects of thermal annealing on structure and properties have not been investigated. We present atomistic molecular dynamics simulations that study the effects of temperature on nanoparticle membrane properties. Nanoparticles are made of a gold core coated with organic oligomer ligands. At high grafting density, ligands with CH_3 end groups exhibit local crystallinity at 300K while those with COOH end groups orient to form dimers due to electrostatics. Both features influence membrane mechanical properties. As temperature increases ligand crystallinity and COOH affinity are disrupted, and mechanical strength is reduced. Immediately after cooling back to 300K, membranes are weaker and measures of ligand interdigitation and COOH affinity are reduced. Over time, interdigitation and end-group interactions rejuvenate and samples that undergo high-temperature annealing have mechanical properties comparable to the original membranes. The structure/property temperature dependence points to ways that membranes could be tailored for temperature-dependent/resistant properties.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's NNSA under contract DE-AC04-94AL85000.

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Date submitted: 14 Nov 2014 Electronic form version 1.4