Mechanical Properties of Two-Dimensional Alkanethiol-Coated Gold Nanoparticle Membranes

K. MICHAEL SALERNO, DAN S. BOLINTINEANU, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — Membranes formed from nanoparticle monolayers have been shown to have mechanical properties that may make them suitable for use in micro-scale devices. Metallic-core nanoparticles with short, organic ligands can form membranes with dimensions up to several micrometers, with large elastic moduli. Experimental tests of membranes with different cores and ligands indicate that ligand length as well as core-ligand and ligand-ligand interactions can influence membrane mechanical response. We use explicit-atom molecular dynamics simulations to examine the properties of membranes formed from a two-dimensional hexagonal array of alkanethiol-coated Au nanoparticles. Results are presented for nanoparticle core diameters from 4-6nm, ligand lengths of 10-18 units and carboxyl and methyl end groups, all of which influence the mechanical properties of the membranes. Knowledge of how microstructure and composition influence membrane properties could lead to efficient membrane manufacture with improved mechanical properties. 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 National Nuclear Security Administration under contract DE-AC04-94AL85000.

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