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Modeling pressure-driven assembly of polymer coated nanoparticles J. MATTHEW D. LANE, Sandia National Labs, K. MICHAEL SALERNO, U. S. Naval Research Lab, GARY S. GREST, HONGYOU FAN, Sandia National Labs — High-pressure experiments have successfully produced a variety of gold nanostructures by compressing polymer coated spherical nanoparticles. We apply atomistic simulation to understand the role of the soft polymer response in determining the pressure-driven assembly of gold nanostructures. Quasi-isentropic experiments have shown that 1D, 2D and 3D nanostructures can be formed and recovered from dynamic compression of fcc superlattices of alkanethiol-coated gold nanocrystals on Sandias Veloce pulsed power accelerator. Molecular modeling has shown that the dimensionality of the final structures depends on the orientation of the superlattice and the uniaxial loading. We describe the role of coating ligand length and grafting density, on ligand migration and deformation processes during pressure-driven coalescence of the cores into permanent nanowires, nanosheets and 3D structures. The role of uniaxial vs isotropic pressure and the effects of compression along various superlattice orientations will be discussed. Sandia National Laboratories is a multimission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

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