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Modeling Ultra-fast assembly and sintering of gold nanostructures J. MATTHEW D. LANE, Sandia National Labs, K. MICHAEL SALERNO, U. S. Naval Research Lab, GARY S. GREST, HONGYOU FAN, Sandia National Labs — We use fully atomistic simulations to understand the role of extreme pressure in the assembly and sintering of fcc superlattices of alkanethiol-coated gold nanocrystals into larger nanostructures. Recent quasi-isentropic experiments have shown that 1D, 2D and 3D nanostructures can be formed and recovered from dynamic compression experiments on Sandias Veloce pulsed power accelerator. Here, we describe the role of coating properties, such as ligand length and grafting density, on ligand migration and deformation processes during pressure-driven coalescence of metal nano 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 Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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