Abstract Submitted for the SHOCK19 Meeting of The American Physical Society

Scale and rate dependence of phase transition pressure in CdS nanoparticles J. MATTHEW D. LANE, JASON P. KOSKI, AIDAN P. THOMP-SON, ISHAN SRIVASTAVA, GARY S. GREST, TOMMY AO, BRIAN S. STOLTZ-FUS, KEVIN N. AUSTIN, HONGYOU FAN, MARCUS D. KNUDSON, Sandia National Laboratories, DANE MORGAN, MSTS — Recent efforts to improve our predictive capability for modeling rate-dependent behavior at, or near, phase transition using molecular dynamics simulations will be described. Cadmium sulfide is a well-studied material which undergoes a solid-solid phase transition from wurtzite to rock salt structures between 3 and 9 GPa. Atomistic simulations are used to investigate the dominant transition mechanisms as a function of orientation, size and rate. The CdS solid-solid phase transition is studied, for both a bulk single crystal and for polymer-encapsulated spherical nanoparticles of various sizes. The transition kinetics, mapped to nanoparticle size and loading rate, will be discussed for particles of diameter 2 to 10 nm. Finally, we will briefly review the experimental effort to investigate this transition using X-ray diffraction on the Thor platform at Sandia. Supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

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Date submitted: 28 Feb 2019

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