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Rapid Compression of Prototype Sand-like Systems using Atomistic Molecular Dynamic Simulations[1] SHINYOUNG KANG, DANIEL ORLIKOWSKI, Lawrence Livermore National Laboratory, LAWRENCE LIVERMORE NATIONAL LABORATORY TEAM — Porous materials offer many challenges in modeling because stress-chains, phase transitions and/or chemical reactions may be occurring. The granular Hugoniot response like for SiO_2 compacts and at low initial macro-densities will yield a stiffer response compared to a fully dense sample [Trunin 2001]. K. Cochrane *et al.* [2017] introduced the hypothesis of surface energy for the initial Hugoniot energy E_o using DFT constrained by a Hugoniot-stat. We test this hypothesis but allowing the system to dynamically respond within the atomistic microcanonical (NVE) ensemble. We use atomistic MD simulations using Tersoff potential for nanometer-sized granules to investigate the underlying mechanism for the SiO_2 Hugoniot. We first establish a Hugoniot baseline for a single crystal SiO_2 system, then we use nearly spherical granules of SiO_2 in close-packed configurations. Additionally, we have applied the similar methodology to SiO_2 systems with voids for comparison.

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