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Rapid Compression of Granular Systems using Atomistic Molecular Dynamic Simulations DANIEL ORLIKOWSKI, Lawrence Livermore Nat'l Lab — The dynamic material response of porous materials has many challenges in modeling because phase transitions and/or chemical reactions/products may be occuring. In particular the Hugoniot response for a granular system like SiO_2 compacts and then has a stiffer response compared to a fully dense sample [Trunin 2001]. A continuum modeling has captured the Hugoniot for these type of systems and was suggested that localized shear may induce phase transitions earlier than hydrostatic compression [Grady 2013]. Recently, atomistic molecular dynamics (MD) are starting to investigate these granular-type, porous sytems [e.g. Lane 2014]. Likewise, we use atomistic MD simulations for nanometer sized granules to investigate the underlying mechanism for the SiO_2 Hugoniot using Tersoff potentials. We first establish a Hugoniot baseline for a single crystal SiO_2 sytem. Then we use nearly spherical granules of SiO_2 in differing packing schemes—close-packed to random configurations—controlling the initial number of contact points. We discuss the observed mechanisms during the compacting and subsequent compression of the porous system. This work performed under the auspices of the U.S. Department of Energy by LLNL under Contract DE-AC52-07NA27344.

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