

Rapid Compression of Prototype Sand-like Systems using Atomistic Molecular Dynamic Simulations

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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 SiO₂ compacts and at low initial macrodensities will yield a stiffer response compared to a fully dense sample [1]. K. Cochrane *et al.* [2] introduced the hypothesis of surface energy for the initial Hugoniot energy E_0 using density functional theory (DFT) calculations 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 molecular dynamics (MD) simulations with the Tersoff potential to investigate the underlying mechanism for the Hugoniot of nanometer-sized SiO₂ granules. We first establish a Hugoniot baseline for a single crystal SiO₂ system, then we use nearly spherical granules of SiO₂ packed in simple cubic

configurations. Additionally, we have applied the similar methodology to SiO₂ systems with voids for comparison. We discuss the observed mechanisms during the compacting and subsequent compression of the porous system.

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References

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