

LA-UR-14-23884

Approved for public release; distribution is unlimited.

Title: Institutional Computing Annual Report 2014 for Project W13_sdtanoc:
Atomic-Scale Design of Shock Damage-Tolerant Nanocomposites

Author(s): Germann, Timothy C.
Cherukara, Mathew J.
Kober, Edward M.
Strachan, Alejandro

Intended for: Web

Issued: 2014-05-31

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Institutional Computing Annual Report 2014

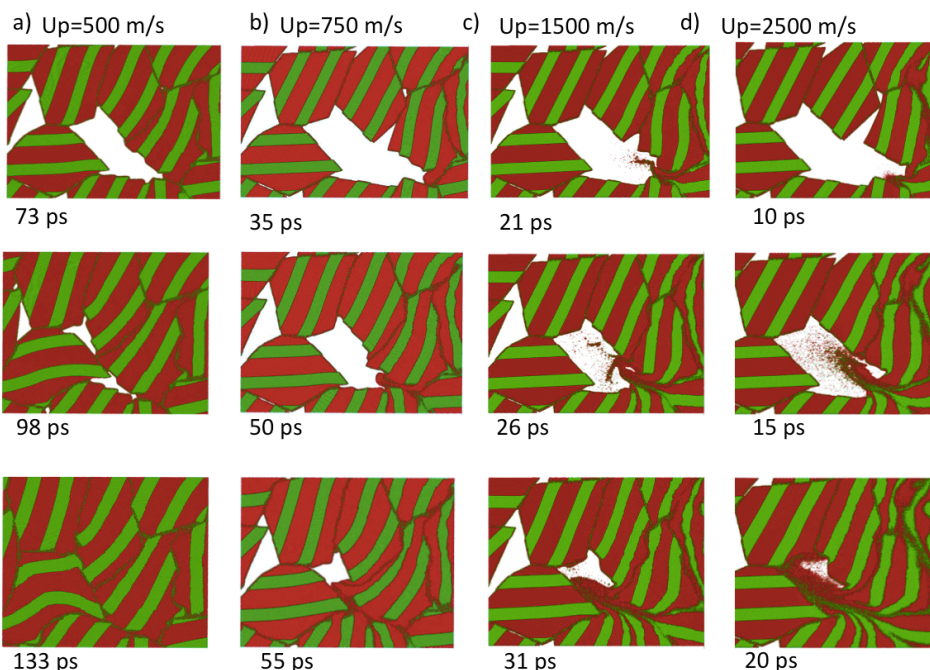
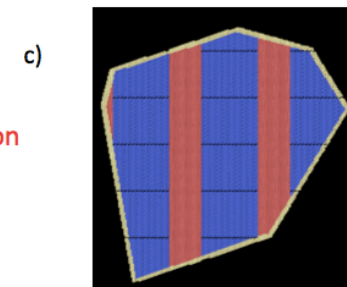
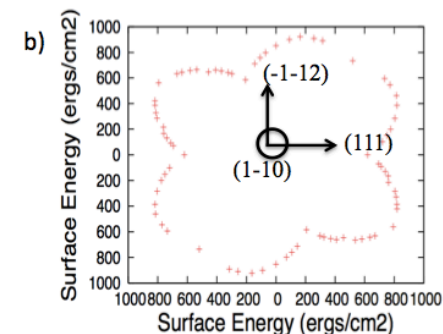
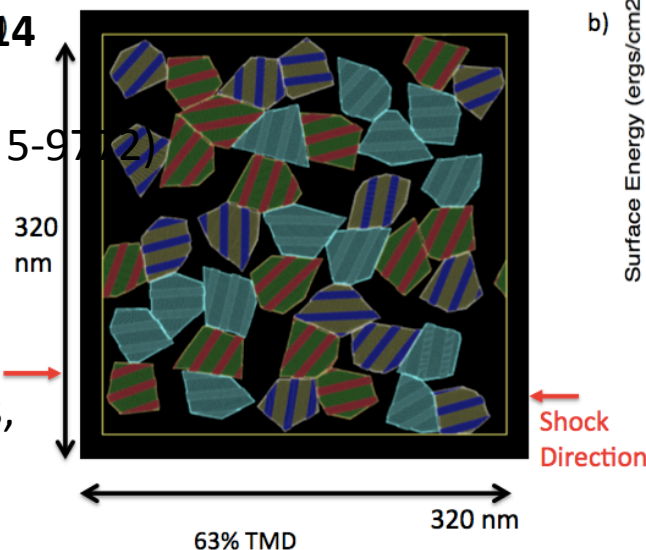
Project: W13_sdtanoc

PI: Timothy C. Germann (T-1, tcg@lanl.gov, 5-977-2)

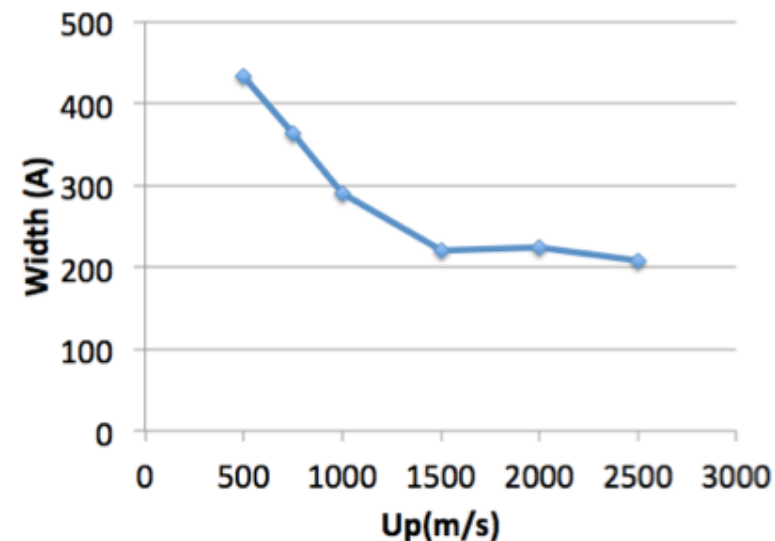
First fully atomistic simulation of a granular material.

Grains built to prefer low energy faces. Diffuse, broad shocks at low piston velocities, but, sharper shocks for stronger impacts.

Consequence of change in nature of ejecta.

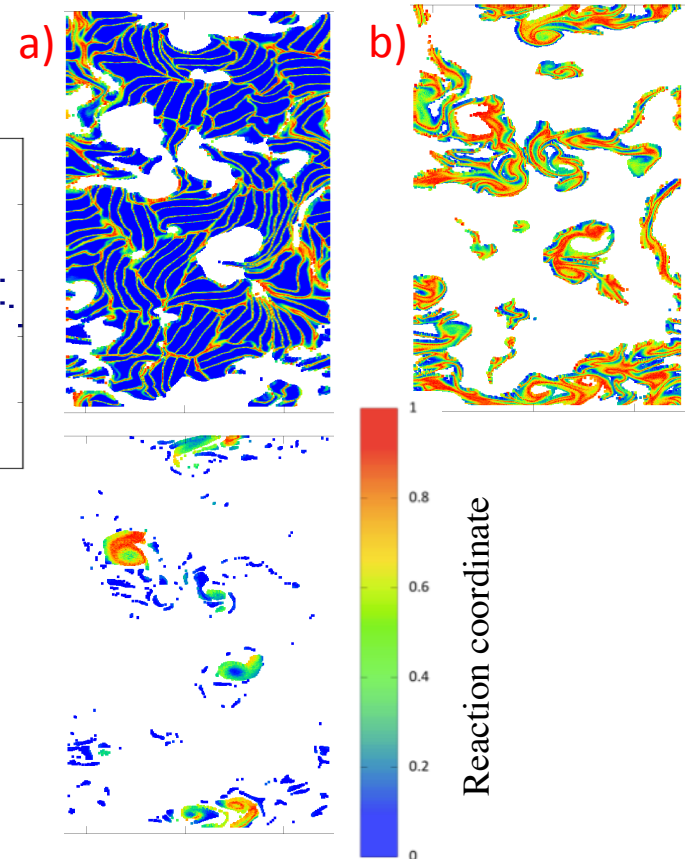
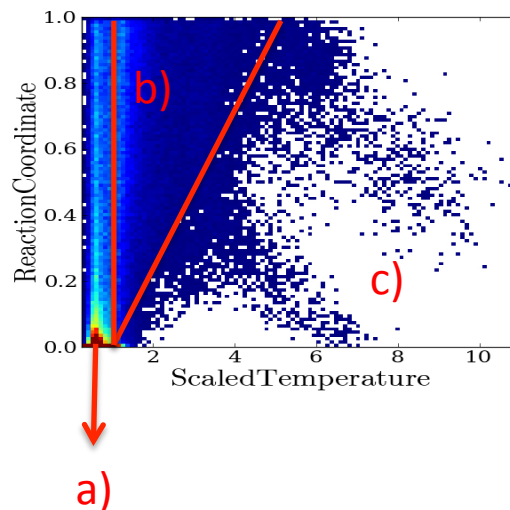


Transition in mechanism of void closure: plastic deformation → extrusion → fluid jetting

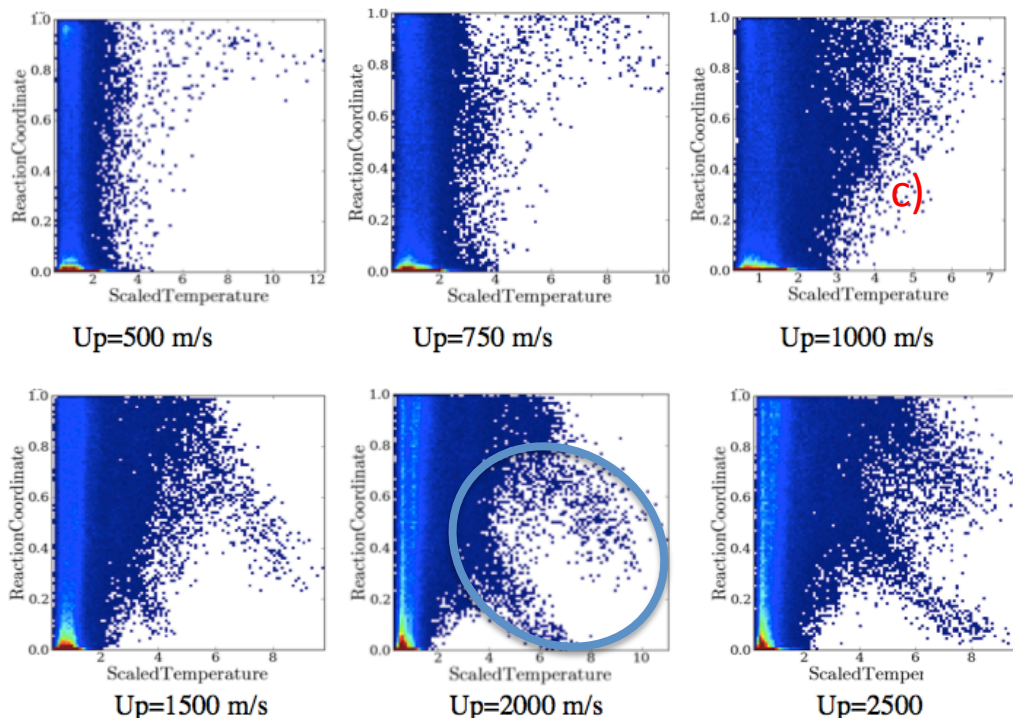


Width of the shock front as a function of piston velocity

- Porosity not just hot-spots.
 - Sites of accelerated mixing.
 - Redirects shock energy to translational K.E.
 - Provide alternate reaction paths.
 - Convective mixing as opposed to diffusive in the bulk.
- Increased non-equilibrium at higher impact velocity.



Alternate reaction paths b) and c) provided by the porosity.



Correlation maps of reaction progress against temperature showing increased non-equilibrium effects at higher impacts.