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Title: Institutional Computing Annual Report 2014 for Project W13_sdtnanoc:
Atomic-Scale Design of Shock Damage-Tolerant Nanocomposites

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Institutional Computing Annual Report 2014

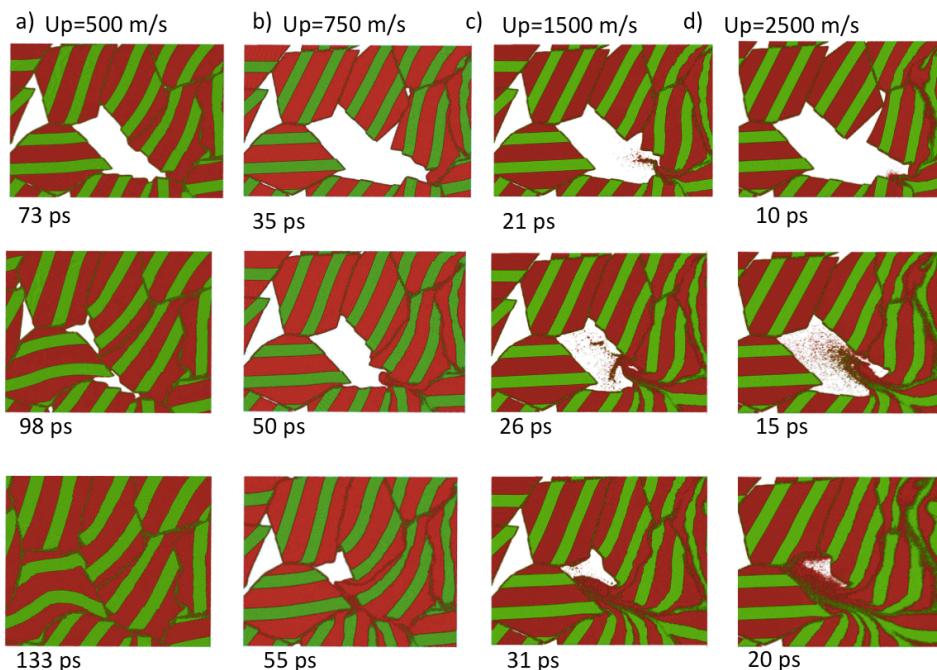
Project: W13_sdtnanoc

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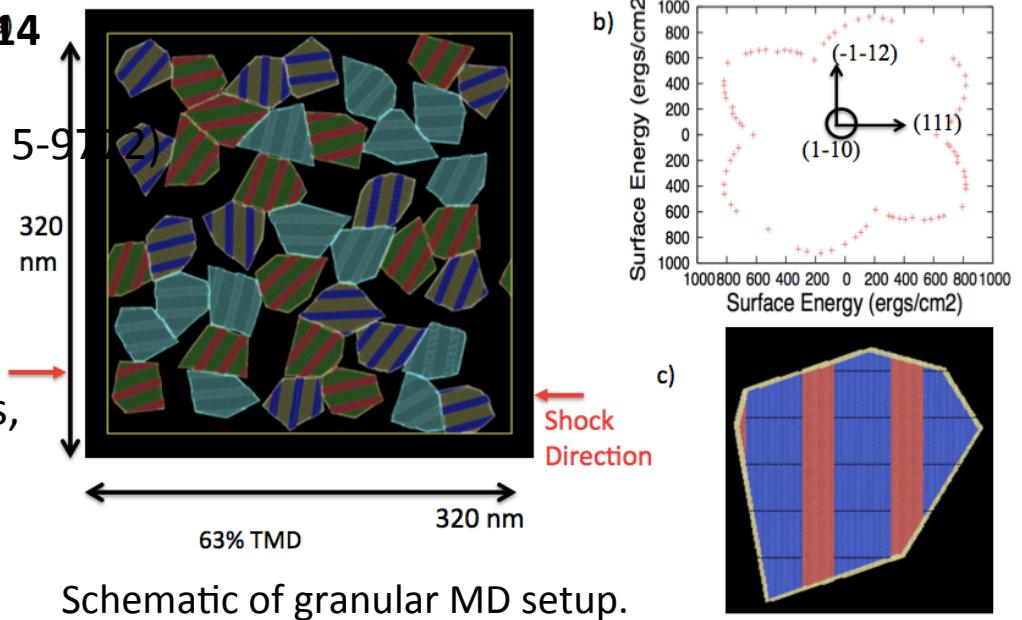
First fully atomistic simulation of a granular material.

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

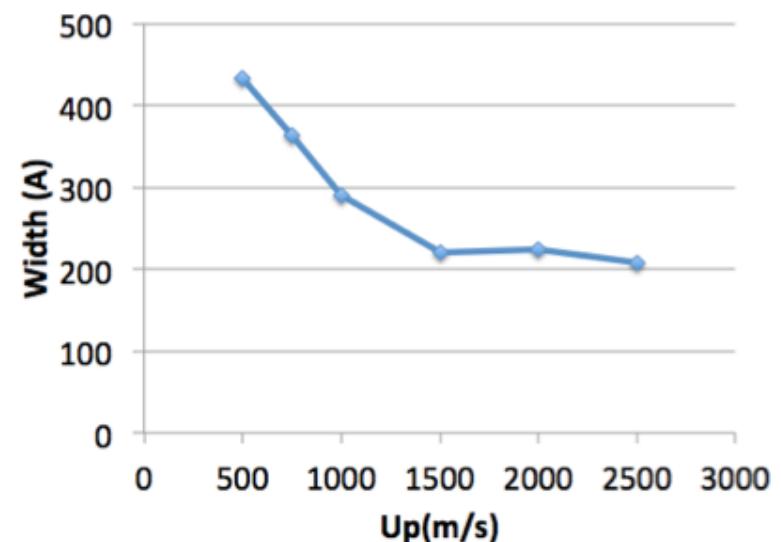
Consequence of change in nature of
 ejecta.



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

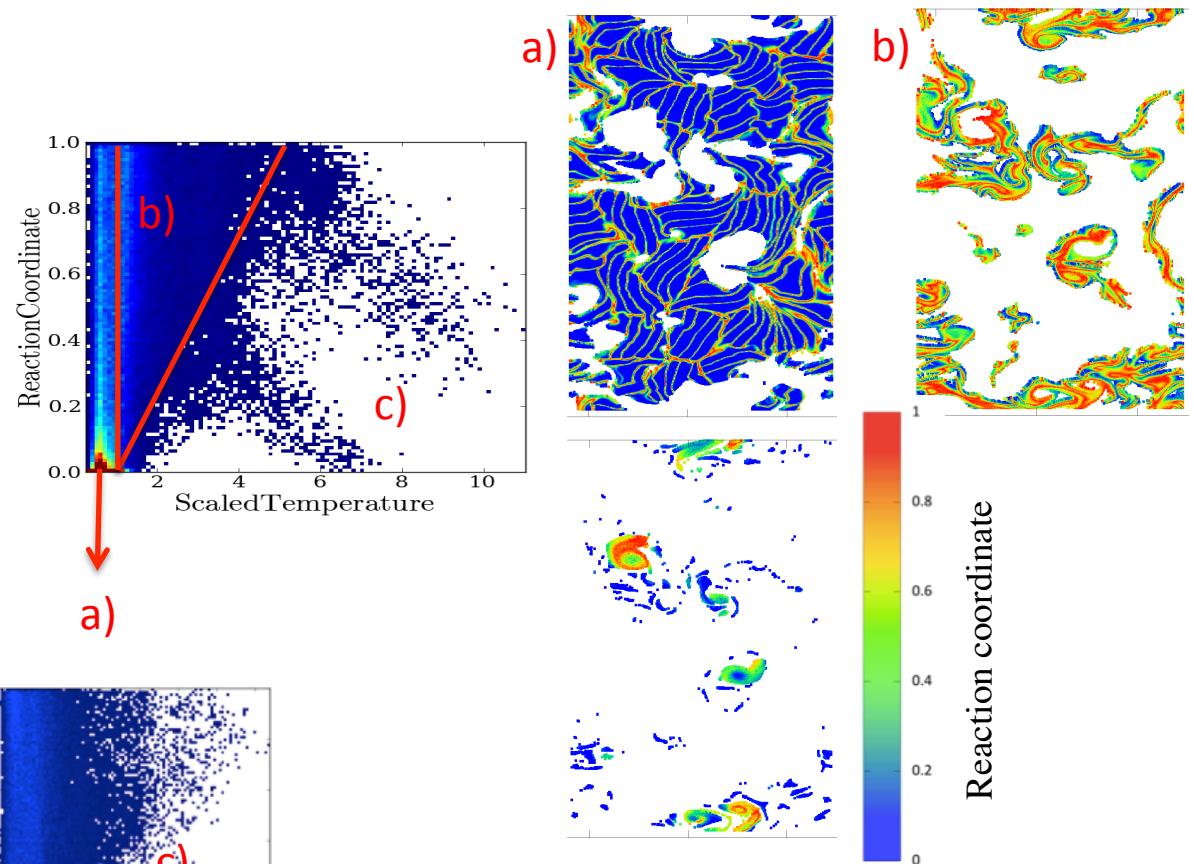
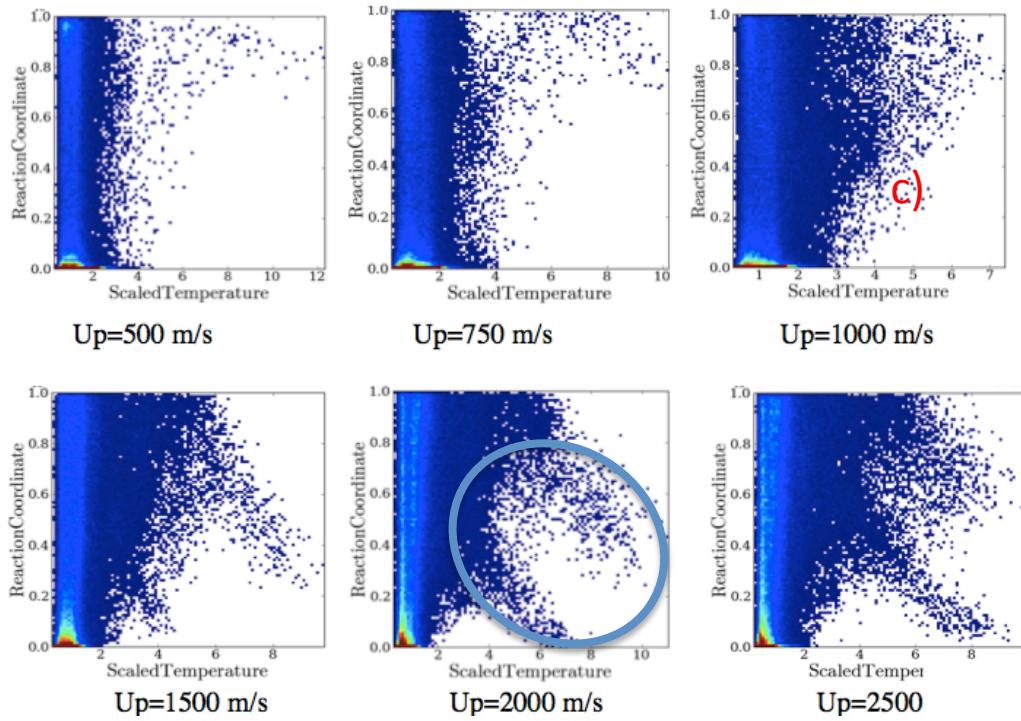


Schematic of granular MD setup.



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.