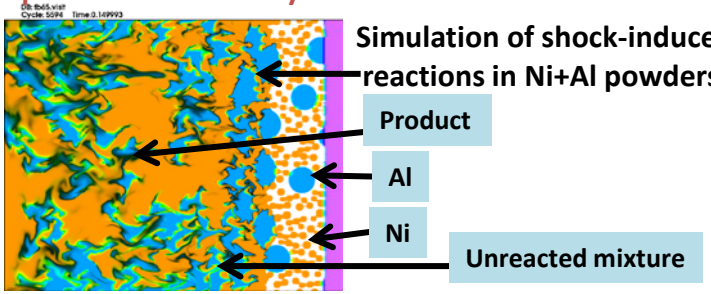
Mesoscale Priority Research Direction

Meso-scale Investigation of Mechanically and Thermally Induced Reactions in Reactive Solid Mixtures and Structures

Opportunity

Certain metal-metal, metal-metal-oxide particulate systems can undergo self-propagating chemical reactions under large deformation and/or high temperatures. Mechanical deformation, diffusivity and reactivity play a complex and critical role in understanding the physical processes underlying chemical reaction. The heterogeneity of particulate materials requires mesoscale investigations since reaction kinetics may be governed by equations dramatically different from molecular chemistry.

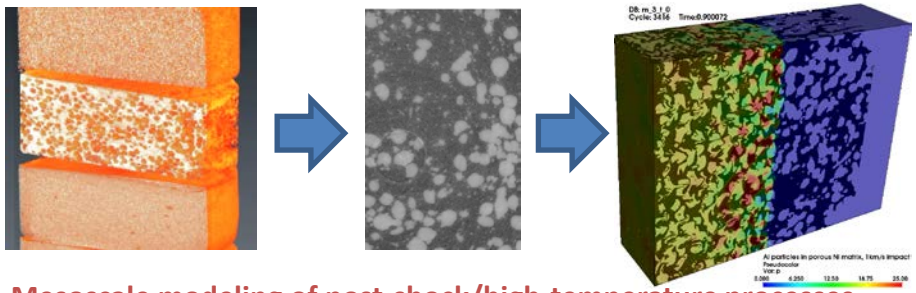


Meso Challenge

- How can chemistry occurring at the atomic scale be coupled to deformation at the micron scale?
- What improvements are necessary in continuum codes to couple reaction, diffusion, heat conduction and material deformation?

Problems involving multiple particles are too large for molecular dynamics (MD) approaches and the deformation and chemistry is not suited for discrete-element methods (DEM) or Lagrangian finite element approaches.

Approach



Mesoscale modeling of post-shock/high-temperature processes in reactive mixtures requires resolving interface phenomena with hybrid algorithms for material diffusion and hydrodynamic mixing and adaptive mesh refinement. Newly developed dynamic transmission electron microscopy (DTEM) and X-ray computed tomography allow exploration of mechano-chemical-thermal processes on the nano-micro length and time scales.

Impact

Experimental data and robust predictive modeling enable virtual design of novel reactive materials and structures and evaluation of performance such as the resulting pressures, temperatures, and impulses. Assessments of reactivity also enhance safety of personnel and equipment in industries relying on these types of reactions (i.e. heat-treating processes in metal factories, metal-forming in automotive industries, remote soldering in computer manufacturing, etc.).

References: 1. Lomov, Herbold, Austin, AIP Proceeedings 1426, 733 (2012).
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3. Herbold, Thadhani, Jordan, J. Appl. Phys., 109, 066108 (2011).

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