Mesoscale Priority Research Direction

Chemistry at extremes

Opportunity

Shock science focuses on bulk materials assumed to be homogeneous when they are inherently heterogeneous, especially after a shock front passes. Post-shock, materials experience extreme gradients in volume, temperature, entropy, pressure, composition. Physical, chemical, and electronic structures are changed. How do these many variables interact? How are electron/energy transport, reaction kinetics, and molecular transport affected?

Meso Challenge

- Many variables (T, P, dP/dt, ionization constant, density, porosity, structure, heterogeneity, material, phase, etc) interacting over sub-ns to 3 s timescales and angstrom to mm sizes
- Examine extreme chemistry/materials; reactions depend on the path followed in these scales.
- Bulk input (compression) leads to quantum-level changes (electronic band structure) and atomistic to mesoscale changes (molecular rearrangement/reactions), which lead back to continuum changes (phase structures). How do we relate energy localization and transfer at each level? How do we use this to control reactions/develop new materials?

Approach

Dynamic compression and Taylor drives will be used to control the reaction path through V, T, P, etc, allowing us to untangle the role of each variable. Experiments are short lived (<10us), which requires sub-ns time resolved XRD, and the development of sub-ns and sub-micron resolution of emission/spectroscopy.

Impact

- Understanding variables' effects on chemical reactions will teach us how energy couples to matter at extremes; application to energy transfer/storage
- develop new materials/synthetic methods for extreme environments
- improve kinetics/dynamics measurements
- Control access to metastable phases
- Improve models for heterogeneity/layered structure in high-P chemistry
- improved fast high resolution techniques

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