SHOCK13-2013-000665

Abstract for an Invited Paper
for the SHOCK13 Meeting of
the American Physical Society

Coupling Instrumented Experiments with Microstructure-based Simulations of Reactant Configuration Effects on Shock-Initiation of Reactions in Intermetallic-Forming Powder Mixtures[1]

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The shock-initiation of reactions in intermetallic-forming powder mixtures is dominated by the configuration of reactants, which is influenced by the intrinsic and extrinsic properties of constituents. Instrumented experiments coupled with microstructure-based simulations can be used to understand the meso-scale processes and effects of reactant configuration on the onset conditions for reaction initiation. Uniaxial-strain impact experiments are performed to monitor the input and propagated stress-wave profiles and to determine changes in compressibility and wave-velocity associated with powder densification and possible reaction, as a function of impact velocity and different reactant configurations such as size, shape, and distribution of constituent powders. Meso-scale computational simulations through discretely represented constituents with real and synthetically generated microstructures of reactants, imported into CTH simulations, are also used to qualitatively and quantitatively probe the local configuration changes and particle-level processes, following validation of macroscopic properties by correlations with experiments. The simulations reveal the dependence of the starting configuration of reactants on the heterogeneous nature of localized deformation and mixing with processes such as forced or turbulent flow, vortex formation, and dispersion of reactants, influencing the onset conditions for reaction initiation. Understanding of these processes as a function of the effects of starting reactant configuration, and correlating those with synthetically-generated microstructural constructs allows reverse design of reactive powder mixture systems for desired macro-scale performance. This presentation will present an overview of our experimental and modeling approach in understanding the mechanistic aspects of impact-initiation of reactions for design of reactive materials systems.

[1]Support provided by AFOSR, DTRA, and ONR.