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Mechanochemical Aspects of Shock-Induced Reactions: Time-Resolved Experiments and Meso-Scale Simulations¹

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Mechanochemical aspects of shock-compression of reactive powder mixtures leading to “shock-induced” reactions will be reviewed. Time-resolved experiments performed on intermetallic-forming mixtures of powders of varying configurations have shown evidence of shock-initiation of reactions inferred on the basis of compressibility changes, shock-velocity increases, or excess pressures. The influence of the characteristics of starting powder mixtures on their densification response, crush-up stress, and type and extent of configurational changes between reactants has also been revealed by experiments. However, the mechanisms responsible for reaction initiation and product formation, extent of reaction and type(s) and amount(s) of reaction products formed, and their correlation with measured changes in shock velocity and/or shock compressibility have not been conclusively demonstrated. Furthermore, while changes in compressibility associated with reactions have been calculated based on an assumed kinetics, and constant volume or constant pressure approximations to account for the heat of reaction, the certainty of high-pressure states and their associated kinetics is a function of the actual reaction product and its amount, which has been lacking. Meso-scale numerical simulations of shock-wave propagation through discretely represented powder mixtures can be used to approximate the configuration of reactants participating in the reaction based on a pre-defined stress, strain, or temperature criterion, and therefore, determine the product and its extent under a given set of loading conditions. Meso-scale numerical analysis can also be used to probe configurational changes and reaction mechanisms, considering processes such as forced or turbulent flow and/or fracture and dispersion of reactant powders of dissimilar properties or morphologies. The understanding can be used for controlling energy release characteristics for design of microstructure or materials with controlled energetics.

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