Computational Modeling of Combustion Wave in Nanoscale Thermite Reaction

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Abstract : Nanoscale thermites such as the composite mixture of nano-sized aluminum and molybdenum trioxide powders possess several technical advantages such as much higher reaction rate and shorter ignition delay, when compared to the conventional energetic formulations made of micron-sized metal and oxidizer particles. In this study, the self-propagation of combustion wave in compacted pellets of nanoscale thermite composites is modeled and computationally investigated by utilizing the activation energy reduction of aluminum particles due to nanoscale particle sizes. The present computational model predicts the speed of combustion wave propagation which is good agreement with the corresponding experiments of thermite reaction. Also, several characteristics of thermite reaction in nanoscale composites are discussed including the ignition delay and combustion wave structures.

Keywords : nanoparticles, thermite reaction, combustion wave, numerical modeling

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