Current challenges and perspectives in modelling the multiphase thermite reactions

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For three decades, significant research efforts have been devoted to thermites and nanothermites using different metal/metal oxide combinations and custom nanostructured architectures. Unlike explosives, these energy-dense materials undergo a rapid deflagration driven by a carbon free oxidation-reduction reaction, which forms stable reaction products (metal oxides or hydroxides). Moreover, these products have stronger mechanical strength and heat resistance than CHNO compounds. They are versatile, different combustion effects (in terms of pressure/gas development, temperature footage, initiation delay) can be obtained by manipulating the reactive system (metal and oxide powders) and their microscopic and mesoscopic morphology. Predictive simulations of the self-propagating reaction of thermite materials is one critical step to achieve their technological maturity and effective deployment into applications[1]. There is however a lack of fundamental understanding on the mechanisms occurring in thermites combustion due to the complexity associated with the material heterogeneities and multiphase (gaseous, condensed phases) and reactive (high energy reaction) flows. Thanks to the constant increase in computing power and progress in numerical methods and modeling techniques, we believe that the most efficient way to address these questions, is to establish a multi-scale modeling approach (nanoscale → cm-continuous scale). DFT based simulations help to decipher localized events (diffusion/reaction)[2] while molecular dynamics simulations mostly based on reaxFF allow exploring more collective phenomena in terms of both the system size (thousands of atoms) and time duration (nanoseconds)[3]. Microkinetic modeling[4,5] can describe the detailed surface and gas phase reaction mechanisms. Finally, the development of numerical CFD continuous models of the self-propagating combustion, is a key step to better test and confront simulations and experiments, to obtain deeper insights into the multiphase physics, thermal and transport processes[6]. The presentation will overview and discuss the multiscale modelling approach adopted by our team to better understand the combustion of Al/CuO thermites and simulate their self-propagating combustion, based on recent publications.

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