

Nanoenergetic: Paving the Way to Smaller and Smarter Pyrotechnics.

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Reactive materials or nanothermites are physical mixtures that demonstrate self-sustaining exothermic reactions upon receiving an initial energy input. This category of materials is distinctive within the realm of energetic materials, differing from explosives: their reaction fronts propagate subsonically and rely on atomic diffusion and other physical transport mechanisms. This dependence on transport mechanisms allows for the engineering of reactive materials to exhibit reactions over a broad range of timescales, depending on the length scale of the reactants. Aluminum (Al) is the most extensively studied metallic fuel, owing to its high reaction enthalpy (84 kJ.cm^{-3} , 31 kJ.g^{-1}), widespread availability and non-toxic nature. Various oxidizers have been studied, including copper oxide (CuO), iron oxide (Fe_2O_3), molybdenum oxide (MoO_3), tungsten oxide (WO_3) and bismuth oxide (Bi_2O_3); the choice depending on the particular application. Reactive materials are promising energetic materials due to their high energy density and tunable reactivity for a wide range of applications, which include self-destructive devices^{1,2}, semiconductor bridges in order to initiate explosives³, pyro-fuze⁴, welding repairs⁵, and many others⁶. On the fundamental science side, with the goal to investigate the combustion mechanisms, research has been conducted at different length scales. At the nanoscale, density functional theory (DFT) calculations⁷, molecular dynamics (MD) simulations⁸, electron spectroscopic transmission electron microscopy (TEM)⁹ and electron energy loss spectroscopy (EELS)¹⁰ have been used to depict pre-ignition reaction mechanisms. Results have highlighted the correlation between oxygen release (from oxidizer decomposition) and ignition and provided very useful insights into the key role of microstructure on the ignition threshold. On the other hand, micro-scale combustion behaviors have been actively investigated in the last decade using high-speed microscopy/thermometry^{11,12}. Research has highlighted the key role of spatial heat transfer mechanisms occurring in the reaction front, which can be affected by local inhomogeneities. In this talk, I will discuss probing both the ignition and combustion processes of aluminum-based nanothermites. The overall aim is to gather essential insights to create Structure – Energetic Properties guidelines for optimizing the safety and performance of such new promising materials. Then, after the illustration of several applications of reactive materials, I will outline the challenges that lie ahead, with a focus on the necessity to advance numerical simulations of nanothermite combustion. This advancement is crucial in providing predictive computational tools for the development of more intelligent and environmentally friendly pyrotechnic solutions¹³. Slides are available upon request at rossi@laas.fr.

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