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### In-detail elaborating the way of titanium in thermite reactions

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#### **Abstract**

In recent years, it has been reported that adding titanium into reactive thermite composites (such as Al/I<sub>2</sub>O<sub>5</sub>, B/CuO) can improve their combustion efficiency and lower their ignition temperature. However, these authors were only able to point out the complexity of the mechanisms governing ternary thermites reactivity but failed to answer the question of the exact role of the Ti reaction with oxidizers in such thermite composites. Due to the fast reaction rate and the difficulties in tracking elemental movements in Ti-based thermite nanoparticles, a full diagnosis from a fundamental standpoint awaits. In this work [1], we put our focus on in-depth understanding the reaction mechanism of Ti-based thermite by employing magnetron-sputtering technique to grow high purity and well-defined CuO/Ti nanolaminates. Contrary to powdered nanothermites in which a thick titania oxide shell layer separates its pure fuel Ti core from the outer surface oxidizer particle, nanolaminates feature a very well controlled interface (in thickness and structure) between the fuel and oxidizer. Furthermore, the multilayer system allows a full contact between the different species compared to particulate system showing random contact, which is crucial to clearly identify and rationalize the different mechanisms taking place during initiation/propagation of the reaction. This provides an ideal model-system to quantitatively describe the TiOx interfacial oxide growing using a host of characterization techniques including microscopy, thermal analysis, spectroscopy and X-ray diffractometric.

Results show that 70% of theoretical heat of reaction of the Ti/CuO system is released within a single strong exotherm at 430 °C, thus confirming the early and fast Ti oxidation. High resolution electronic microscopy reveals that the titania, terminal reaction oxide, is grown and propagates into the Ti layer, driven by the diffusion/reaction of oxygen atoms released by CuO at 300 °C. Spectroscopy measurements show that CuO/Ti redox reaction undergoes a two-step oxidation process: at 300 °C, Ti is first oxidized into TiO and further oxidized into crystalline TiO<sub>2</sub> at 500 °C. At a similar initiation temperature, the Ti-based sample supports more oxygen transport, thus a greater number of elementary exothermic reactions, causing a greater amount of heat per unit volume. In turn, this drives the system into the self-sustaining reaction mode where sufficient energy is present to activate mass transport across the continuously forming terminal oxide until the reaction is completed. This study confirms that Ti can be of great interest in addition or replacement of Al in nanothermites, for applications where it is desirable to lower the ignition temperature. Adding two CuO/Ti bilayers prior to the deposition of CuO/Al multilayers allows decreasing ignition time below the ms (200  $\mu$ s) against 15 ms without CuO/Ti. Also, a burn rate enhancement factor of  $\times$  3, and a reduction of the ignition delay by  $\times$  700 is obtained when replacing Al by Ti in standard CuO/Al multilayers.

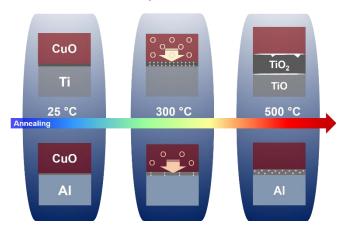


Figure 1. Schematic of the reaction mechanism of CuO/Ti compared with CuO/Al.

**Keywords**: Titanium, nanolaminates, energetic materials, thermite reaction mechanism

[1] T. Wu, V. Singh, B. Julien, C. Tenailleau, A. Estève, C. Rossi, Pioneering insights into the superior performance of titanium as a fuel in energetic materials, Chemical Engineering Journal. 453 (2023) 139922.

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