

Unraveling the Oxidation Dynamics in Zr/CuO Nanothermites Using Correlative Spectroscopies

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Refractory metal fuels like zirconium (Zr) possess the capability to undergo rapid oxidation and exhibit exceptional combustion efficiency, making them highly reactive when combined with a strong oxidizer such as CuO. The rapid reaction rates, however, have hindered a comprehensive understanding of the reaction mechanisms from a fundamental perspective.

In this study, Zr/CuO reactive multilayer films (RMF) are deposited via a carefully controlled physical vapor deposition (PVD) process, ensuring precise regulation of film thicknesses. The fabricated CuO/Zr stacks are annealed at temperatures (Figure 1) corresponding to key oxidation events, followed by a detailed analysis of each interface. This study then delves into the evolution of oxidation states of zirconium (Zr) in Zr/CuO nanothermites, shedding light on their reaction mechanisms.



Figure 1. STEM micrographs of CuO-Zr-CuO-Al reactive multilayer films at various temperatures. Al is used as a capping layer.

Utilizing correlative spectroscopies, including electron energy-loss spectroscopy (EELS) and energydispersive X-ray spectroscopy (EDX), we also examine the Zr layer within reactive multilayer stacks. EELS proves instrumental in analyzing both high-loss and low-loss (N) edges of Zr, providing valuable insights into its oxidation states. Complementing this, EDX offers a deeper understanding of the diffusion behaviors of heavier metals such as copper (Cu) and zirconium (Zr). Though oxygen quantification remains challenging, within the signal-to-noise ratio, we can assess oxygen saturation qualitatively and infer oxidation states accurately.

Our research highlights the efficacy of EELS and EDX techniques in unraveling the complex interplay of oxidation states as well as the elemental tracing across the interfaces. By elucidating the mechanisms governing Zr/CuO redox reaction, we contribute to advancing our understanding of its energetic properties. Furthermore, these spectroscopic tools offer promising applications in various fields where precise control over combustion processes is paramount for system optimization and material design. This study underscores the importance of leveraging advanced spectroscopic techniques for an in-depth characterization of materials, paving the way for enhanced performance and efficiency in reactive materials engineering.

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