

Investigating the Local Structure and Phase Evolution of Mesoporous Gamma Alumina Using Pair Distribution Function (PDF) Analysis

Mesoporous gamma alumina ($\gamma\text{-Al}_2\text{O}_3$) is widely used as a support in catalytic applications because of its high surface area, large pore volume, acid-base characteristics, and thermal stability. Our laboratory has developed a highly effective method of synthesizing $\gamma\text{-Al}_2\text{O}_3$, and work over the last few years has demonstrated that both pore properties and thermal stabilities are significantly improved by the addition of silica dopants. Nevertheless, the interactions between alumina crystallites and the silica dopants are still not well understood due to the poorly crystallized nature of the material. To enhance our understanding of the structural features responsible for improved thermal stability, we are applying Pair Distribution Function (PDF) analysis to a series of both pure and silica-doped aluminas calcined between 50-1300°C to determine the differences in local structure and phase evolution caused by the dopant and thereby identify the location and role of the silica dopant. We are simultaneously investigating how our aluminas differ structurally from those currently offered commercially, allowing us to separate general trends in alumina local structure from idiosyncrasies based on synthetic method/conditions. Our PDF analyses along with ab-initio calculations of gamma phase stability are leading us to suspect that the silica dopant stabilizes defects in the gamma structure originating from the boehmite-to-gamma phase transition.

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