On the Cobalt Carbide Formation in a Co/TiO\textsubscript{2} Fischer–Tropsch Synthesis Catalyst as Studied by High-Pressure, Long-Term Operando X-ray Absorption and Diffraction

Fischer-Tropsch synthesis (FTS) is a process used to synthesize ultra-clean diesel from crude-oil alternative feedstocks, such as biomass, municipal waste and natural gas. The application of FTS in the chemical industry is experiencing a resurgence, due to increased environmental awareness, an ever-growing demand for (increasingly cleaner) transportation fuels, and the environmental impact from burning fossil carbon. FTS converts synthesis gas, a mixture of CO + H\textsubscript{2}, over a catalyst to produce the heavier hydrocarbons. An industrially relevant catalyst for this process is in the form of cobalt nanoparticles supported on titania. It is known that this catalyst slowly deactivates but many questions remain regarding details of the deactivation mechanisms.

In this study, a collaboration between Prof. Bert Weckhuysen (Utrecht University) and Simon R Baré (SLAC National Accelerator Laboratory), we examined possible deactivation mechanisms of the Co/TiO\textsubscript{2} catalyst over the course of one-week continuous operation under FTS conditions of CO:H\textsubscript{2} 1:1, 220°C, 16 bar pressure. The intent was not only to provide insight into the deactivation mechanism, but also to illustrate methods to study atomic-level details of long-term deactivation. Over this time the cobalt nanoparticles transformed into cobalt carbide nanoparticles, as determined by both X-ray absorption spectroscopy (XAS) at Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC National Accelerator Laboratory, and XRD in the laboratory at Utrecht University. At SSRL we used a Hiden HPR-20 to detect the gas phase products from the catalysis. It was determined that the product formation does not noticeably change when cobalt carbide formation is detected, suggesting that cobalt carbide formation is not a major deactivation mechanism for this catalyst.

This study shows that it is feasible to conduct longer term catalyst deactivation experiments at a synchrotron facility. Indeed, as a result of the success of this pilot experiment, we are planning on making this capability available to catalyst researchers and use the learnings from this study to develop a user-friendly capability at SSRL.
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