Three-dimensional view of catalysts in action

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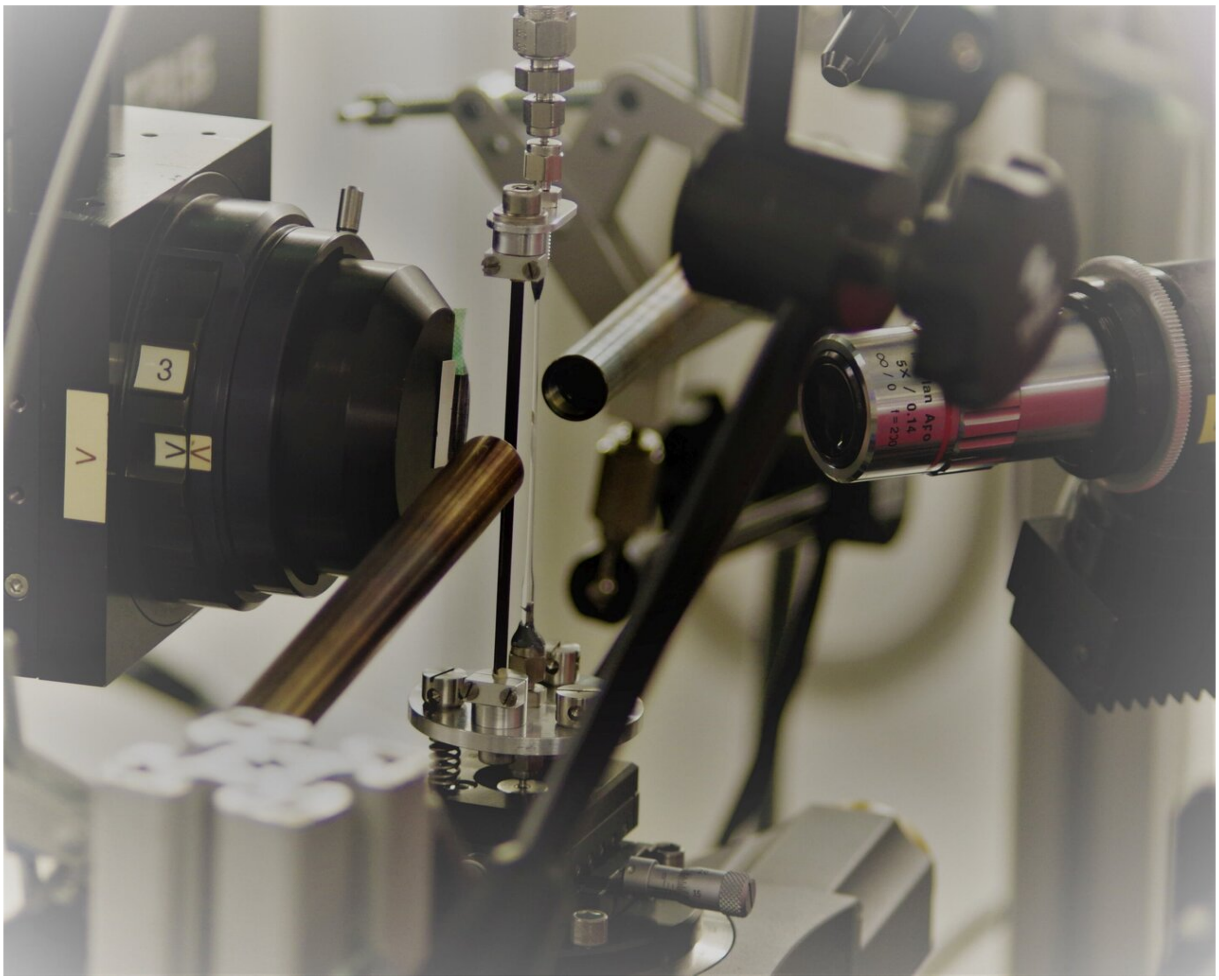

Operando X-ray spectroscopy shows what happens in each single part of a working catalyst. Credit: Dr. Dmitry Doronkin, KIT

For understanding the structure and function of catalysts in action, researchers of Karlsruhe Institute of Technology (KIT), in cooperation with colleagues from the Swiss Light Source SLS of Paul Scherrer Institute (PSI) in Switzerland and the European Synchrotron Radiation Facility (ESRF) in France, have developed a new diagnostic tool. Operando X-ray spectroscopy visualizes the structure and gradients of complex technical catalysts in three dimensions, thus allowing us to look into functioning chemical reactors. The results are reported in *Nature Catalysis*.

Catalysis is indispensable for many branches. 95% of all chemicals are produced using catalysts. Catalysts also play a key role in energy technologies and environmental protection. Catalysts are materials used to accelerate chemical reactions in order to reduce energy consumption and undesired byproducts. This chemico-physical principle is the basis of entire systems, examples being catalytic converters in cars or catalysts in power plants to remove pollutants from their exhausts. Technical and industrial catalysts are also applied in fertilizer and polymer production. Often, they must exhibit high pressure resistance and mechanical strength, while additionally operating under dynamic environmental condi-tions. Even smallest efficiency increases in the removal of pollutants, such as carbon monoxide, nitrogen oxides, and fine dust, from exhaust gases or in the production of green hydrogen will result in major advantages for humans and the environment. To improve existing catalytic materials and processes, however, exact understanding of their function is required. "Whether in a large chemical reactor, in a battery, or underneath your car—technical and industrial catalysts often have a highly complex structure," says Dr. Thomas Sheppard from the Institute for Chemical Technology and Polymer Chemistry (ITCP) of KIT. "To really understand how these materials function, we need to take a look inside the reactor when the catalyst is working, ideally with an analytical tool to detect the complex 3-D structure of the active catalyst."

Operando X-ray Spectroscopy Provides 3-D Images

and Major Chemical Information

Thomas Sheppard directed a study on automotive catalytic converters, the results of which are now reported in *Nature Catalysis* by the researchers involved from KIT, PSI, and ESRF. For their studies, the team used a newly developed setup and carried out tomography experiments at synchrotron radiation facilities in Switzerland and France. Computer tomography produces 3-D images of a sample, including the exterior and interior, without needing to cut it open. By using a special reactor, the researchers performed tomography and X-ray spectroscopy to track an active catalytic pro-cess. In this way, they succeeded in observing the 3-D structure of an emission control catalyst under conditions just like those in a real automotive exhaust. This so-called operando X-ray spectroscopy provides not only the 3-D structure of the sample, but also important chemical information.

Method Suited for Various Catalysts

"Since catalysts often have a rather complex and non-uniform structure, it is important to know whether the entire catalyst volume or only parts of it are performing their chemical function as intended," explains Johannes Becher from ITCP, one of the main authors of the study. "Operando X-ray spectroscopy lets us see the specific structure and function of every single piece. This tells us whether the catalyst is performing at maximum efficiency or not and, more importantly, it helps us understand the underlying processes." During reaction, the team observed a structural gradient of the active copper species within the catalyst, which could not be detected previously using conventional analytical tools. This is important diagnostic information in the performance of emission control catalysts. The method itself can be applied to many different catalysts and chemical processes.

New Opportunities for Materials and Reaction Diagnostics

The team's studies show how visualizing the chemical state of an active catalyst in 3-D can bring new opportunities for materials and reaction diagnostics. "Until now, it was not possible to freely select any piece of a working catalyst and understand which reactions take place in there without disturbing it. Now, we can follow exactly which reactions are occurring, where, and why," says Professor Jan-Dierk Grunwaldt from ITCP. "This is the key to improving our understanding of chemical processes and designing better and more efficient catalysts in future." Studies using operando X-ray spectroscopy can be carried out at different synchrotron radiation sources, provided that an appropriate sample environment exists. The groups of Jan-Dierk Grunwaldt and Thomas Sheppard will continue their investigations as part of the new Collaborative Research Center TrackAct at KIT. TrackAct is aimed at understanding and improving the design and efficiency of emission control catalysts.

More information: Johannes Becher et al. Chemical gradients in automotive Cu-SSZ-13 catalysts for NOx removal revealed by operando X-ray spectrotomography, *Nature Catalysis* (2020). DOI: 10.1038/s41929-020-00552-3

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