PRESS RELEASE

Three-Dimensional Characterization of Catalyst Nanoparticles

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Depiction of catalyst nanoparticles: The particles (coloured) adhere to a substrate (grey). They are imaged by electron tomography. For imaging, the data are processed using novel algorithms.

Photo: HZB

Catalysts will forever be a part of modern technology. They are crucial to industrial chemical processes, are fundamental to low-emission cars and will be essential for energy production inside next generation fuel cells. In a cooperative between Helmholtz Zentrum Berlin (HZB) and the Federal Institute for Materials Research and Testing (BAM), scientists have produced the first three-dimensional representations of ruthenium catalyst particles only two nanometres in diameter using electron tomography. Employing new processing algorithms, the scientists were then able to analyze and assess the chemically active, free surfaces of the particles. This detailed particle study provides insights into the action of catalysts that will play a key role in the fuel cell-powered cars of the future. The results are published in the Journal of the American Chemical Society (JACS).

To gain a fuller understanding of the action of catalyst particles and to enhance them accordingly, it is extremely important to know their three-dimensional shape and structure. The problem is these particles are typically only around two nanometres in size, some ten thousand times smaller than the thickness of a human hair. As part of his doctoral work, HZB physicist Roman Grothausmann, together with colleagues from HZB and BAM, has managed to analyze in three dimensions special catalyst nanoparticles developed at HZB for use in polymer electrolyte membrane (PEM) fuel cells in cars and busses. The scientists employed a special technique called electron tomography. This technique is similar to computer tomography (CT), as used in medicine, with the difference that the nanoparticles are scanned at much higher resolution. Grothausmann took many individual electron micrographs from different angles. Scientists from BAM then calculated 3D images in very sharp detail using a novel mathematical reconstruction algorithm.

Inside a fuel cell, catalysis takes place on the surface of the catalyst material. Since catalyst materials are often very expensive – platinum, for example – the aim is to obtain as large a surface area on the tiny particles as possible. Nanoparticles have an especially large surface area compared to their volume. At the atomic scale, however, not all areas of the particle surface are equal: Some parts of the surface allow a higher conversion rate of chemical to electrical energy than other areas, depending on their specific properties. Since the particles of a heterogenic catalyst do not float around freely but rest on a substrate instead, only a portion of each catalyst nanoparticle's surface is available for catalysis. The reactive materials can only reach these uncovered surfaces. Yet, the electrically conductive connection between the nanoparticles and substrate is just as important for closing the circuit of the fuel cell. Grothausmann and colleagues measured both the uncovered and covered surfaces of a few thousand nanoparticles to determine the size and shape distribution of the nanoparticles. It turns out many of the nanoparticles deviate from spherical symmetry, which increases their surface to volume ratio. Next, they analyzed the alignment of the nanoparticles to the local surface of the substrate. Statistically, this shows how frequently the rough and particularly reactive surface areas of the nanoparticles remain uncovered.

Electron tomography is a method for directly imaging 3D structures, and serves as a reference for better understanding data obtained using other methods. The catalyst studied in this case accelerates the reduction of oxygen to water in PEM fuel cells. Instead of the typically used and very expensive platinum, the more affordable material ruthenium was used. This doctorate helps to understand these novel materials and how to optimize them for use in the next generation of fuel cells.

Publication: R. Grothausmann, G. Zehl, I. Manke, S. Fiechter, P. Bogdanoff, I. Dorbandt, A. Kupsch, A. Lange, M. Hentschel, G. Schumacher, J. Banhart
Quantitative Structural Assessment of Heterogeneous Catalysts by Electron Tomography
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