Tracking in-situ morphological changes of nanoparticles in a variable gaseous environment at the atomic scale

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Nanomaterials attract more and more attention over the last few decades thanks to their improved properties and utility in a plethora of scientific areas including catalysis. In catalytic reactions unwanted structural, morphological and compositional changes take place which in turn affect dramatically the catalytic performance. A detailed characterization of these parameters in-situ is of utmost importance if one wants to obtain a better insight concerning the structure-to-property connection.

Transmission Electron Microscopy (TEM) is an ideal technique to investigate materials at both the nanometer and atomic scale and has therefore been widely used in the study of nanomaterials both ex-situ and in-situ. By combining the technique with tomography, a technique which derives three-dimensional (3D) information from two-dimensional (2D) projections, one is able to determine the structure and shape of nanostructures in 3D, even with atomic resolution. Although TEM has often been used to characterize nanoparticle catalysts, unfortunately most observations so far have been performed at room temperature and in ultra-high vacuum, conditions which are completely irrelevant for the use of NPs in real catalytic applications. By using dedicated in-situ holders which became recently commercially available, one can reach higher pressures and temperatures and also introduce liquids in the microscope, and therefore create an environment which is identical to that during actual catalytic reactions.

In my talk, a methodology which was very recently developed in our group to quantify variations of the 3D atomic structure and morphology of nanoparticles under the flow of a selected gas, will be presented.[1] 2D atomic resolution Scanning TEM (STEM) projection images were acquired in an aberration-corrected microscope in different gaseous environments and elevated temperatures using an in-situ gas holder. These images were used as an input for atom counting with the purpose to quantify the 3D shape and structure of the catalyst nanoparticles at different steps of a redox reaction. Prior to their use for quantification, the images were corrected for drifting and other distortions using a novel methodology based on deep convolutional neural networks (CNNs).

[1] Altantzis, T., Lobato, I., De Backer, A. et al., Nano Lett. 19 (2019) 477-481.