In situ surface structure determination during catalytic reactions using high-energy surface X-ray diffraction

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Surface X-ray diffraction (SXRD) is one of few methods available for surface structure determination under ambient conditions. Using conventional SXRD, however, exploring 2D maps from a substantial part of reciprocal space is extremely time-consuming, and mapping of the 3D reciprocal space with high resolution is currently impossible even with synchrotron radiation. As a result, the probed surface structure has to be known qualitatively from other measurements, and an unexpected structure may easily be left unnoticed, especially under harsh conditions.

In this contribution I will demonstrate how the use of high-energy X-rays (85 keV) in combination with a large 2D detector accelerates the data collection by several orders of magnitude and enables full surface-structure determination by 3D mapping of reciprocal space on a time scale suitable for in situ studies [1]. In addition, the small diffraction angles, resulting from the high photon energy, and the large detector result in data that are easily presented in a more intuitive way, since each detector image contains the projection of a full plane in reciprocal space and straight lines in reciprocal space correspond to straight lines on the detector.

We have used this method to analyse the structure of ultra-thin surface oxides formed on Rh(111), Pd(100) and Cu(111). Especially, we have followed how the presence and nature of these oxide varies with the catalytic activity towards CO oxidation and CO_2 reduction.

References:

[1] J. Gustafson, M. Shipilin, C. Zhang, A. Stierle, U. Hejral, U. Ruett, O. Gutowski, P.-A. Carlsson, M. Skoglundh, and E. Lundgren, Science **343**, 758 (2014).