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Spectroscopic Bragg Coherent Diffraction Imaging of Single Nanoparticles

Characterizing nanoscale displacement fields, compositional variations, and defects in heterogeneous catalysts remains a central challenge in materials science and energy-conversion research. Bragg coherent diffraction imaging (BCDI) [1] can deliver three-dimensional strain maps with nanometre resolution, yet chemical inhomogeneities often blur the distinction between strain and compositional contributions. This is an especially acute issue for chemically heterogeneous structures such as NiFe and PtPd, climate-critical alloyed bimetallic catalysts used in CO_2 hydrogenation. This underscores the need for high-resolution chemical and spatial analysis of catalysts during catalytic reactions.

We are therefore developping a nano-focused 3D spectroscopic Bragg coherent imaging technique at the nanoprobe ID01-EBS beamline of The European Synchrotron (ESRF). By combining BCDI with multiwavelength anomalous diffraction (MAD) [2], the spectro-BCDI technique will be used to reveal both chemical (oxidation states and bond structure) and structural (lattice strain, defect(s), morphology, composition) information of nanocatalysts under in-situ conditions to extract a mechanistic understanding for designing both effective and selective catalysts. By applying 3D spectroscopic BCDI, we aim to uncover critical information about the dynamic behavior of catalysts under working conditions. Nano-focused diffraction anomalous fine structure (DAFS) and fluorescence spectroscopy are applied as well [3].

This talk will present the application of the spectro-BCDI technique through simulations, complemented by experimental results.

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