



Structural evolution of nanoparticles under realistic conditions observed with Bragg coherent X-ray imaging

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Structural evolution of nanoparticles under realistic conditions observed with Bragg coherent X-ray imaging
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Abstract

The advent of the world's first coherent hard X-ray sources represents an unprecedented opportunity to conduct *in situ* and *operando* studies on the structure of nanoparticles in reactive liquid or gas environments in synchrotrons. In this talk, I will illustrate how Bragg coherent X-ray imaging [1] allows to image in three dimensions (3D) and at the nanoscale the strain and defect dynamics inside nanoparticles as well as their refaceting during catalytic reactions [2–5]. I will also highlight the potential of machine learning to predict characteristic structural features in nanocrystals just from their 3D Bragg coherent diffraction patterns [6].

References

- [1] I. Robinson and R. Harder, Coherent X-Ray Diffraction Imaging of Strain at the Nanoscale, *Nat. Mater.* 8, 291 (2009).
- [2] S. Fernández et al., In Situ Structural Evolution of Single Particle Model Catalysts under Ambient Pressure Reaction Conditions, *Nanoscale* 11, 331 (2018).
- [3] M.-I. Richard et al., Crystallographic Orientation of Facets and Planar Defects in Functional Nanostructures Elucidated by Nano-Focused Coherent Diffractive X-Ray Imaging, *Nanoscale* 10, 4833 (2018).
- [4] J. Carnis, L. Gao, S. Fernández, G. Chahine, T. U. Schülli, S. Labat, E. J. M. Hensen, O. Thomas, J. P. Hofmann, and M.-I. Richard, Facet-Dependent Strain Determination in Electrochemically Synthesized Platinum Model Catalytic Nanoparticles, *Small Weinh. Bergstr. Ger.* e2007702 (2021).
- [5] J. Carnis et al., Twin Boundary Migration in an Individual Platinum Nanocrystal during Catalytic CO Oxidation, *Nat. Commun.* 12, 5385 (2021).
- [6] B. Lim et al., A Convolutional Neural Network for Defect Classification in Bragg Coherent X-Ray Diffraction, *Npj Comput. Mater.* 7, 1 (2021).