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

M.-I. Richard[1,2], C. Atlan[1,2,3], C. Chatelier[1,2], M. Grimes[1,2], E. Bellec[1,2], K. Olson[1,2], M. Dupraz[1,2], S. Labat[4], I. Martens[2], A. Viola[3], F. Maillard[3], E. Rabkin[5], S. J. Leake[2], T. Schülli[2], J. Eymery[1]

[1]Univ. Grenoble Alpes, CEA Grenoble, IRIG, MEM, NRX, 17 avenue des Martyrs, F-38000 Grenoble, France.
[2]ESRF - The European Synchrotron, 71 Avenue des Martyrs, F-38000 Grenoble, France.
[3]Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, 38000 Grenoble, France.
[4]Aix Marseille Université, CNRS, Université de Toulon, IM2NP UMR 7334, 13397 Marseille, France
[5]Department of Materials Science and Engineering, Technion-Israel Institute of Technology, 3200003 Haifa, Israel.
mrichard@esrf.fr

Keywords: Coherent imaging, nanoparticles, catalysis

The advent of the new 4th generation x-ray light sources represents an unprecedented opportunity to conduct *in situ* and *operando* studies on the structure of nanoparticles in reactive liquid or gas environments. 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 [2–4]. As an example, we successfully mapped the lattice displacement and strain of a Pt nanoparticle in electrochemical environment (see Figure 1). Our results reveal that the strain is heterogeneously distributed between highly- and weakly-coordinated surface atoms, and propagates from the surface to the bulk of the Pt nanoparticle as (bi)sulphates anions adsorb on the surface [5].

We will also discuss the possibility to measure particles as small as 20 nm [6] and to enable high-resolution and high-energy imaging with Bragg coherent x-ray diffraction at 4th generation x-ray light sources [7]. Finally, I will highlight the potential of machine learning to predict characteristic structural features in nanocrystals just from their 3D Bragg coherent diffraction patterns [7].

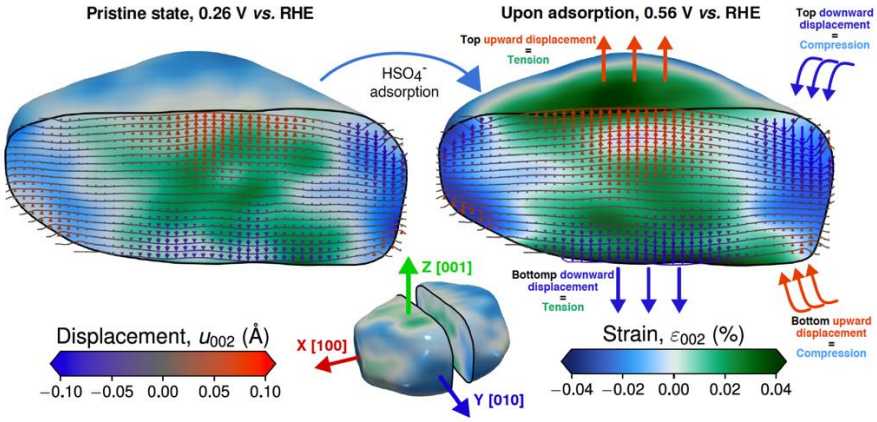

Figure 1. Evolution of the lattice displacement and strain of a Pt nanoparticle in its pristine state and under potential control (0.56 V *vs.* RHE) and in 0.05 M H_2SO_4.

We acknowledge funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 818823).

[1] I. Robinson and R. Harder, *Coherent X-Ray Diffraction Imaging of Strain at the Nanoscale*, Nat. Mater. **8**, 291 (2009).
[2] 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 Synthetized Platinum Model Catalytic Nanoparticles*, Small Weinh. Bergstr. Ger. e2007702 (2021).
[3] J. Carnis et al., *Twin Boundary Migration in an Individual Platinum Nanocrystal during Catalytic CO Oxidation*, Nat. Commun. **12**, 5385 (2021).
[4] M. Dupraz et al., *Imaging the Facet Surface Strain State of Supported Multi-Faceted Pt Nanoparticles during Reaction*, Nat. Commun. **13**, 1 (2022).
[5] C. Atlan et al., *Imaging the Strain Evolution of a Platinum Nanoparticle under Electrochemical Control*, Nat. Mater. **22**, 6 (2023).
[6] M.-I. Richard et al., *Bragg Coherent Diffraction Imaging of Single 20 Nm Pt Particles at the ID01-EBS Beamline of ESRF*, J. Appl. Crystallogr. **55**, 621 (2022).
[7] M.-I. Richard et al., *Taking Bragg Coherent Diffraction Imaging to Higher Energies at Fourth Generation Synchrotrons: Nanoscale Characterization*, ACS Appl. Nano Mater. **6**, 10246 (2023).
[8] B. Lim et al., *A Convolutional Neural Network for Defect Classification in Bragg Coherent X-Ray Diffraction*, Npj Comput. Mater. **7**, 1 (2021).