Three-Dimensional Imaging of Gold/Palladium Nanocatalysts by Coherent X-ray Diffraction at the CATERETÊ Beamline @ SIRIUS

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Understanding catalysts strain dynamic behaviours is crucial for the development of cost-effective, efficient, stable and long-lasting catalysts.

Chemical properties of supported metallic catalysts can be modified by lattice strain that alters the reactivity of metal surfaces [1,2]. As shown theoretically on extended surfaces, the adsorption and dissociation energies can be optimised for enhancing a particular chemical reaction by neatly controlling the degree of lattice surface strain [3]. This is explained by the d-band model [1], with a change in the surface d-band center due to lattice distortion. For example, gold (Au) is a late transition metal with a d-band more than half-filled. Tensile strain leads to a narrowing of the d-band and consequently an increased population of the d-band.

In nanoparticles (NPs), strain can emanate from intrinsic factors such as nanoparticle's size, morphology, exposed crystallographic facets, crystalline defects and the material itself [4–7]. Besides extrinsic strain can emerge from lattice mismatch induced at interfaces, nanoparticle-support interface, core-shell structures… Strain information are mostly obtained by X-ray diffraction while under reaction conditions, the nanoparticle structure can present dynamic restructuration, faceting process, requiring *in situ* and *operando* imaging tools.

We have recently shown using *in situ* coherent diffraction imaging techniques (Figure 1) that the three-dimensional strain of single gold nanocrystals evolves during the catalytic CO oxidation reaction[8–10].

To deepen our understanding of the atomic strain evolution of nanocatalysts, we propose that the student will develop and apply colloidal chemistry synthesis approach to prepare shape-controlled gold/palladium nanocrystals. In a second step, the student will perform the in situ 3D coherent diffraction imaging measurements on the Cateretê beamline during the CO oxidation reaction.

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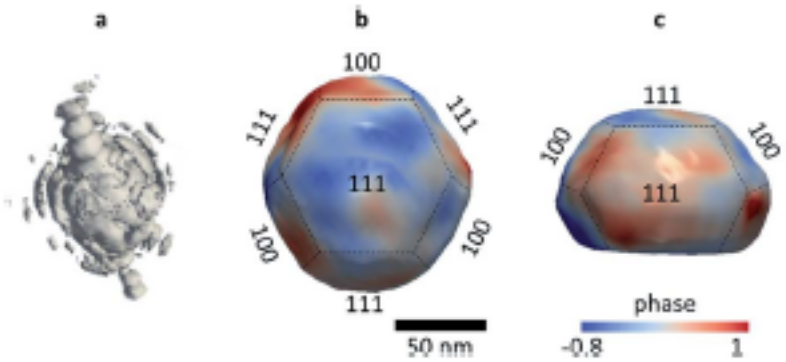

Fig. 1 (a) 3D diffraction pattern obtained by rocking scans around the (111) Bragg peak of a 120 nm Au/TiO2 nanoparticle in air at RT. The corresponding 3D reconstruction with a 30% isosurface seen from (b) top and (c) side views scaled with the phase. The facet orientations are shown.