3D strain dynamics of catalysts driving CO oxidation

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Catalytic materials can present dynamic restructuration under reaction conditions that can directly alter their chemical properties. Understanding the correlation between three-dimensional strain fields and the catalytic activity of nanocrystals is essential to improve the efficiency of catalysts. Bragg coherent X-ray diffraction imaging (Bragg-CDI) enables the determination of lattice strain and defects dynamics at the surface and inner core of nanocrystals. Bragg-CDI benefits from the use of coherent hard X-rays to unveil changes at the single nanoparticle level under *operando* conditions with a spatial resolution of the order of 10s of nanometers and picometer precision for lattice displacements.

In this work, we will present how Bragg-CDI in combination with mass spectrometry can reveal nanoscale peculiarities tuning the catalytic properties of nanomaterials. In particular, we will discuss the highly dynamic 3D strain distribution of noble metal catalysts during the CO oxidation reaction [1]. We will show how the hysteresis observed at the single particle level is directly correlated to the normal/inverse hysteresis loop of the catalytic performances or its inversion (Fig. 1).

With the higher coherent flux available at 4th generation synchrotron sources, such as the Brazilian synchrotron radiation facility SIRIUS [2] and the latest generation of pixels detectors, faster acquisitions will allow time-resolved *operando* imaging of catalysts enabling a deeper knowledge of catalytic property-structure relationships of various dynamic or transient systems.

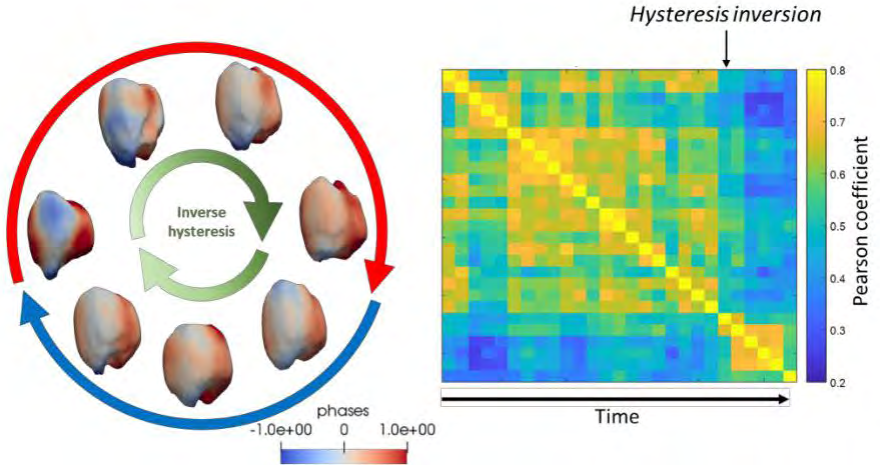

Figure 1. Left: Evolution of Bragg-CDI reconstructions of the displacement field of the same Pd nanoparticle during CO oxidation reaction cycle. Right: Cross-correlation map of the displacement fields as a function of the time showing the hysteresis inversion at the nanoscale.

[1] Passos, A. R., Rochet, A., Manente, L. M., Suzana, A.F., Harder, R., Cha, W., Meneau, F. (2020). *Nature Comm.*, 11, 4733.

[2] Lin, L., Milas, N., Mukai, A. H. C., Resende, X. R., De Sá, F. H. (2014). *J. Synchrotron Rad.*, **21**, 904.