Arriving at 5D tomographic diffraction imaging of functional materials

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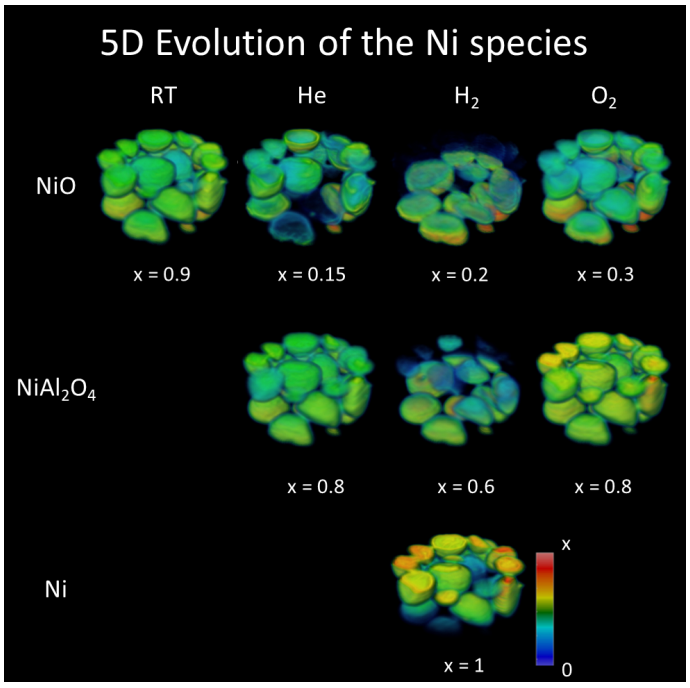
Heterogeneous functional materials, like catalytic solids, fuel cells and batteries usually possess complex structures where the 3D spatial distribution of the various components is rarely uniform. Such materials are known to change with time under operating conditions and in order to gain an insight into the complex structure-function relationships, it is essential to study them *in situ* with spatially-resolved techniques. X-ray diffraction computed tomography (XRD-CT) is such a technique that can provide spatially resolved physico-chemical information from within the interiors of intact objects [1]. The main advantage of XRD-CT though lies on the fact that it allows to track the chemical changes taking place in a functional material under operating conditions as a function of time and/or chemical environment [2]. For example, as shown in the Figure 1, ultra-fast XRD-CT measurements allowed us to study a complex Ni–Pd/CeO_2–ZrO_2/Al_2O_3 catalyst used for methane processing reactions under various operating conditions (i.e. ambient and at 800 °C under He, H_2 and O_2 flow) and observe the evolving solid-state chemistry of the Ni-containing phases in 3D.



Phase distribution volumes of NiO, $NiAl_2O_4$ and Ni as obtained from the Rietveld analysis of the 3D-XRD-CT datasets collected at the four different operating conditions.

References

[1] A. M. Beale *et al.*, Coord. Chem. Rev. 277-278 (2014), 208-223

[2] A. Vamvakeros *et al.*, Chem. Commun. 58 (2015), 12752-12755.