REAL-TIME CHEMICAL IMAGING OF FUNCTIONAL MATERIALS AND DEVICES: CATALYTIC REACTORS, FUEL CELLS AND BATTERIES

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ABSTRACT

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. In the past decade, a lot of effort has been put into developing novel reactor cells that allow for chemical imaging of functional materials and devices under industrially-relevant operating conditions. It is now possible to obtain the desired spatially-resolved chemical information by combining X-ray scattering and spectroscopic techniques with computed tomography [1]. Such techniques are considered to fall under the umbrella of "chemical tomography" as each pixel (or more precisely voxel) in the reconstructed images corresponds to a chemical signal [2]. The main advantage of these techniques though lies on the fact that they allow to track the chemical changes taking place in a functional material or device under operating conditions as a function of time and/or chemical environment. 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 [3].

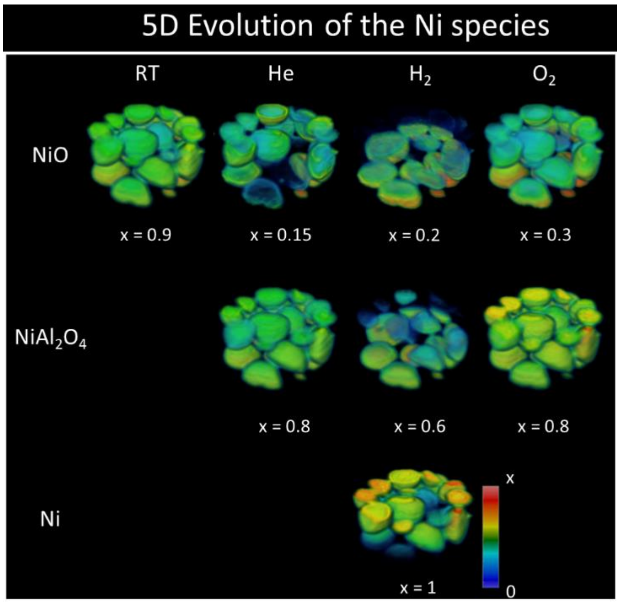

Figure 1: Phase distribution volumes of NiO, $NiAl_2O_4$ and Ni as obtained from the Rietveld analysis of the 3D-XRD-CT data collected at the four different operating conditions. The values in the colorbar axes have been chosen to achieve the best possible contrast.

REFERENCES

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