

## **Multimodal Chemical Imaging: Linking Microscopic Chemistry to Materials Properties and Reactivity**

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Nearly all natural and engineered materials exhibit pronounced physical and chemical heterogeneities at various length scales. These heterogeneities potentially dictate the physical properties as well as the chemical reactivity of the macroscopic material. Consequently, being able to image and visualize spatial variations of physicochemical characteristics is fundamental to advance our understanding of the properties, function, and reactivity of materials. Quite commonly though, imaging analysis is limited to 'physical imaging' providing information related to physical properties such as morphology or physical structure. Often however, in particular in the context of materials reactivity, microscopic chemical properties and their spatial framework turns out to be determinative.

Over the most recent years, micro-analytical facilities based on synchrotron X-ray beams advanced to be indispensable instruments in the context of micro-analytical imaging in general. The exceptional brilliance of modern synchrotron sources in combination with advanced design and production of hard X-ray focusing optics allowed the construction of dedicated high-flux microprobe beam lines. Opportunely, concerning chemical imaging, such synchrotron-based X-ray microprobe facilities possess several intrinsic advantages. Most important, the element-specific absorption resonances accessible within the X-ray energy range provide an element-specific chemical sensitivity. The fine structure of an absorption edge reveals specific chemical information of the target atom such as molecular structure and electronic state. These speciation-dependent features provide a chemical contrast that can be used for chemical imaging going beyond elemental composition mapping. Several X-ray techniques providing chemical contrast, including X-ray fluorescence (XRF), X-ray absorption or emission spectroscopy (XAS, XES) or X-ray diffraction (XRD), can be applied synchronously allowing the recording of multimodal datasets.

Due to the considerable penetration power of (hard) X-rays, not only two-dimensional scanning studies ('chemical images') based on spectro-microscopy and/or XRD-imaging. investigations in 3D ('chemical tomography') are feasible. Combining computed tomography approaches with the afore mentioned chemical X-ray techniques provides means to derive local chemical information from within intact, undisturbed objects or materials. Moreover, in most cases X-ray techniques can be considered as being non-invasive and non-destructive. This important feature allows the undisturbed recording of multiple, consecutive three-dimensional chemical and structural images of an evolving reactive system – corresponding to a 4D visualization of chemistry in space and time. Time-resolved chemical imaging allows diverse scientific communities to gain unrivalled insights into the chemical complexity of hierarchical, heterogeneous materials, including corresponding chemical reaction pathways and kinetics ('reactivity').

In this presentation, recent progress and achievements in the field of 2D/3D chemical imaging and speciation analysis using various synchrotron radiation microprobe techniques will be demonstrated. Examples from a wide range of scientific disciplines, including materials science and energy systems, will be used to illustrate the potential of chemical imaging. Recent progress in time-resolved chemical imaging

will be detailed based on *in-situ* observations of physicochemical processes occurring during advanced manufacturing and machining<sup>1,2</sup>.

*Example of relevance of multimodal chemical imaging:  
Degradation of Solid Oxide Fuel Cell.*

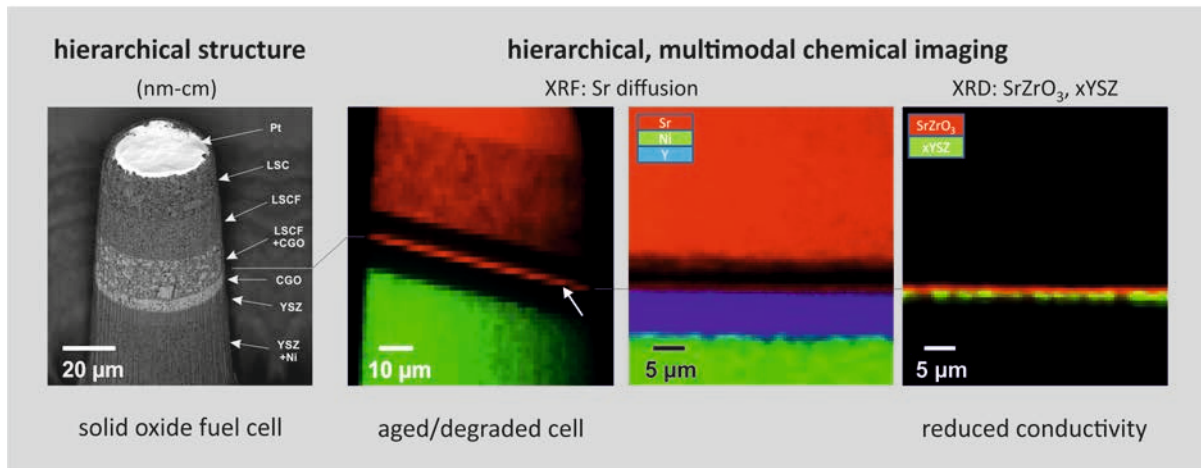


Figure 1: XRF based imaging identifies unexpected Sr-diffusion process. Simultaneous XRD imaging reveals SrZrO<sub>3</sub> precipitation and a linked chemical modification of YSZ at the electrolyte/diffusion barrier interface. These reaction products build a thin resistor layer, drastically reducing the device performance<sup>3, 4</sup>.

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