Structural dynamics of nanoalloy catalysts for Fuel Cells and CO oxidation by *in situ* Total x-ray scattering

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Many catalysts for energy related applications, in particular metallic nanoalloys, readily undergo atomic-level changes during electrochemical and gas-phase reactions. The origin, dynamics and implications of the changes for the performance of the catalysts inside operating devices though are not well understood. This is largely because they are studied on model nanocatalysts under controlled laboratory conditions. We will present results from studies on the dynamic behavior of Pt-3d transition metal nanoalloys inside i) an operating proton exchange membrane fuel cell (**Figure 1**), and ii) reactor for gas-phase oxidation of CO (**Figure 2**). The results indicate that the nanoalloys change profoundly, from the initial pristine state to the catalytically active form and further along their utilization. The studies employ a combination of x-ray and diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), electrochemical and total synchrotron x-ray scattering techniques. The advantages of this experimental approach will also be discussed.

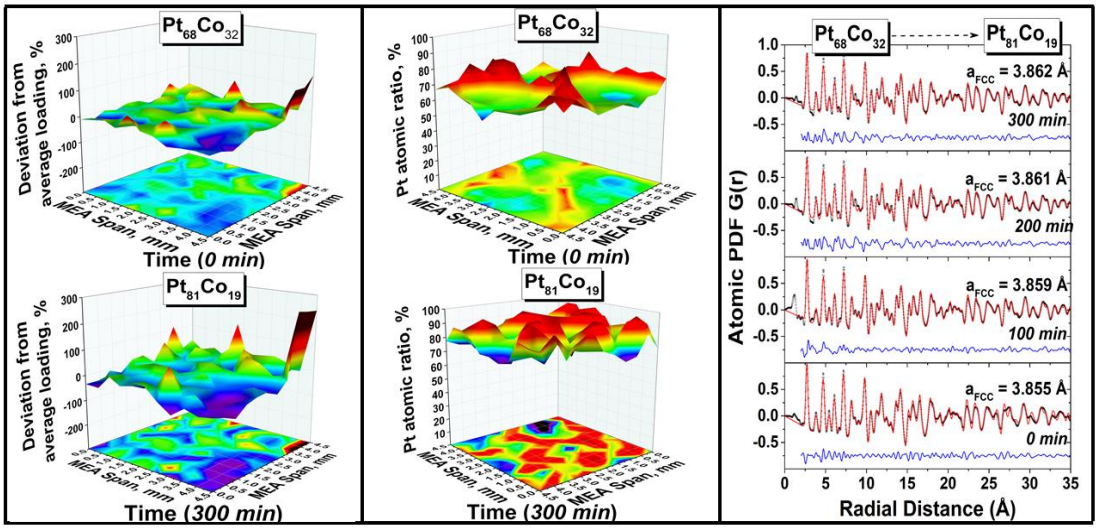

Figure 1. ***(left)*** Mass distribution of fresh (top row) and 5 h cycled (bottom row) $Pt_{68}Co_{32}$ alloy nanoparticles (NPs) over a 4.5 mm x 4.5 mm area of the membrane electrode assembly (MEA). ***(middle)*** Distribution of Pt species over the same MEA area for fresh and 5 h cycled NPs (bottom row) NPs. ***(right)*** Experimental (symbols) and computed (red line) atomic pair distribution functions for fresh and 5 h cycled NPs.

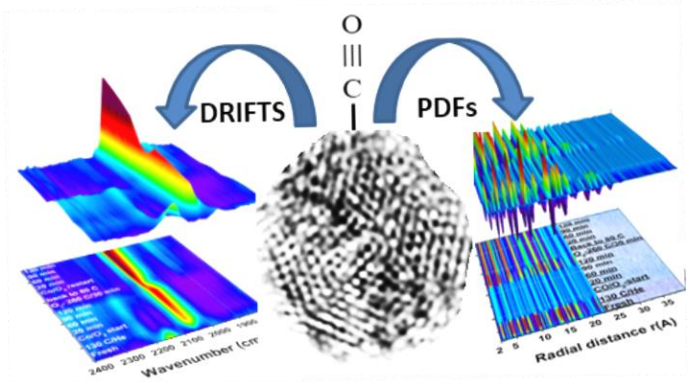

Figure 2. *In situ* DRIFTS spectra (left) and atomic pair distribution functions (right) for Pt-Au-Ni nanoalloy partciles (middle) annealed in pure He atmosphere at 130 °C for 30 min, used as a catalyst for low-temperature (80 °C) CO oxidation for 2 hours, reactivated in oxygen-rich atmosphere at 260 °C for 30 min, and then re-used as a CO oxidation catalyst for 2 more hours.