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Machine-Learning Aided Evolution Studies of Nano-composite Electrodes and Nano-particle Catalysts for Fuel Cell Applications

David Rossouw[1], Lidia E. Chinchilla[1], Sagar Prabhudev[1] Tyler Trefz[2], Natalia Kremliakova[2], and Gianluigi A. Botton[1].

[1] McMaster University, Department of Materials Science and Engineering, Hamilton, ON, Canada.
[2] Automobile Fuel Cell Cooperation, 9000 Glenlyon Parkway, Burnaby, BC V5J 5J8 Canada

Automotive vehicles powered by proton exchange membrane fuel cells are approaching commercial viability but further improvements are necessary for a practical technology that can be mass-produced cost effectively. The bottleneck limiting their commercialization is the notorious cathodic cell reaction, called the oxygen reduction reaction (ORR), which is a multi-electron pathway reaction with inherently sluggish kinetics. Platinum (Pt) has been used as a catalyst to accelerate the ORR, but despite its exceptional catalytic activity, it is cost prohibitive for commercialization. The search for more affordable fuel cell cathode materials has focused on controlling the surface structure and composition of novel multi-metallic catalytic nanoparticles on high surface area support membranes. However, such nano-structured heterogeneous systems are notoriously challenging to characterize. In addition to difficulties associated with interpreting spatially and spectrally overlapping analytical signals, samples can be beam-sensitive, so care must be taken to limit the beam dose.

Here, we overcome these challenges by using a machine learning technique, called independent component analysis (ICA) implemented in HyperSpy [1], applied to electron energy loss spectroscopy (EELS) signals obtained using a transmission electron microscope (TEM) [2]. We characterize a proposed fuel cell cathode material, promising improved corrosion resistance and durability, containing nano-particulate platinum on a NbO_x-carbon hybrid support. We unambiguously separate spatially and spectrally overlapping platinum and niobium EELS signals then map their distribution in the electrode before and after fuel cell loading (Fig. 1). The separation and mapping of the various electrode components provides valuable insight into the role of the various material components in the fuel cell ORR.

The ICA technique has also been used to study gold-platinum (AuPt) nano-particles which show great promise as durable catalysts in the ORR at the fuel cell cathode. Unlike Pt alloyed with 3d transition metals [3,4], AuPt nano-particles do not undergo leaching in the harsh chemical environment in the fuel cell. Recent studies have revealed that AuPt particles, less than 10 nm in size, exhibit properties notably different from AuPt bulk alloys. However, progress in understanding the relationship between nano-scale composition and enhanced electrocatalytic properties, has been hindered by the lack of advanced analytical techniques with both sufficiently high spatial and chemical specificity [5]. Here, ICA is used to separate the spectrally and spatially overlaying gold and platinum EELS signals acquired from Pt@Au (Pt clusters seeded on Au) nano-particles. These particles were annealed *in-situ* using a dedicated TEM sample holder and nanoscale phase transformations were tracked over the course of a thermal treatment. This *in-situ* study of nano-scale compositional and morphological changes in individual Pt@Au nanoparticles provides valuable insight towards the understanding of the enhanced surface reactivity of these nanoparticles [6].

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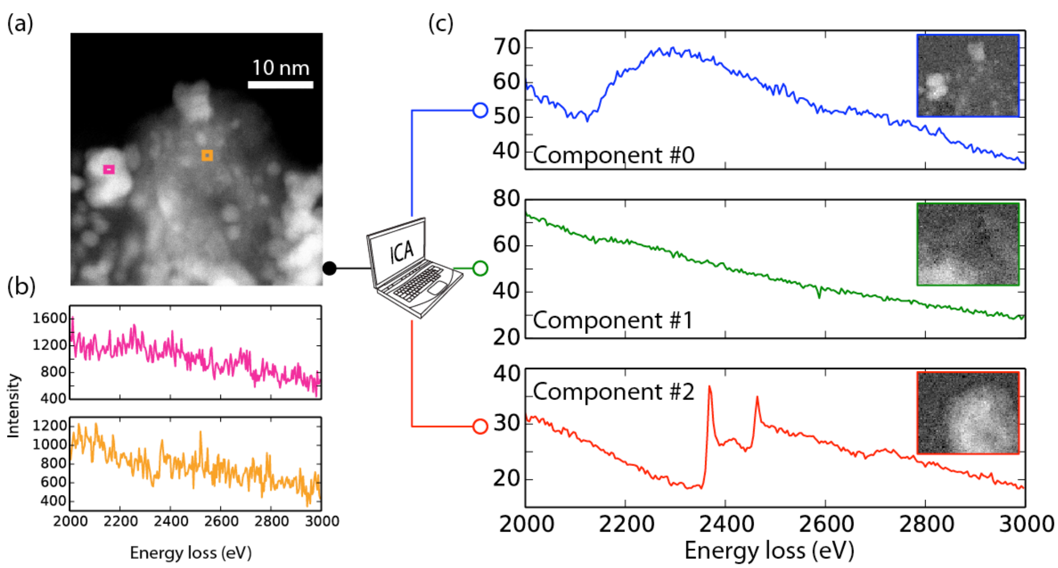

Figure 1. (a) TEM-EELS analysis of a fuel cell cathode material containing nano-particulate platinum and niobium oxide on a NbO_x-carbon hybrid support. (b) The raw spectral data are noisy due to limited beam dose to avoid sample damage. (c) ICA finds three main components in the spectral mixture, belonging to platinum and niobium.

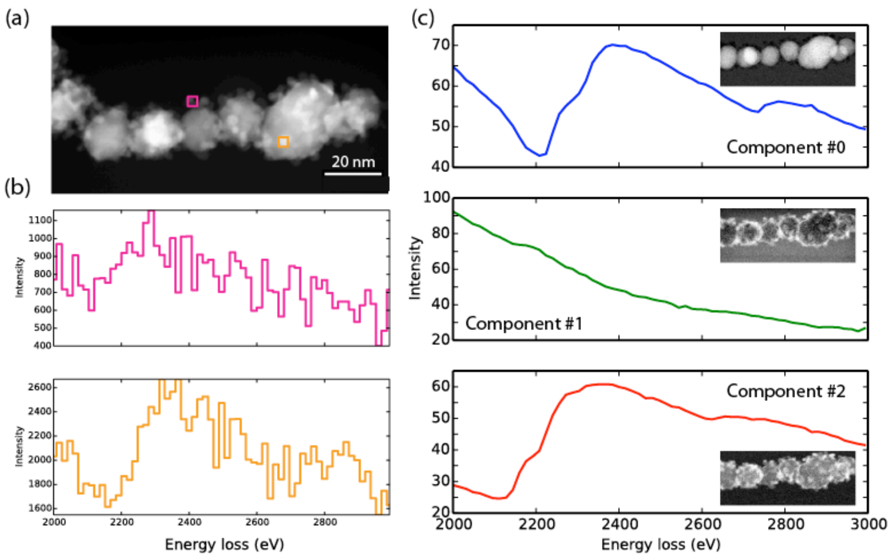

Figure 2. (a) TEM-EELS analysis of a AuPt nanoparticle ensemble. (b) Trace evidence of gold and platinum edges are present in the noisy raw EELS spectra. (c) ICA successfully separates the spectrally and spatially overlapping gold and platinum edges in the EELS signals present in the raw data.