**Combined EELS and EDX datasets probed by advanced data mining techniques**

Braidy, N.[1], B. Lavoie, F.[1] and Gosselin, R.[1]

[1] Université de Sherbrooke, Canada

TEM hyperspectral images are typically processed using background removal and peak-integration techniques or linear least-square (LLS) fitting from known references. Latent variable models such as principal component analysis (PCA) are becoming interesting alternatives capable of resolving complex mixtures into pure component contributions. Here, we demonstrate the advantages of using some of these methods for the joint analysis of EELS-EDX co-registered linescans.

EELS and EDX acquisition were simultaneously acquired from a 31 nm linescan (100 pixels) from an Intel Xeon Ivy Bridge tri-Gate 22 nm process (Fig. 1a: false color STEM image). Both EELS (Fig. 1b) and EDX (Fig. 1c) spectra exhibit strongly overlapping features and low signal-to-noise ratio. A typical peak integration failed to produce meaningful interpretation. As shown in Figs. 2a and 2b, LLS using internal references resulted into noisy elemental profiles that lack internal consistency.

Here, we jointly processed the two datasets by splicing them rather than analyzing them independently. A combination of K-means clustering and N-FINDR [1] produced an initialization set of 7 spectral components. These were then used as initial guesses in an iterative process identifying the individual spectral contributions for each pixel by maximizing the Poisson log-likelihood under the constraints of closure and non-negativity [2]. This method is particularly well-suited for low signal-to-noise ratio spectra for which the Poisson nature becomes prominent.

Fig. 3 shows the output of the algorithm: the component profiles (Fig. 3a) with their respective EELS (Fig. 3b) and EDX (Fig. 3c) components. The nature and the shape of the profiles are consistent with the expected PMOS architecture. The method successfully extracted the expected EELS and EDX spectra of Ti, Hf, La and W based layers. In addition, Si and $SiO_2$ could be discriminated, without the use of internal references. The end-member spectra associated to the $HfO_2$ layer highlights the presence of Si, which was not visible using LLS, demonstrating the systematic presence of Si in that layer. We note that the featureless exponential EELS background associated with the Ti layer over the 1100-2100 eV energy range (Fig. 3b) could be isolated thanks to the contribution of the respective EDX component. In this case, removing the exponential background prior to analysis result in the loss of the Poisson character of the signal and makes it impossible to uncover the Ti signal in EELS (in the 1100-2100 eV range).

This technique allows high quality spectra of the components to be isolated with their corresponding maps using only the number of components as free parameter. It then becomes easier and more appropriate to conduct elemental and quantitative analyses. In addition to enabling the extraction of meaningful spectral components (unlike PCA), this method makes it possible to carry out a single analysis of several co-registered datasets. Work is under way to consider non-linear phenomena associated to changes in thickness, known to impact the EELS post-edge structures and the EDX background.

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**References** [1] Winter M. E. N-FINDR: an algorithm for fast autonomous spectral end-member determination in hyperspectral data. *Proc. SPIE* **3753** 266-275

[2] Lavoie F. B., Braidy N., Gosselin R. (2016). Including noise characteristics in MCR to improve mapping and component extraction from spectral images. *Chemometrics and Intelligent Laboratory Systems* **153** 40-50.

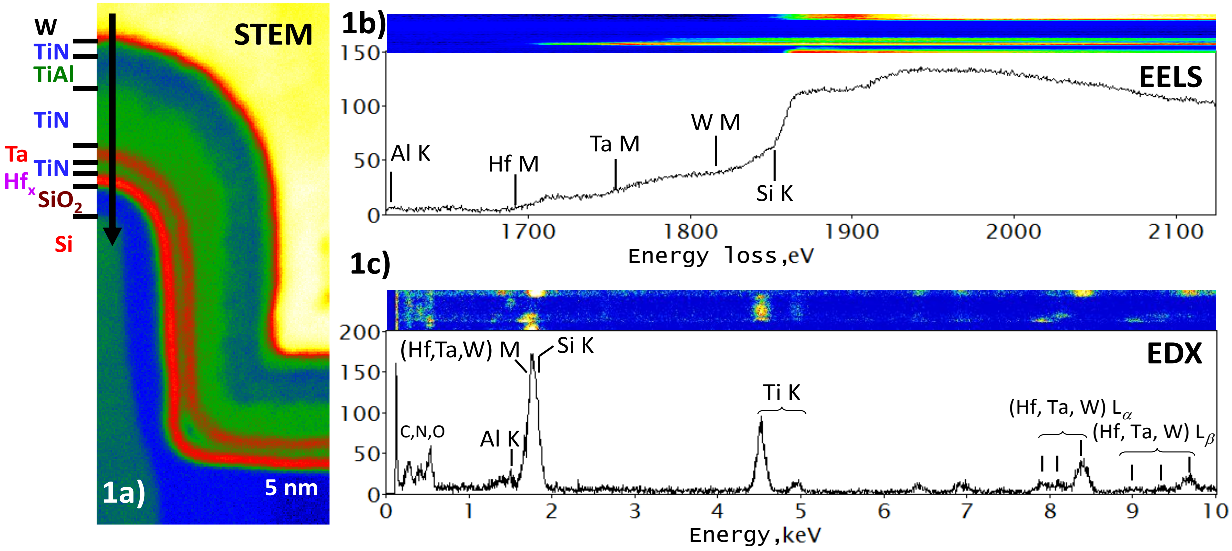


*Fig. 1. (a) False color representation of STEM image of PMOS gate stack showing the scan location.(b) EELS and (c) EDX spectrum images and sum spectra.*

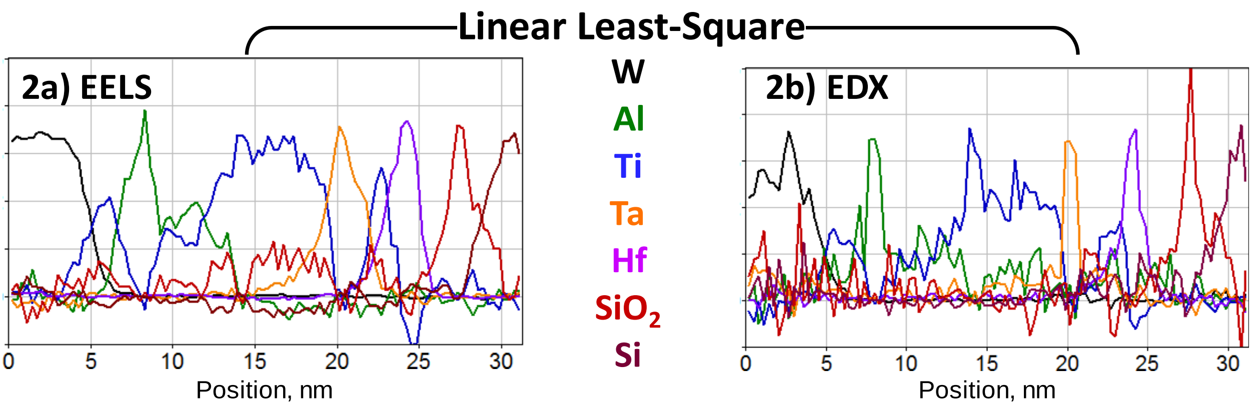


*Fig. 2. (a) EELS and (b) EDX elemental profiles produced by linear least-square fitting using internal references.*

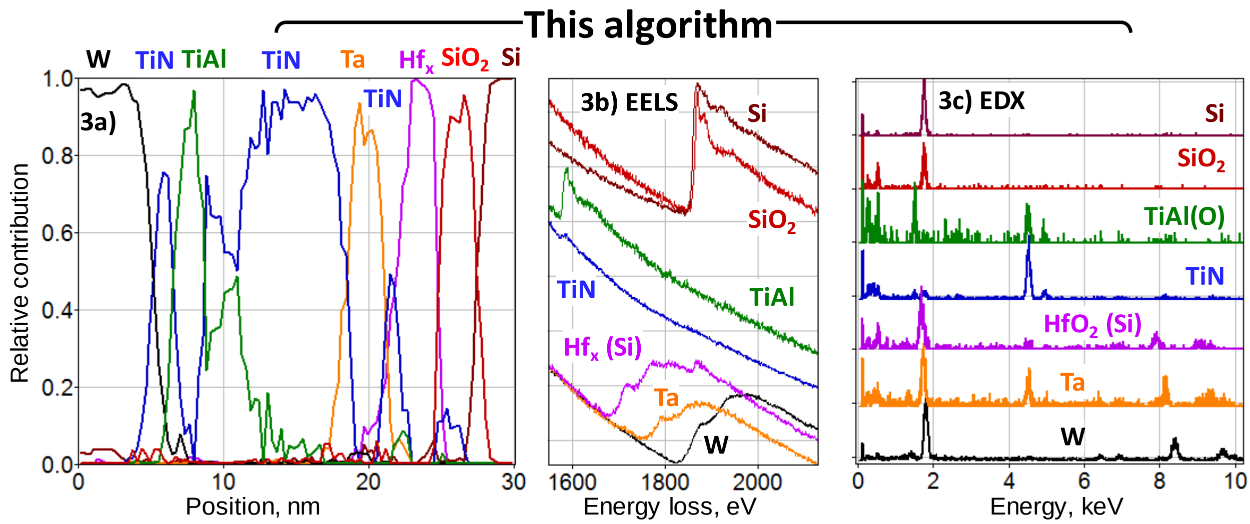


*Fig. 3. (a) Component profiles with corresponding (b) EELS and (c) EDX component spectra extracted using K-means followed by N-FINDR and the maximum likelihood algorithm.*