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A Method of Component Extraction of EDS and EELS maps

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In microanalysis, we generate elemental maps from analytical data, such as EDS and EELS, to show the spatial distribution of elements of interest. In either EDS or EELS, the intensity of a map pixel may have contributions from multiple components. For example, overlapping signals, x-ray fluorescence (for EDS), or spatial mixture can form mixture maps. To obtain a map for each individual component, we need to find a way to calculate each individual contribution. A commonly used method to separate overlapping signals is to deconvolute the source signal. For situation of x-ray fluorescence or spatial mixture, spectral deconvolution is not applicable.

Here we demonstrate a component extraction method on EDS and EELS maps. Let $I(x,y)$ be the intensity function of a map. Suppose $I(x,y)$ has contributions from two components, $A(x,y)$, and $B(x,y)$, from signal a and b, respectively. Mapping is obtained through integration of a signal over a fixed window and integration is a linear operation, we thus have, $I(x,y) = A(x,y) + B(x,y)$. If we know $B(x,y)$, we get a pure $A(x,y)$ through a simple subtraction, $I(x,y) – B(x,y)$. The way to find $B(x,y)$ is to form a map $C(x,y)$ over the same region. $C(x,y)$ is a map generated from signal c. The criteria of choosing c are: (1) the map $C(x,y)$ has a region free of contribution of a, (2) c has no signal overlap with a, and (3) the intensity of c is linearly proportional to b. With $C(x,y)$, we can strip the contribution of b, and obtaining the $A(x,y)$ through the following equation,

$$A(x,y)= I(x,y) - k\cdot C(x,y) \qquad (1)$$

Where, k is a constant independent of spatial coordinates and its value is $B(x,y)/C(x,y)$. $A(x,y)$ can be explicably solved since $I(x,y)$ and $C(x,y)$ are simply the pixel reading of maps. The key is finding the constant k. This is through the region free of contribution of a, in which $B(x,y)/C(x,y)$ is a constant. By comparing the pixel intensity ratio, we compute the value k. With the value k being a constant, eq. (1) is simply image subtraction.

For EDS or EELS, it is always possible to find such a component like c. For example, Fig. 1 (A) is "*Si-kα* map". Because *Si-kα* peak overlaps with *W-Mα1* peak, the map contains *W* component. From examination of local EDS spectrum, we know the vertical bright structure is pure W. Thus we pick a *W-Lα1* signal to be our c (Fig. 1B). The ratio k is found by comparing pixel intensities of *W-Lα1* map and "*Si-kα* map" at a Si-free region (such as the area marked by the box in Fig. 1(B). If the component c is not readily available on the sample, we can put a piece of material containing c onto the sample by FIB manipulation. There are two methods in choosing c: (1) c can be a different signal, such as different EDS peaks, EELS edges, or from different type of detector, of the same element; (2) c can be from a different element of a chemical compound.

The process described by Eq. 1 can be readily extended to maps with more than two components. Fig. 2 shows the result of pure component maps involving signal overlaps and x-ray fluorescence. With iterative application of Eq. 1, a clean spatial distribution of each individual element is obtained (Fig. 2B).

Through computer programming, the calculation of Eq. 1 can be easily automated. Fig. 3 shows a program written with Gatan® DigitalMicrograph scripting language. When a user selects a region for c, a subtraction image is formed by $I – k\cdot C$, with k value selected such that the average intensity of the same selected area in the subtraction image is zero. The application of this method is limited to thin samples, when $b:c$ linearity requirement is satisfied. For thick sample, this method losses its accuracy and eventually becomes not applicable when the linearity between b and c does not hold due to absorption.

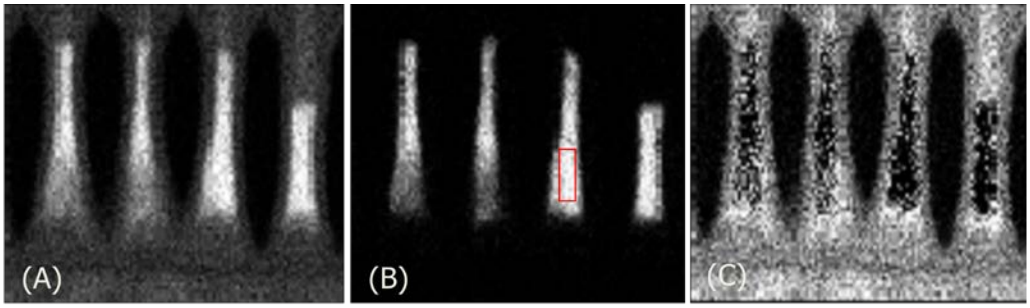

Fig. 1. EDS maps. (A) Si-Kα map, contaminated by W-Mα1 signal. (B) W-Lα1 map. (C) Si map stripped of W component.

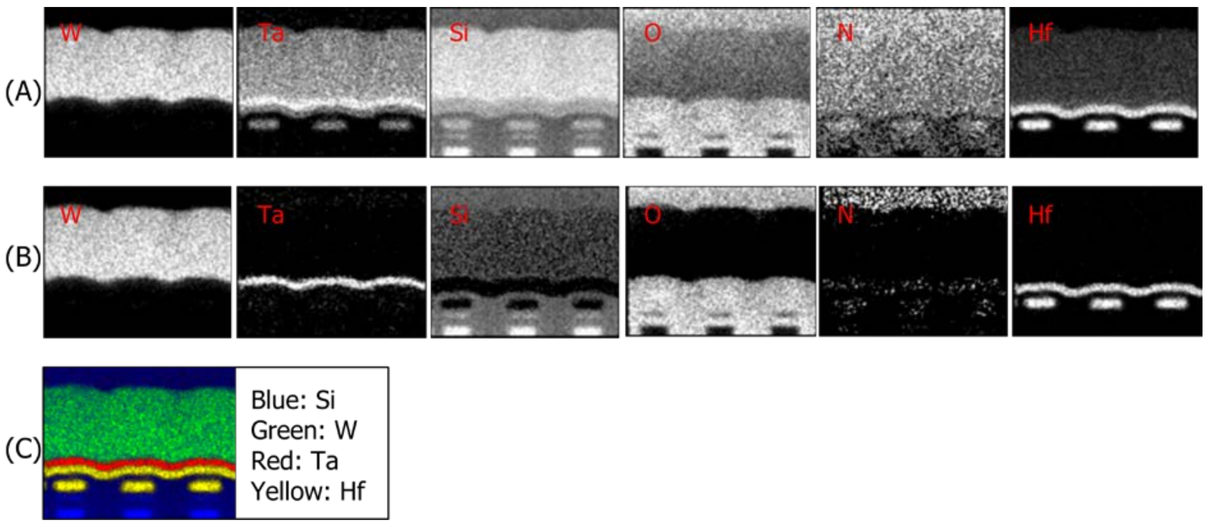

Fig. 2. EDS maps. (A) Original unprocessed maps. (B) pure component maps. (C) color overlays of true elemental maps.

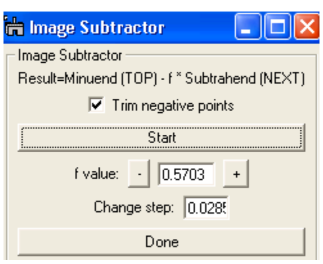

Fig. 3. A computer program to carry out the map component extractions interactively.

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