

## 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,

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

Where,  $k$  is a constant independent of spatial coordinates and its value is  $B(x,y)/C(x,y)$ .  $A(x,y)$  can be explicitly 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-ka* map”. Because *Si-ka* peak overlaps with *W-Ma1* 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-La1* signal to be our  $c$  (Fig. 1B). The ratio  $k$  is found by comparing pixel intensities of *W-La1* map and “*Si-ka* 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.

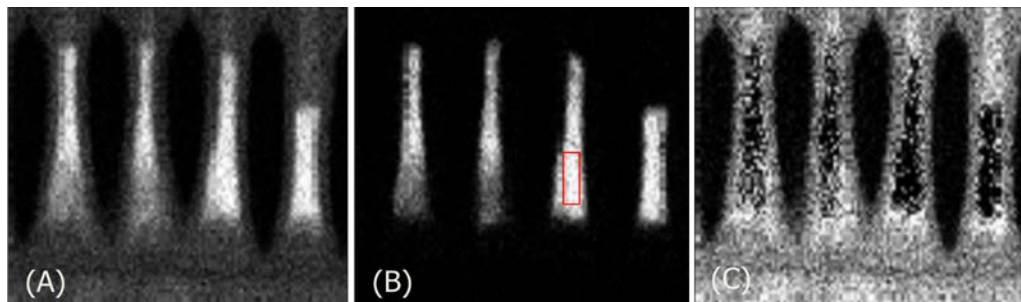


Fig. 1. EDS maps. (A) Si-Kα map, contaminated by W-Mα1 signal. (B) W-Lα1 map. (C) Si map stripped of W component.

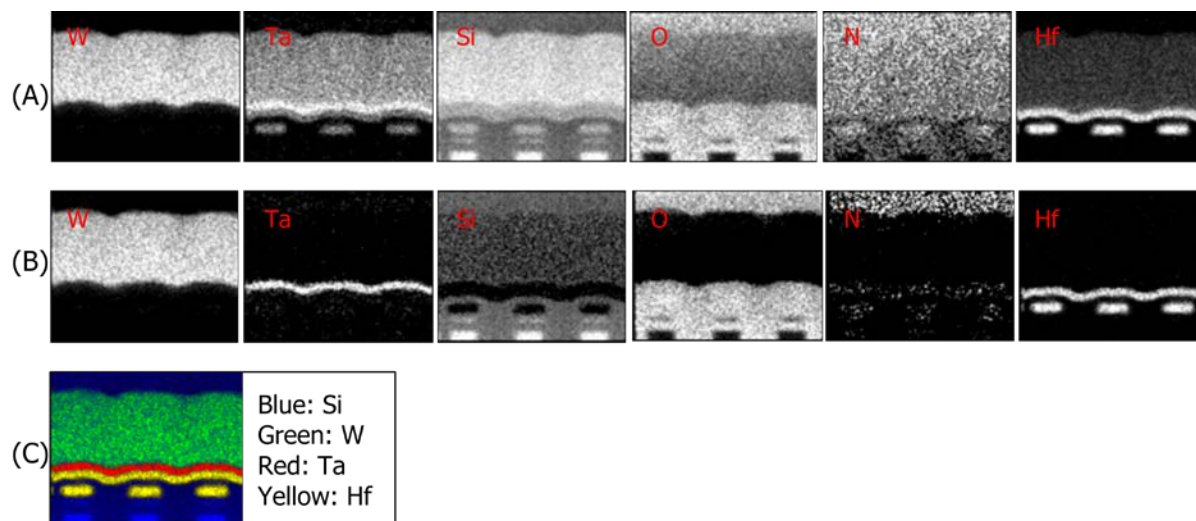


Fig. 2. EDS maps. (A) Original unprocessed maps. (B) pure component maps. (C) color overlays of true elemental maps.

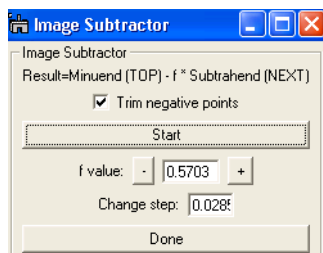


Fig. 3. A computer program to carry out the map component extractions interactively.