

# COMPASS: More Accurate than Elemental Mapping

## Key Words

- COMPASS
- Component Analysis
- Peak Overlaps
- Spectral Imaging
- X-ray Mapping

A primary concern for many investigators is understanding the spatial distribution of elements within a sample. The method to obtain these distributions in the SEM with EDS has been through the use of X-ray maps provided by traditional means or as extractions from a Spectral Imaging data set. There are, however, some potential problems with elemental mapping that must be considered to correctly understand the sample.

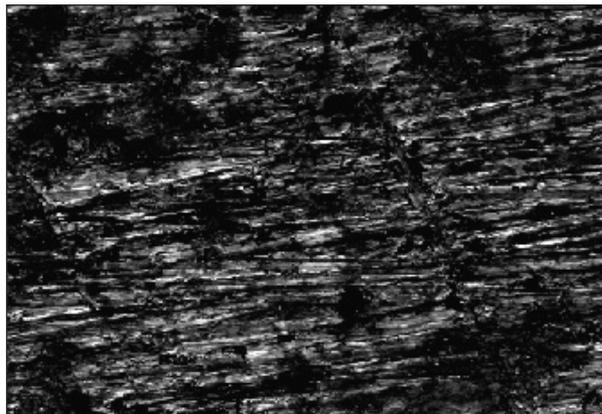
The COMPASS statistical analysis option on the Thermo Scientific NORAN System 7 avoids these problems while simplifying the interpretation of the Spectral Imaging data set.

## Problems with Elemental Maps

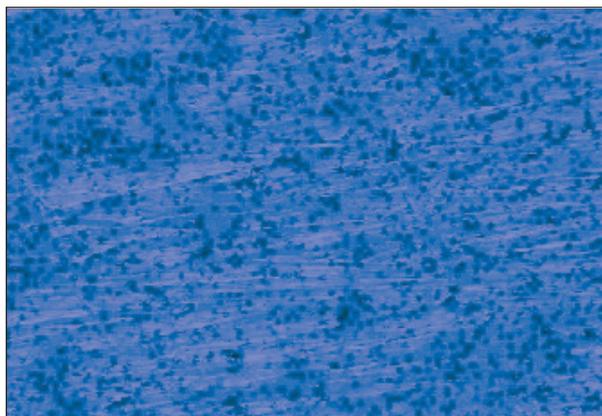
The biggest problem with traditional mapping is the need to know all the elements of interest that exist in your sample before the data collection is started. If an element is not expected but is present, a “black hole” may appear in the maps at its location or the element may go totally unnoticed. The use of Spectral Imaging data acquisition reduces this problem by collecting complete spectrum at each location. This permits elemental map extraction of the unexpected element days or even years after the data was collected. However, it is still the responsibility of the user to identify and choose the element(s) for mapping.

An additional problem with maps is the high background signal, usually for low energy X-rays, arising from the Bremsstrahlung. Maps of features from peaks located on the high Bremsstrahlung that have a low concentration will have a high background intensity and low signal-to-noise ratio. Visual delineation of the features within the maps may be either difficult or impossible. This will lead to bad interpretation of the data and faulty conclusions.

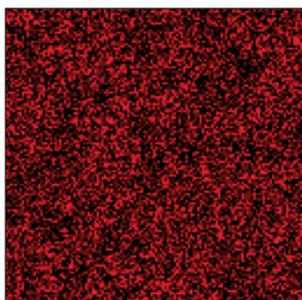
The final problem can arise from pathological peak overlaps. If there is a need to map multiple elements which have important peaks that are closely spaced in energy, improper contributions of each element into the map of the other will occur. Manual adjustment of the



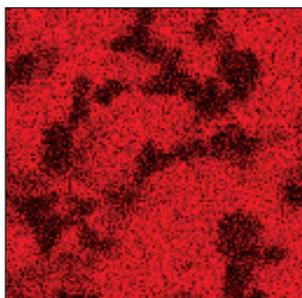
SEM image with few features



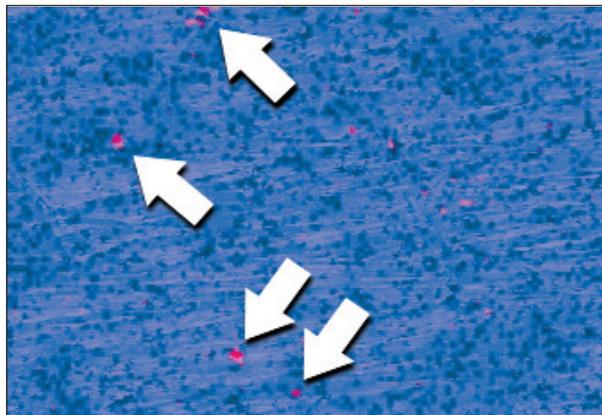
Map of all expected elements



Low signal Mn L map



High signal Mn K map

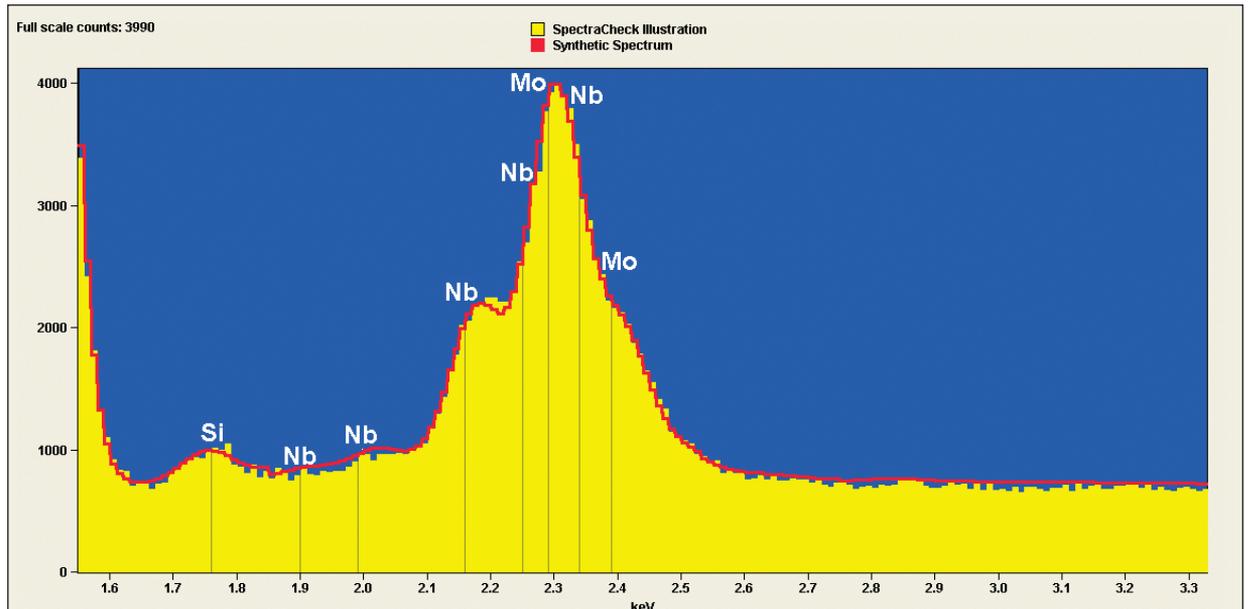


Map of ALL elements

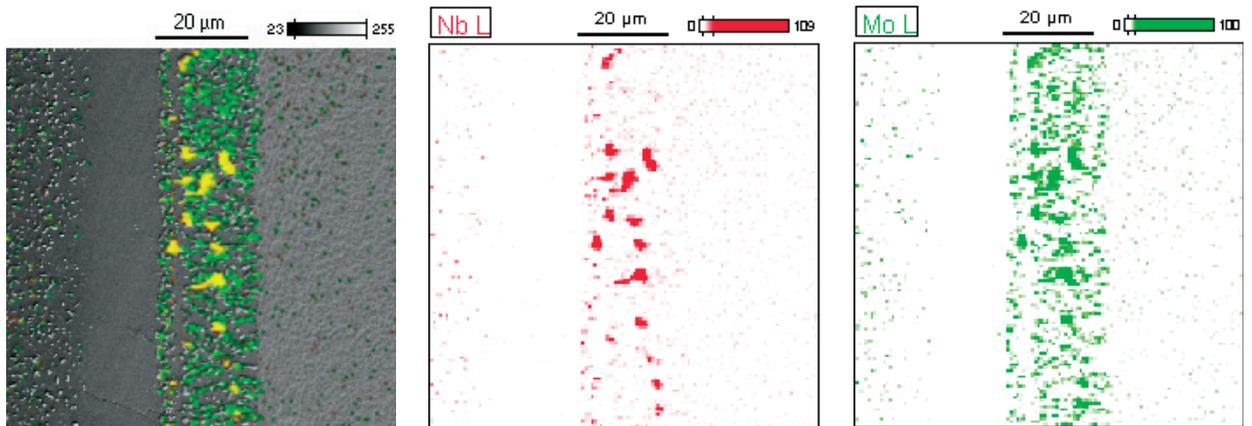
energy region-of-interest will only help slightly, but will not eliminate the problem. Visual delineation of the features from the maps may be either difficult or impossible. This will lead to bad interpretation of the data and faulty conclusions.

This can be shown for a multiphase material that has both Nb and Mo which have a peak overlap near 2.25keV.

Extracting simple X-ray maps of the elements indicates that there are regions which contain only Mo (pure green) and regions where the Nb and Mo overlap (yellow), but no regions where Nb (red) is alone. The analysis below will demonstrate that this interpretation is flawed.



Spectrum of multiphase material showing Nb and Mo peaks



SEM image with map overlays

Nb X-ray map

Mo X-ray map

## COMPASS to the Rescue

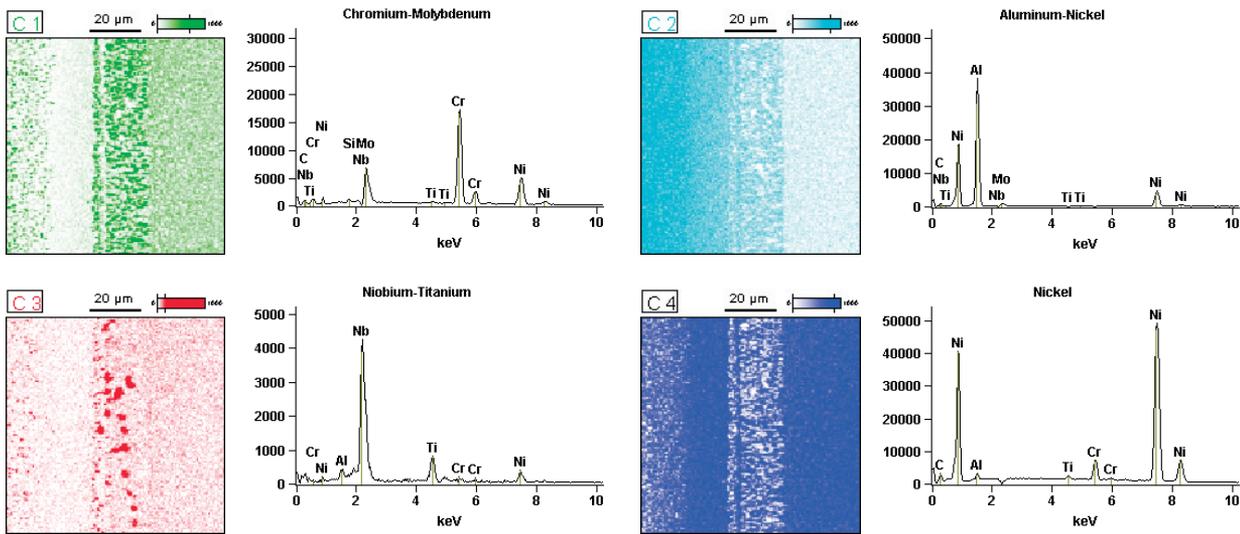
The previous examples show that user interpretation can be either biased (missing elements) or distorted (background and overlaps) by inexact methodology. What is required to avoid such pitfalls is a robust principal component statistical analysis that analyzes all of the data and provides meaningful and interpretable results for the user. COMPASS is the premier method for analyzing Spectral Imaging data sets.

The COMPASS analysis does not start with X-ray maps, because user bias may have already been introduced. COMPASS analyzes the whole of the Spectral Imaging data set and compares every spectrum to every other spectrum looking for similarities. No *a priori* knowledge about possible or expected elements or peaks is required. Nor are any “user-selectable sensitivity” factors needed where the analyst may have no idea of the range of values or final effect. COMPASS performs the direct comparison for you, automatically.

The results produced by COMPASS (shown below) are easily interpretable. They consist of probability maps of the identified components (phases) and a related pure component spectrum.

Results important for this discussion are the data for the chromium-molybdenum and niobium-titanium components. The maps appear similar to the Nb and Mo maps discussed previously. Upon closer examination, however, significant differences exist.

Where the pure X-ray maps indicated no exclusive Nb regions, the COMPASS results show distinct regions of Nb-rich (red) and Mo-rich (green) material but little if any overlapped regions (yellow). Another interesting result is that the spectra for the two pure components have the proper peak shapes that are expected for the elemental species. They are not abruptly cut-off at a central energy as would occur if X-ray map regions-of-interest were manually chosen by the user but are well-formed peaks that are easily identified by the automatic qualitative analysis routine.



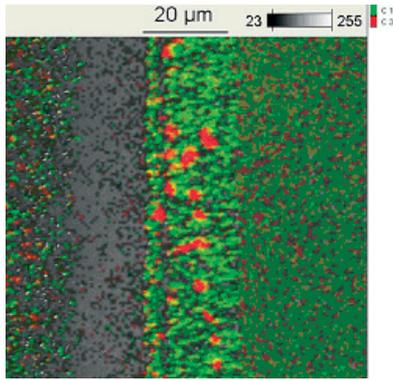
COMPASS Results

These results indicate that COMPASS is intelligent enough to find the compositionally distinct components (phases), can spatially separate components that have severe peak overlap problems, and can spectrally separate the X-rays of the components, all without user intervention. And the results are correct.

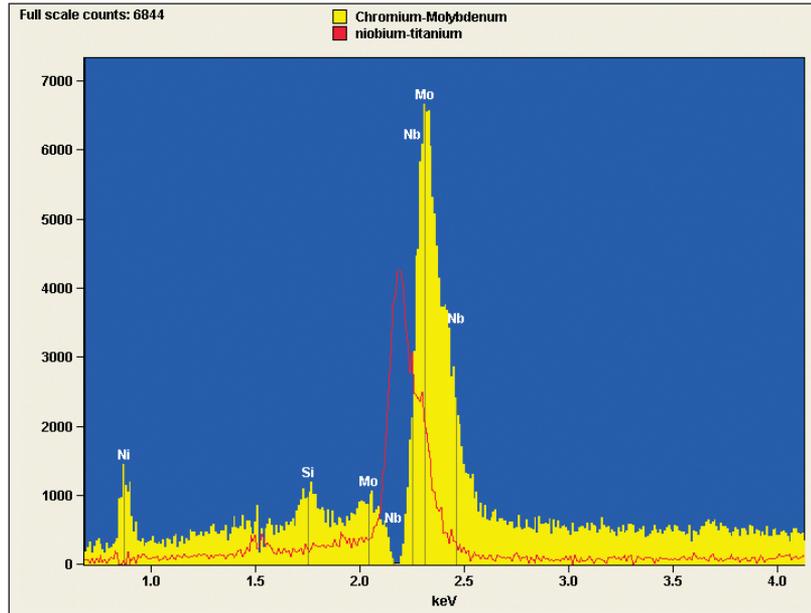
## Conclusions

Phase determination using X-ray maps is burdened with problems. Any conclusions drawn must still be verified.

The COMPASS option on the NORAN System 7 automatically performs primary component analysis without user intervention. The user is confident that any conclusions drawn from the results are accurate.



COMPASS results showing distinct regions of Nb-rich (red) and Mo-rich (green) material



Spectra for the two pure components with proper peak shapes expected for the elemental species

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