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Automatic Phase Labeling During Spectral Imaging Acquisitions

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Analysts using any technique would prefer that the instrumentation uniquely characterize the measured results using familiar phase nomenclature. For instance, a materials analyst in an analysis laboratory for a steel company who is tasked with identifying a material would prefer a report using a common label that has more meaning to them (304 Stainless Steel) in place of a report of elemental compositions (Fe – 18 Cr – 8 Ni). While phase labeling for spectral analyses has been routine for many years, phase detection from spectral imaging data cubes, with phase labeling is a recent development. Most of these schemes, however, have typically been performed after the acquisition is complete, i.e. in analysis mode. Finally, automatic phase identification and labeling has now been implemented for spectral imaging acquisitions.

Phase labeling for spectra has typically required the two-step process of acquiring the complete spectrum and then labeling, although the labeling could be done during the acquisition. The labeling operation could be done in at least two ways. The fastest method is to compare the elemental quantification values of the spectrum to a list of expected composition values input by the user. This method can be called “Chemical Typing”. The second method is to compare the whole acquired spectrum against user-stored spectra in a database, called “Spectral Match”. The advantage of this method is the lack of user-input in correctly identifying the elements for quantification. The disadvantage is the need to collect a spectrum to add to the database.

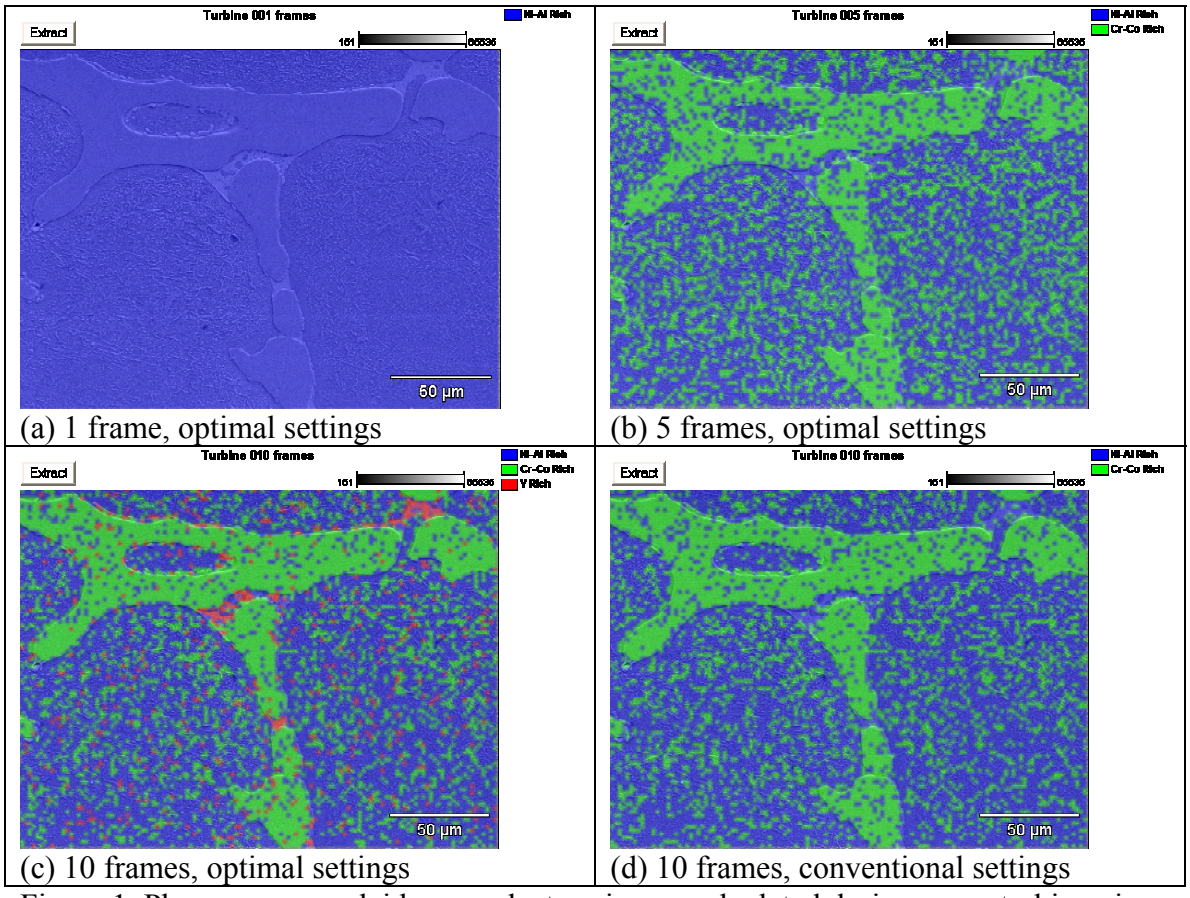
Phase discrimination for mapping acquisitions has been available for many years as a post-acquisition analysis technique. The discrimination operation involves comparing the intensity values of the elemental maps and looking for unique overlaps or combinations. This operation has even been adapted to use quantitative elemental maps. The disadvantage of these techniques is the requirement that the user select all of the relevant elements. If a key element is not selected, a phase may not be found. No automatic labeling of the phases has been reported.

For spectral imaging data cubes, phase discrimination is becoming routine and automatic labeling of the phases is possible. The discrimination is typically performed using multi-variant statistical analysis (MSA or COMPASS) which provide phase maps and spectra. These spectra can then be labeled using the techniques described previously. The advantage of using a MSA approach is the lack of user bias on the input data and the ability of the algorithm to provide phase identification for features that the analyst did not know exists in the sample. As powerful as this technique has become, it was still a post-acquisition analysis technique primarily due to the calculation time and the minimum number of x-ray events necessary to obtain meaningful phase results.

The advent of faster computers and refinements in MSA routines now permit automatic phase discrimination and labeling to be permitted during a spectral imaging acquisition. As the spectral imaging data cube is being filled, the MSA analysis is performed

periodically. Because the amount of data is limited at the beginning of the acquisition, internal MSA parameters are adjusted during the acquisition to provide the greatest level of phase detail possible from the amount of data available at that moment. These new parameter adjustments also provide better phase discrimination with less data than was available previously. From the instantaneous phase maps and spectra, phase labeling is performed as described above. All of these operations can be performed on a regular basis even while the x-rays are detected at the maximum storage rate of the analyzer.

Automatic phase labeling is the desire of most analytical analysis reporting. Automatic phase discrimination and labeling of mapped regions has developed into a routine operation. The ability to finally perform automatic phase labeling during a spectral imaging data acquisition is the pinnacle of sample analysis reporting.



(a) 1 frame, optimal settings

(b) 5 frames, optimal settings

(c) 10 frames, optimal settings

(d) 10 frames, conventional settings

Figure 1. Phase maps overlaid on an electron image calculated during a spectral imaging acquisition. Each frame time was selected as the first frame in which the number of phases changed. As the amount of data increases, more phases appear. The new optimal MSA settings permit the identification of more phases with less data than conventional settings.

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