



Accelerating Ion Beam Analysis with Artificial Intelligence

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Ion Beam Analysis (IBA) is a group of spectroscopy techniques that allows non-destructive elemental analysis of any solid material. The good knowledge of the underlying physics governing elastic and inelastic interactions of a light ion beam with a target gives access to absolute elemental concentrations and depth profiles, from H to U, either present as major or trace elements. These data are generally accessible using simultaneously at least two IBA spectroscopy techniques. Fitting these spectra is commonly a heavy duty since one needs to keep a consistency between them, each technique being sensitive to a specific range of elements. Moreover, up to date, no software is available to process conveniently these spectra in a unified way. Consequently, users have to iterate between various software programs until reaching a global coherence.

These difficulties are even more amplified when IBA is performed in micro-beam mode, where each analyzed pixel represent a set of spectra. Here we need an additional step to extract similar pixels corresponding to the same chemical phase before going to spectra fitting.

We recently investigated the use of artificial intelligence techniques to automatically process the raw data and obtain the desired quantities, based on unsupervised hyperspectral imaging segmentation for micro-IBA mode, and neural network based machine learning for simultaneous spectra processing.

We found that chemical phases from micro-IBA experiments and corresponding spectra mappings are efficiently extracted using multi-dimensional principal component analysis (PCA).

For spectra processing, we performed various optimizations with a special care on computing time. For this, we employ both data augmentation that efficiently increases the learning set size used to train a neural network. We also optimize the neural network by using dimensionality reduction through input data PCA conversion, a process that permit to limit substantially the neural network size without affecting performances.

We recently overcame a remaining difficulty linked to the prediction accuracy. When trained with a large number of elements, the neural network fails in discriminating between effectively present elements in the experimental targets. We added in the learning process a classification step, where a first neural network is trained at classifying the spectra depending on the effective elements.

Finally, using standard signal processing techniques, we are also able to detect and quantify trace elements that have tiny signatures in the spectra.

All these processes, when fully automatized and chained, should allow extremely fast and nearby “on the fly” IBA and micro-IBA processing.