

Combining Ion Beam Analysis and Artificial Intelligence: a route to high throughput material screening

Hicham Khodja

Université Paris-Saclay, CEA, CNRS, NIMBE, LEEL, 91191 Gif-sur-Yvette, France

hicham.khodja@cea.fr

High throughput Ion Beam Analysis (IBA), for which automated data processing is mandatory, has already been implemented by some groups but is generally restricted to a similar matrix composition and/or a fixed analytical arrangement. Moreover, the analytical information is frequently provided by a single IBA technique or is limited to a narrow range of chemical elements. Extension to strongly contrasted matrixes and to coupled IBA techniques, in particular when performed simultaneously, cannot be implemented with currently available tools. These difficulties are even more amplified when IBA is performed in microbeam mode, where each pixel represents a set of spectra.

Artificial Intelligence (AI) techniques became this last decade very popular since building blocks are much more accessible thanks to comprehensive computing packages, and found numerous applications in spectroscopy. In the case of IBA and micro-IBA, these techniques can efficiently help to overcome most of the listed limitations. We will present here the AI-based tools developed in the laboratory that help at automatically processing (micro-) IBA data in few seconds. We are developing these tools, based on unsupervised methods and neural network arrangements, with the ambition of being operative with any analytical setup and any sample composition.

We will also discuss uncertainty evaluation, a central, but sometimes neglected, aspect in IBA spectroscopy, and explore how we can address this point within the framework of AI.