Multivariate analysis of X-ray diffraction and XAFS data

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The structural dynamics of chemical systems can be investigated by in situ or operando X-ray experiments. Advanced and fast computational methods are needed to cope with the huge amount of data collected, and to extract precious information hidden in data through a model-free analysis. Data analysis approaches based on multivariate analysis are particularly suited to this aim, as they are able to efficiently process in a probe-independent way multiple measurements, by considering them as a whole data matrix [1].

We have developed a fully automatic and big-data set of computing procedures based on principal component analysis, which is able to process with the same algorithms in situ/operando X-ray diffraction and XAFS data to extract qualitative and quantitative information. The multivariate approach has been adapted to treat crystallographic data, by optimizing the directions of the principal components [2], or by including kinetic models in the extraction of the reaction coordinate [3]. The procedure includes several pre-processing strategies that can be applied on crystallographic and XAFS data; among them a peak-shift correction to disentangling lattice variations from changes of the atomic parameters [4]. The procedures have been implemented in the computer program RootProf [5], available from www.ic.cnr.it/ic4/en/software/. It can be also used for fast on-site analysis while running in situ experiments (Fig.1).

Here we show how in situ experiments coupled with new data analysis methods can disclose the structural mechanism underlying: i) the thermal adsorption of gas in zeolites [4]; ii) the non-isothermal solid-state synthesis of materials based on poly-aromatic molecular complexes [6]; iii) the temperature-induced transitions of metal halide perovskites [7].

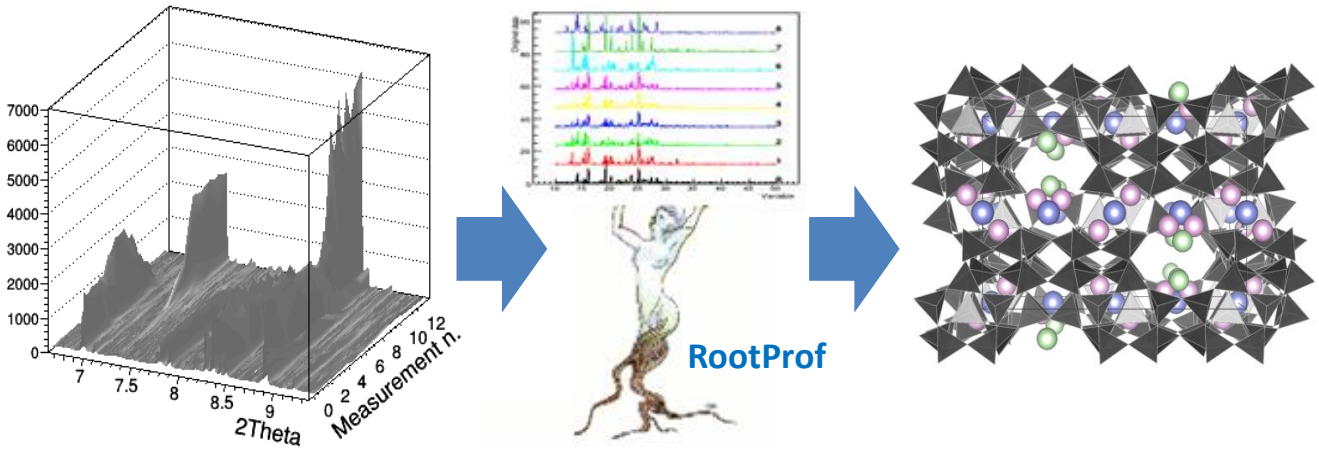

Figure 1. The RootProf program processes data from in situ experiments to locate atoms responding to an external stimulus.

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