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Principal component analysis used for structural and elementary datas coming from iron corrosion products layer

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Predict how corrosion evolves for centuries in iron materials is decisive as well in nuclear field in order to evaluate the nuclear waste containers thickness and in heritage for conservation of metal items. Our goal is to describe the Corrosion Product Layers (CPLs) which grew up under natural conditions in order to understand atmospheric corrosion mechanisms and the role of the layer in those phenomena.

For that, we decide to find correlations between minor chemical elements and mineralogical compositions localization in iron CPLs. For data collection, we use Raman spectroscopy and MEB-EDS with a micrometric resolution. Ferrihydrite (FeOOH, nH_2O) is one of the most reactive oxidized phases of iron which can see its reactivity be inhibited by adsorption of phosphorus. On a little area of cross section of a clamp coming from a French Cathedral, one shows there are correlations between phosphorus and ferrihydrite [1] in iron CPLs.

In order to check this observation, we propose to acquire, on large areas, Raman and MEB-EDS hyperspectral images. By a self-made program in Python, those data are analyzed by multiway analysis like Principal Component Analysis (PCA) [2]. After pretreatments following by a PCA, we localize minor chemical elements (Mg, P, Cl) and phases in CPL by projecting data on principal components. We are trying to quantify these observations and developing a multiblock analysis to ensure there are correlations between minors elements and specific phases in CPLs.

[1] Bouchar, M., *Mécanismes de la corrosion atmosphérique multiséculaire des alliages ferreux : Le cas des renforts de la cathédrale de Metz.* 2015

[2] Massart, D.L., et al., *Handbook of Chemometrics and Qualimetrics,* 1997: Elsevier Science Inc.