**MS43 Crystallography for cultural heritage materials**

MS43-04

Application of multivariate analysis to X-ray diffraction tomography: the study of medieval applied brocades

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Abstract

X-ray diffraction tomography (XRD-CT) is a recognized technique for structural investigation of heterogeneous materials, which makes it a tool of choice for the non-destructive analysis of cultural heritage micro-samples. Characterization of such complex samples with a sufficiently high spatial resolution requires the acquisition of a large number of diffraction images (typically several tens of thousands), followed by a sequence of multiple data manipulations and corrections to locate the various phases in the samples. Here we propose to use multivariate analysis to automatically break down the data into a small set of components, each representing the diffraction pattern of one or a small number of phases. This makes the identification of phases and the quantification of each component much more efficient and leads to a quantitative determination of the phase content of each voxel of the tomographic reconstruction, without a priori knowledge about the sample composition. We show that the NMF (Non-negative Matrix Factorization) method is very effective for this purpose, with a computation time suitable for online data analysis in order to e.g. assess the quality of measurements during synchrotron experiments. Here, we apply this method to the study of micro-samples of medieval applied brocade decorations taken from a wooden statue [1,2] which was found to contain as many as 11 different phases. The figure shows an exemple of tomographic reconstruction of the 11 phase concentrations after 6-component NMF multivariate analysis. From left to right and top to bottom: gypsum, cinnabar, beeswax, romarchite, cassiterite, cerussite, hydrocerussite, goethite, minium, gold, chlorargyrite.The results are validated a posteriori by comparison with analytical techniques requiring sample preparation and therefore destructive (SEM- EDX, IRTF, Raman) and sequential Rietveld refinement.

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References

[1] Martinetto, P., Blanc, N., Bordet, P., Champdavoine, S., Fabre, F., Guiblain, T., Hodeau, J.-L., Lelong, F., Leynaud, O., Prat, A., Pouyet, E., Uher, E., Walter, Ph. (2021). J. Cult. Herit., 47, 89-99.

[2] Bordet P., Kergourlay F., Pinto A., Blanc N., Martinetto P. (2021). J. Anal. At. Spectrom., 36, 1724

Phase concentrations from NMF