Contribution ID: **86** Type: **not specified**

Comparison of different methods for evaluating quantitative XRF data in copper-based artefacts

Friday, 23 June 2023 12:40 (20 minutes)

X-ray Fluorescence (XRF) analysis with energy dispersive spectrometers (ED-XRF) is a versatile, multi-elemental analytical technique able to determine the major, minor and trace elements of a broad range of different materials in a non-invasive way and in short measuring times. The non-destructive capabilities of XRF are indeed particularly suited to research in the field of cultural heritage where the sample is unique, or its integrity has significant technical or esthetic value [1]. In the last decades, technological developments in X-ray generation and detection have led to the production and commercialization of different types of portable instruments [2], such as the so-called hand-held XRF devices, which allow both qualitative and quantitative analysis of samples in situ. In the cultural heritage field, the opportunity to avoid sampling by on-site field analyses through a non-destructive and non-invasive method is significant, and for this reason, different hand-held XRF devices are employed and performed ad hoc also for this sector.
Quantitative XRF analysis requires the conversion of measured intensities of the characteristic radiation to the concentrations of the elements to be determined [3]. Numerous methods, both empirical and theoretical, have been proposed for quantitative X-ray fluorescence analysis [4] and all hand-held analyzers are equipped with programs providing quantitative results using one of them. Usually, the results of measurements are derived from the X-ray spectra of the sample using either an empirical calibration or one based on the Fundamental Parameter approach [5].
In this study, we compare the quantitative XRF results, obtained by a commercial hand-held XRF device "Bruker Tracer 5g", using these two different approaches methods.
In detail, the XRF data were achieved by the analysis of twenty-six (26) certified standards, compositionally significant of heritage copper-based artefacts. The measured elemental concentrations were derived using three different calibrations. Two of them are based on empirical coefficients: one was loaded into the device by Bruker when instruments were purchased, whereas the other is a customized calibration from us through the "Bruker EasyCal software"; while the third one was performed with the fundamental parameter-based PyMCA software [6], which was used properly configured to account for all the required set-up and spectrometer characteristics.
The results of this study will be very useful for future in situ measurements of copper-based manufact in order to select the most suitable quantitative method.

[1] Liritzis I, Zacharias N, "Portable XRF of archaeological artifacts: current research, potentials and limitations", In: ShackleyMS (Eds), "Xray fluorescence spectrometry (XRF) in geoarchaeology", Springer, New York, 2011, pp. 109–142.
[2] Francesca Gherardi, "Handheld X-Ray fluorescence analysis of archaeological artefacts: challenges, advantages and limitations", Analytical Methods, vol.13, pp. 3731- 3734.
[3] A.Markowicz, "An overview of quantification methods in energy-dispersive X-ray fluorescence analysis", Pramana –J. Phys., Vol. 76, No. 2, 2011, pp. 321-329.
[4] Sitko Rafal, Zawisza Beata, "Quantification in X-Ray Fluorescence Spectrometry", In: Shatendra K. Sharma (Eds.), "X- Ray Spectroscopy", IntechOpen, 2012, pp. 137-162.
[5] S.Piorek, "Handheld X-Ray Fluorescence (HHXRF)"In: R.A.Crocombe, P.E.Leary, B.W.Kammrath (Eds.), "Portable Spectroscopy and Spectrometry 2: Applications", 1st edition, John Wiley and Sons Ltd, 2021, pp. 423–453.
[6] V.A.Solé, E.Papillon, M.Cotte, P.Walter, J.Susini, "A multiplatform code for the analysis of energy-dispersive X-ray fluorescence spectra", Spectrochimica Acta B, vol.62, 2007, pp.63-68.

Summary

Primary author: Dr KONSTANTAKOPOULOU, Eleni (Polytechnic School, Aristotle University of Thessaloniki (AUTH), University Campus, 54124 Thessaloniki, Greece)

Co-authors: Dr CASANOVA MUNICCHIA, Annalaura (Institute of Heritage Science (CNR-ISPC), National Research Council of Italy, Area della Ricerca di Roma 1, Montelibretti, Via Salaria Km 29,300, 00015 Rome, Italy); Dr LUVIDI, Loredana (Institute of Heritage Science (CNR-ISPC), National Research Council of Italy, Area della Ricerca di Roma 1, Montelibretti, Via Salaria Km 29,300, 00015 Rome, Italy); Dr FERRETTI, Marco (Institute of Heritage Science (CNR-ISPC), National Research Council of Italy, Area della Ricerca di Roma 1, Montelibretti, Via Salaria Km 29,300, 00015 Rome, Italy)

Presenter: Dr KONSTANTAKOPOULOU, Eleni (Polytechnic School, Aristotle University of Thessaloniki (AUTH), University Campus, 54124 Thessaloniki, Greece)

Session Classification: X-ray applications in various fields