Trace Analysis: Quantification Problems in 1, 2 or 3 Dimensions

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X-ray fluorescence (XRF) analysis based characterization and quantification of numerous types of specimens is a well-established (mostly) destruction-free technique used for a long time already. However, the occurrence of deviations in results between two (nominally) identical samples, between labs and even the same sample measured at different times may rise concerns about the reliability and questions how to improve it. While the physics is of course the same, all parts of the analysis can have significant effects and need to be regarded closely, e.g.

- sampling and sample distribution (selection of representative sample fractions of the specimen, sample mass [1], lateral distribution on the sample carrier (droplet, pico/nano-droplets, layer-like))
- instrumental parameters (beam size and shape (parallel, focused), detector field-of-view [2], convergence/divergence, monochromaticity/bandwidth, coherence [3])
- measurement procedure (sample orientation on the carrier and relative to beam and detector, spectrum evaluation, secondary fluorescence, internal/external standards, fundamental parameters (FPs))

XRF instruments equipped with the possibility to modify the beam incidence angle let new effects occur that were not known or at least not too obvious in previous fixed angle devices. On the other hand, this option for grazing incidence XRF (GI-XRF), in the past mainly restricted to synchrotrons [4,5], is now possible in numerous labs. This provides the opportunity for deeper analysis and understanding of such effects. A current cooperation project within the framework of the German "WIPANO (Wissens- und Technologietransfer durch Patente und Normen)" program aims at addressing several of those aspects. Further, a COST action [6] was started on new methods and instrumentation for screening of hazardous elements in the health & food area. Some of the mentioned aspects will be discussed in this presentation together with ideas and motivations for future works and possible cooperations.

References:

- [1] R. Klockenkämper, A. von Bohlen, Spectrochimica Acta 44B, 1989, 461-469
- [2] B. Beckhoff, R. Fliegauf, M. Kolbe, M. Müller, J. Weser, G. Ulm, Analytical Chemistry 79, 2007, 7873-7882
- [3] A. von Bohlen, M. Krämer, C. Sternemann, M. Paulus, Journal of Analytical Atomic Spectrometry 24, 2009, 792-800
- [4] M. Krämer, A. von Bohlen, C. Sternemann, M. Paulus, R. Hergenröder, Journal of Analytical Atomic Spectrometry 21, 2006, 1136-1142
- [5] M. Krämer, A. von Bohlen, C. Sternemann, M. Paulus, R. Hergenröder, Applied Surface Science 253, 2007, 3533-3542
- [6] COST Action CA18130, European Network for Chemical Elemental Analysis by Total Reflection X-Ray Fluorescence ENFORCE TXRF, www.cost.eu/actions/CA18130