

Can laboratory-XAFS compete with XRD and Mössbauerspectroscopy for quantitative analysis?

Background

While Mössbauer- and XRD-spectroscopy are frequently used Methods for quantitative analysis, X-ray Absorption Fine Structure (XAFS) Spectroscopy is not a common technique due to its limited access at synchrotron radiation facilities.

The advent of powerful laboratory instrumentation [1] may change this and make quantitative XAFS attractive for a wide range of research field, such as catalysis, mineralogy, etc. or industrial applications. Quantitative analysis via XASF has a great advantage over XRD, since it can operate on amorphous and liquid materials as well. With this work we compare these three methods for quantitative analysis of solid state samples

Methods

Different techniques for quantitative analysis have been performed on a Mexican mineral to determine the magnetite and hematite content. The XAFS Spectroscopy has been performed at our laboratory setup at the Berlin Laboratory of innovative X-ray Technologies (BLIX) at the Technical University of Berlin. The quantification was done by a linear combination of reference spectra. Mössbauer- and XRD-spectroscopy were carry out at the Leibnitz University in Hannover.

Results

The results shows quantitative Analysis can be done by laboratory-XAFS spectroscopy. Repeated measurements confirmed the reproducibility of this technique. Comparisons with XRD- and Mössbauer-spectroscopy were used to verify the results. While the first Mössbauer-spectroscopy results deviate from the XAFS results, the XRD-Spectroscopy supports them.

Conclusion

After the successful application of the Laboratory-XAFS quantification methods via linear combination of references on modeled samples [1], it was possible to use that technique on more complex real samples like the Mexican mineral. For a successful application certain knowledge of the sample, elemental concentration of the analyte and possible species, is helpfull. With further development this techniques has great potential in the quantitative analysis. Its big advantage comparing to other techniques is, that you can use this technique on almost any sample type, e. g. crystalline, liquid or amorphous samples.

[1] Schlesiger, C., et.al., Journal of Analytical Atomic Spectrometry 30(5), 2015, 1080-1085