X-ray absorption spectroscopy applications on a versatile laboratory X-ray diffractometer

L. Ding [1], G. Nénert[1], M. Gateshki [1], C. Zarkadas [1], H. Hussain [1]

1 Lelyweg 1, 7602 EA Almelo, Malvern Panalytical B. V.

lei.ding@malvernpanalytical.com

As a powerful method for analysing the structure and properties of new materials [1,2], X-ray absorption spectroscopy (XAS) examines how the absorption coefficient behaves near the absorption edge of a specific element, providing valuable insights into the oxidation state, coordination chemistry, electronic and local atomic structure. As a complementary technique to X-ray Diffraction (XRD), it is especially useful for non-crystalline and highly disordered materials. Compared to the X-ray Pair Distribution Function (xPDF) method—which also probes local structural features but yields signals averaged over all atomic species—XAS is element specific. Usually, XAS data are collected at synchrotron beamlines or by means of dedicated laboratory instruments. In this contribution, we propose a novel experimental setup that enables the acquisition of high-quality XAS data in transmission mode using a standard laboratory-based XRD system-Empyrean. The method has been used to analyse successfully the K absorption edges of many different compounds with transition metal elements, ranging from Ti to Mo, for example different Fe oxides (Fig.1)[3], as well as L-edges of heavier elements such as Ba, Pt and Au. In this work, XAS application examples will be presented and discussed. This approach may broaden the use of XAS in materials research, especially among users already employing diffraction methods.

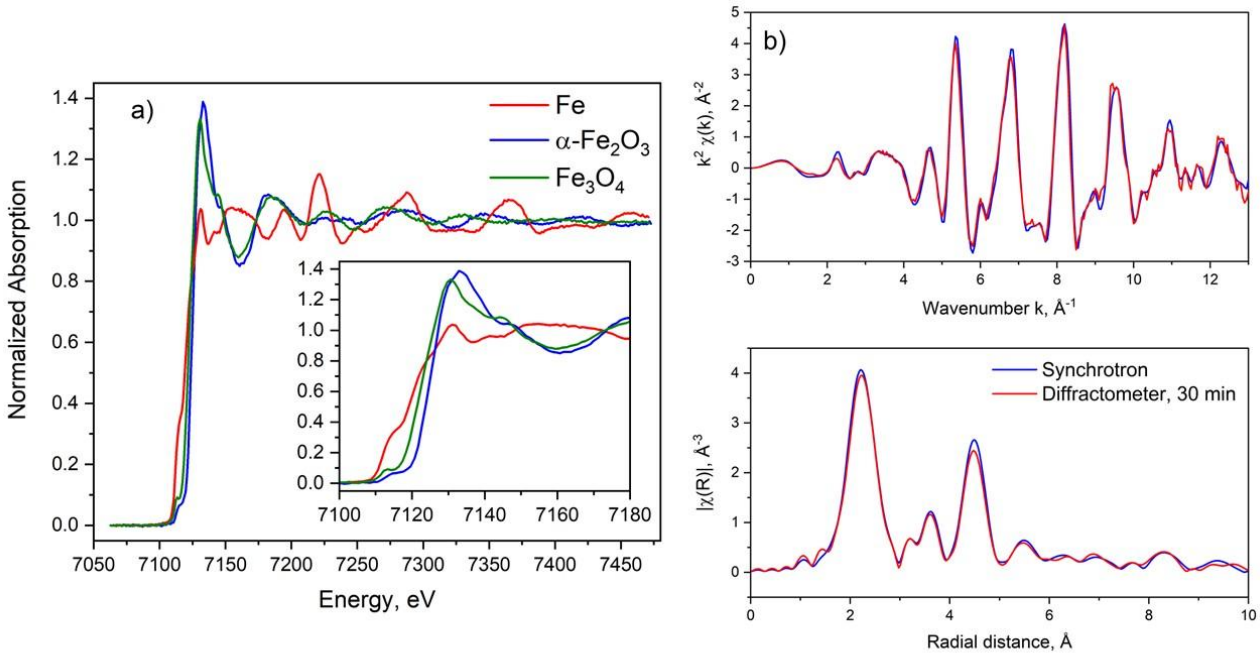


Figure 1. *a) XAS spectra of α-Fe_2O_3 (blue) and Fe_3O_4 (green) powder samples, compared with the corresponding spectrum of a 7.5 µm Fe reference foil (red) measured on Empyrean. The inset shows a magnified view of the XANES range. b) EXAFS signal and the corresponding Fourier transform of Fe compared with the result of a synchrotron measurement adjusted to the same k range (blue) [4].*

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