T-REX for advanced QEXAFS data analysis

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Quick-scanning EXAFS (QEXAFS) [1,2] is used by many groups to investigate fast processes in physics and chemistry, especially in the field of catalysis [3,4]. Due to recent developments in the QEXAFS technique it is possible to acquire tens of full EXAFS spectra each second in a very accurate and user-friendly way [5,6]. Thereby, huge amounts of data are generated which have to be processed with adequate software tools. On the one hand, these tools have to cover the typical steps of EXAFS analysis, i.e. background subtraction, spline fits, Fourier transformations and atom shell fittings. On the other hand, studying time-resolved data requires additional approaches as e.g. determining the number of independent components with principal component analysis and tracking the weights of sample components by successively fitting the spectra with linear combinations of reference spectra. Valuable approaches are also to determine edge jump, edge position and whiteline intensity as function of time. All these operations have to be performed in an automatized way with thousands of spectra in order to effectively analyze QEXAFS data. Furthermore, with respect to signal processing the large amount of spectra along the time axis provides unique possibilities for the application of digital filters. Thus, it is possible to apply accurate low pass operations or e.g. median filters to achieve the best compromise between time-resolution and noise characteristics.

The new software package T-REX (**T**ime-**R**esolved **EX**AFS analysis software) with a graphical user interface was designed using Microsoft Visual C# in order to provide the mentioned and additional unmentioned operations for QEXAFS data analysis. Thereby, for some of the tools interaction with IFEFFIT [7] is established, which provides a powerful set of methods for the EXAFS data treatment as - known from ATHENA [8]. These methods were adapted for the convenient processing of thousands of spectra. The complete data analysis starting with the QEXAFS raw data files in ASCII format can be performed with T-REX. Thereby, each project can be stored making it possible to save progress and to rapidly navigate through the results. The software will be presented along with several typical QEXAFS applications as (i) a Cu/Al_2O_3 catalyst that was periodically reduced and re-oxidized at various temperatures and (ii) Cu layers that were dc sputtered on glass and thereafter oxidized, whereby both surface processes were followed by in-situ QEXAFS measurements in grazing incidence reflection mode.

[1] R. Frahm, *Nucl. Instrum. Methods Phys. Res. A* **270,** 578-581 (1988)
[2] R. Frahm, *Rev. Sci. Instrum.* **60,** 2515-2518 (1989)
[3] J.-D. Grunwaldt, M. Beier, B. Kimmerle, A. Baiker, M. Nachtegaal, B. Griesebock, D. Lützenkirchen-Hecht, J. Stötzel and R. Frahm, *Phys. Chem. Chem. Phys.* **11,** 8779 (2009)
[4] J. Singh, E. M. C. Alayon, M. Tromp, O. V. Safonova, P. Glatzel, M. Nachtegaal, R. Frahm and J. A. van Bokhoven, *Angew. Chem. Int. Ed.* **47,** 9260 (2008)
[5] J. Stötzel, D. Lützenkirchen-Hecht, E. Fonda, N. de Oliveira, V. Briois and R. Frahm, *Rev. Sci. Instrum.* **79,** 083107 (2008)
[6] J. Stötzel, D. Lützenkirchen-Hecht and R. Frahm, *J. Synchrotron Rad.* **18,** 165 (2011)
[7] M. Newville, *J. Synchrotron Rad.* **8,** 322 (2001)
[8] B. Ravel and M. Newville, *J. Synchrotron Rad.* **12,** 537 (2005)