pseudopotentials (projected augmented waves, PAWs). The calculated ρ(r) function is equidistant 3D grid. The dimension of 3D grid can be easily adjusted by internal keywords of the VASP program and it is limited by the size of the system RAM only.

To compare the experimental and theoretical ρ(r) functions we carried out the high-resolution X-ray studies and DFT calculations of crystal structures of coordination compounds containing group 14 elements. The present work covers the results obtained for two complexes with formally divalent Ge and Sn and six formally tetravalent Si, Ge and Sn. We used the ρ(r) function calculated for the corresponding isolated molecules as reference points to evaluate the influence of crystal packing and possible systematic errors. The topological parameters (the values of ρ(r), its Laplacian ($\nabla^2\rho(r)$), kinetic and potential energy densities) in CP(3,-1) were compared. The most prominent differences are revealed for the $\nabla^2\rho(r)$ values. The latter are defined by dimension of 3D grid. On the other hand, the values of atomic volumes and charges are in good agreement. In our opinion the usage of our methodology is allowed to investigate the chemical bonding in any crystal with volume of the unit cell to be up to 4000-5000 $Å^3$.

Keywords: DFT calculations, charge density, topological analysis

MS.77.1

Acta Cryst. (2011) A**67,** C171

Advances in instrumentation, automation and validation of fast XAFS experiments

Ronald Frahm, *Dept. of Physics, Bergische Universität Wuppertal, Wuppertal (Germany).* E-mail: frahm@uni-wuppertal.de

Time resolved X-ray absorption spectroscopy can be performed in the so-called Quick-EXAFS (QEXAFS) mode, where the spectrum is collected "on-the-fly" using fast monochromators at synchrotron radiation facilities [1]. Such experiments yield e.g. structural information during fast chemical decomposition reactions, thin film deposition, solid-state reactions and phase transformations. Currently, most scientific applications focus on catalyst research [2], [3]. A dedicated facility is available at the Swiss Light Source (SLS) [4], several other are currently under development worldwide.

Depending on photon flux and sample quality, repetition rates of about 100 Hz can be realized for the XANES range. A new optimized monochromator enables the acquisition of full high quality EXAFS spectra with a scan range of typically 1 keV - up to about 2.5 keV - in only 50 ms per spectrum. This setup employs a channel cut crystal, a cam driven tilt table for rapid angular oscillations and a novel fast readout system for the Bragg angle. Latest developments also allow a user friendly variation of the scanned energy range within experiments by remote control [5]. Since a fast sequential energy scanning technique is used, the detection of fluorescence radiation or surface sensitive techniques like X-ray reflection measurements can be applied. A reference sample can be monitored simultaneously with each measurement to detect minor edge shifts reliably. Even XANES microtomography becomes feasible, using the fast scanning monochromator with refractive X-ray lenses for beam focusing. Using cryogenic cooling, the monochromator crystal can cope with the full heat load from third generation undulator sources, and excellent data quality can be obtained. Currently, a new dedicated setup using an insertion device at the PETRA III storage ring (DESY, Hamburg, Germany) is under development.

However, such measurements require very fast high precision detection systems with low noise level, and the photon energy at each instant must be known with high accuracy. Special care is necessary to avoid dynamic distortions of the measured absorption spectra. In addition, the high data acquisition rates make special software developments necessary for fast continuous measurements [6].

The most recent technical developments of fast XAFS measurements, the current states and different experimental realizations of hard- and software are discussed. Experimental factors which are influencing the data quality like the homogeneity of real samples, photon flux and beam stability are evaluated.

[1] R. Frahm, *Nucl. Instrum. Methods Phys. Res. A* **1988**, *270*, 578-581, *Rev. Sci. Instrum.* **1989**, *60*, 2515-2518. [2] B.S. Clausen, H. Topsøe, R. Frahm, *Advances in Catalysis* **1998**, *42*, 315-344. [3] S. Reimann, J. Stötzel, R. Frahm, W. Kleist, J.-D. Grunwaldt, A. Baiker, *J. Am. Chem. Soc.* **2011**, *133,* 3921-3930. [4] R. Frahm, M. Nachtegaal, J. Stötzel, M. Harfouche, J.A. van Bokhoven, J.-D. Grunwaldt, *AIP Conf. Proc.* **2010**, *1234*, 251-255. [5] J. Stötzel, D. Lützenkirchen-Hecht, R. Frahm, *Rev. Sci. Instrum.* **2010**, *81*, 073109/1-7. [6] J. Stötzel, D. Lützenkirchen-Hecht, R. Frahm, *J. Synchrotron Rad.* **2011**, *18*, 165-175.

Keywords: XAS, synchrotron_radiation, in-situ_measurement

MS

MS.77.2

Acta Cryst. (2011) A**67,** C171

Standardizing Data Formats for X-ray Absorption Spectra and Libraries

Matthew Newville,[a] Bruce Ravel,[b] V. Armando Sole,[c] Gerd Wellenreuther,[d] James R. Hester,[e] Darren S. Dale,[f] [a]*CARS, The University of Chicago, Chicago, IL (USA).* [b]*NIST, Gaithersburg, MD,* [c]*ESRF, Grenoble, (France).* [d]*DESY, HASYLAB, Hamburg, (Germany).* [e]*ANSTO, Menai, (Australia).* [f]*CHESS, Ithaca, NY (USA).* E-mail: newville@cars.uchicago.edu

As the number of high-quality facilities for collecting x-ray absorption spectra (XAS) and the size of the community using XAS grow, there is an increasing need for transferring measured XAS data between different beamlines and different analysis applications. This is particularly true for spectra measured on "model compounds" which are often used as reference spectra for XANES analysis or for calibrating analysis procedures. Unfortunately, there is no standardized file format to exchanging data. We present the efforts of a working group to define and implement a standardized file format for XAS format that can be used to exchange XAS data between researchers and analysis programs. The XAS Data Interchange (XDI) format defines a structured plain-text column data file. A header contains meta-data as keyword, value pairs with pre-defined keywords describing the spectra and experimental conditions. Numerical data is represented in white-space delimited text, with each row of data corresponding to an energy value at which the measurement was taken. Any of several pre-defined column data types can be stored for the most common types of XAS scans. For example, either energies or monochromator angles can be stored as the primary dependent variable. Sampled intensities or calculated absorption values (or both) can be stored. Normalized absorption spectra and isolated χ(k) spectra can also be stored. The format and a programming interface to it will be shown. With this format for a plain-text file which represents a single spectrum, we also show efforts to build libraries of spectra using the free and portable SQLite relational database engine. A prototype application to build and manage spectral libraries which can be either used for individual storage or easily shared between researchers will be shown.

Keywords: XAS, XANES, database