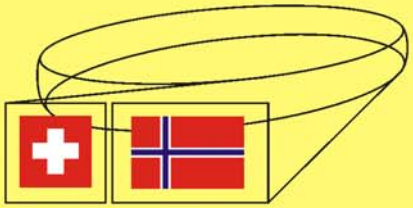

Swiss-Norwegian Beam Lines
at ESRF

Swiss-Norwegian Seminar

Synchrotron Radiation in Studies of Nanoscaled Materials

June 22-23, 2006

Grenoble, France

Program and Abstracts

Thursday, June 22
(Auditorium 500, Central Building)

10:00 **Welcome**
D.Nicholson
SNX Foundation

10:15 **X-ray scattering from nano wires and guides**
R.Feidenhans'l
Niels Bohr Institute, Copenhagen University, Denmark

11:00 **Coffee**

11:25 **Investigating the transformation mechanism of Alanates using synchrotron radiation**
A.Léon
Institute for Nanotechnology, Research Centre Karlsruhe, Germany

12:10 ***In situ* SR diffraction studies of the phase-structural transformations in hydrogen storage materials**
V.Yartys
Institute for Energy Technology, Kjeller, Norway

12:35 **Hydrogen storage in light complex hydrides - structural studies**
M.Pitt
Institute for Energy Technology, Kjeller, Norway

13:00 **Lunch**

14:15 **Small-angle x-ray scattering for nano-scale materials**
A.V. Petukhov
van ’t Hoff laboratory, Utrecht University, The Netherlands

15:00 ***In-situ* synchrotron X-ray powder diffraction studies: So far and further**
P.Norby
Centre for Materials Science and Nanotechnology University of Oslo, Norway

15:30 **Coffee**

16:00 **More than skin deep: The surface structure of Perovskites**
B.D.Patterson
Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

16:40 **Observation of the ferroelectric stripe domains in thin PbTiO3 films by using a standard x-ray diffraction**
T.Tybell
NTNU Nanolab, Department of Electronics and Telecommunications, Norwegian University of Science and Technology, Trondheim, Norway

17:20 **Diffraction studies of ferroic materials under an electric field**
F.Mo
Deptartment of Physics, NTNU, Trondheim, Norway

17:45 **Micro-Raman spectroscopy of ferroelectric thin films**
Yu.Yuzyuk
Centre de Recherche sur les Matériaux à Haute Température, Université Orléans, France

20:00 **Dinner**

Friday, June 23
(Control Room)

09:00 **Nanocrystallography**
W.Steurer
Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland

9:45 **Synthesis and Characterization of Nano-Sized WO_3**
V.Dmitriev
SNBL at ESRF, Grenoble, France

10:10 **XRD characterization of iron-oxide nanoparticles for ferrofluids**
A.Vorobiev
ESRF, Grenoble, France

10:25 **Instrumentation for investigating nanoscale materials on SNBL (BM1A) illustrated with some recent examples**
D.Chernyshov
SNBL at ESRF, Grenoble, France

10:50 **Coffee**

11:20 **Structure defines the nano-world: Investigation of very small semiconductor nanoparticles**
C.Kumpf
Experimentelle Physik II, Universität Würzburg, Würzburg, Germany

12:05 **3D local structure of nanomaterials: advanced XANES analysis**
A.Soldatov
Laboratory for Nanoscale Atomic Local Structure Analysis, Faculty of Physics, Rostov State University, Rostov-Don, Russia

12:50 **Concluding Remarks**
D.Nicholson
SNX Foundation

13:00 **Lunch**

14:15 **DUBBLE: another multipurpose beam line**
W.Bras
DUBBLE at ESRF, Grenoble, France

14:40 **SNBL setup: open discussion**

X-ray scattering from nano wires and guides.

Robert FEIDENHANS'L
Niels Bohr Institute, Copenhagen University, Denmark
E-mail: robert@fys.ku.dk

In this talk I will discuss how x-ray scattering can be applied to obtain structural information about nano structures using the crystal truncation rod scattering from their facets. I will focus on GaAs nano wires grown on GaAs(111)B and GaAs(100) surfaces catalysed by Au nano clusters and discuss how information about their crystal structure, shape and orientation can be obtained. I will also discuss the necessary experimental setup in particular the advantage using modern 2-dimentional detectors.

The second topic of my talk will concern x-ray waveguides. I will discuss how x-ray wave guides can be fabricated by use of wafer bonding and show how they work both as planar and as 2-dimensional waveguides.

Investigating the transformation mechanism of Alanates using synchrotron radiation

Aline LEON, Christoph FROMMEN, Jörg ROTHE and Maximilian FICHTNER
Institute for Nanotechnology, Research Center Karlsruhe, Germany
E-mail: Aline.Leon@int.fzk.de

The development of a hydrogen storage material, which fulfils all requirements for mobile applications, is a challenge. So far, the system, which is the most advanced with respect to thermodynamics, kinetics and storage capacity, is the sodium alanate ($NaAlH_4$) doped with Ti-based precursor by ball milling. However, the mechanism underlying the reversible decomposition reaction is still not elucidated. The understanding of the catalytic activity would allow an optimization of the precursor and in turn increase the efficiency of the material.

Ti K-edge XAS has been applied to investigate the evolution of the dopant structure in nanoscale hydrogen storage materials at different stage of the hydrogen release and uptake cycles. $TiCl_3$, nano-sized $Ti_{13}{\cdot}6THF$ and a novel catalyst $Al_xTi_{(1-x)}$ have been used as precursors for doping sodium alanate. It has been shown that the chemical state of Ti is relevant for the evolution of the reversible storage capacity and the desorption/absorption reaction rate. We observe that the reduction to the metallic state favors some nano-scale alloy formation between Ti and Al. We correlate the formation of these local defects in the alanate structure to the decrease in the hydrogen storage capacity and reaction rate with increasing number of cycles.

In situ SR diffraction studies of the phase-structural transformations in hydrogen storage materials

V.A.YARTYS and J.P.MAEHLEN
Institute for Energy Technology, Kjeller, NO 2027, NORWAY
E-mail: volodymyr.yartys@ife.no

Phase–structural composition of the metal-hydrogen systems depends on a number of variable parameters including hydrogen pressure, applied static pressure, and temperature and is time-dependent. *In situ* SR diffraction studies of these systems are very valuable allowing control and modification of the specific applied conditions and even studies of the kinetics of the hydrogen-involving processes. In this paper we will give a review of the results received during our studies of hydrogen storage materials performed at SNBL and ESRF. The majority of these studies were based on the use of a specially designed cell for *in situ* studies in H_2-atmosphere. The cell is attached to a metal hydride hydrogen storage unit developed at IFE providing hydrogen gas at convenient pressures.

We will present the data for the *in situ* studies of the following systems:

- Intermetallic hydride with the shortest known H-H separation, 1.6 Å: $LaNiInH_{1.3}$ at applied static pressures up to 40 GPa;
- Hexagonal-monoclinic low temperature order-disorder transition in $ErMn_2D_2$ Laves phase deuteride;
- Hydrogen desorption studies from alanes, α-AlH_3 and γ-AlH_3, releasing up to 10 wt.% H;
- $LaNi_{4.7}Sn_{0.3}$-based hydrides with fast rates of hydrogen absorpion and desorption.

We gratefully acknowledge collaboration in these studies with M.Stange (IFE), P.Norby (University of Oslo), M.Fichtner and Ch.Frommen (Research Centre Karlsruhe), B.M.Bulychev (Moscow State University), H.Fiegel (University of Mining, Poland), H.Emmerich, W.van Beek, Ya.Filinchuk, D.Chernyshov, Ph.Pattison and V.Dmitriev (SNBL) and M.Hanfland (ESRF).

Hydrogen storage in light complex hydrides - structural studies

M.P. PITT and B.C. HAUBACK
Institute for Energy Technology, P.O. Box 40, NO-2007, Kjeller, Norway
E-mail: mark.pitt@ife.no

Efficient and safe storage of hydrogen remains as the most challenging unsolved problem for the introduction of the Hydrogen Economy. Among the most promising materials are the Alanates, compounds based on the tetrahedral AlH_4 unit. The use of Ti based catalysts has shown much improved kinetics at temperatures below 200°C, and made re-hydrogenation possible in some cases. Detailed structural studies are vital in understanding the hydrogen absorption/desorption processes, and the role of the catalyst. Crystal structures of $MAlD_4$, (M=Li,Na,K), Li_3AlD_6, $Mg(AlH_4)_2$, and mixed complexes, such as $(M1)_2(M2)AlD_6$, (M=Li,Na,K), have been determined by simultaneous Rietveld refinements, using the PUS neutron diffractometer at the JEEP II reactor, at IFE in Norway, and the high resolution BM01B diffractometer at the Swiss-Norwegian Beam Line at the ESRF. As well as crystal structure solution, we have focussed on in-situ diffraction measurements, such as thermal desorption and H cycling studies using both neutrons and X-rays at IFE and SNBL, and the study of high pressure phase transitions in $LiAlD_4$ and $NaAlD_4$, using the TOF neutron diffractometer PEARL, at the Rutherford Laboratories at ISIS. This presentation will review the current state of research for Alanates as potential H storage materials. We will also focus on future research goals and experimental plans for the SNBL.

Small-angle x-ray scattering for nano-scale materials

Andrei V. PETUKHOV
van 't Hoff laboratory for physical and colloid chemistry, Utrecht University, The Netherlands
E-mail: a.v.petukhov@chem.uu.nl

In the first part of the talk I shall present a simple introduction to small-angle x-ray scattering (SAXS), which is widely applied to characterise materials with organisation at length scales between approximately a nanometre and a micrometre. The applications of SAXS are therefore very wide and range from biology and soft condensed matter to various topics in nanotechnology. The demand for synchrotron SAXS is very high and the competition for the beamtime is often tough. After giving a few simple examples, a few words will be spent on the instrumentation. The Dutch-Belgium beamline BM-26 DUBBLE, which closely collaborates with BM-01 SNBL, offers possibilities for widely needed SAXS studies.

In the second part I shall concentrate on the self-organisation of colloids, which is the main topic of our activity at BM-26. Colloids can be seen as giant atoms or molecules, which are slow and seeable. The particles can be made sufficiently large so that one can watch them in an optical microscope! Colloids are much slower than atoms so that one can study their dynamics in real time. One can also tune the interactions between colloidal particles in fine details. Therefore, colloids provide an important model system, which allows studying various aspects of, e.g., crystallisation and melting on a much more convenient time and length scale. Furthermore, I would like to discuss the similarities between ordinary (atomic) nano-crystals and colloidal crystals.

***In-situ* synchrotron X-ray powder diffraction studies: So far and further**

Poul NORBY
Department of Chemistry and Centre for Materials Science and Nanotechnology University of Oslo, Norway
E-mail: p.a.norby@kjemi.uio.no

In-situ powder diffraction, especially utilizing synchrotron X-ray sources, has become a valuable tool for studying materials synthesis, and chemical or physical reactions involving crystalline materials. This includes studies of materials synthesis, for instance under hydrothermal conditions, studies of solid-gas and solid-liquid reactions, ion exchange, adsorption and intercalation. In addition, the possibility of studying materials under real working conditions, e.g. selective diffraction from materials inside working devices, may be utilized. This could be studies of catalytic reactors, batteries, fuel cells or membranes.

The talk will describe some results from *in-situ* studies using e.g. SNBL. In addition some plans and possibilities for studying synthesis and transformation of nanomaterials using *in-situ* powder diffraction will be outlined.

More than Skin Deep: The Surface Structure of Perovskites

Bruce D. PATTERSON
Swiss Light Source, Paul Scherrer Institute Villigen, Switzerland.
E-mail: bruce.patterson@psi.ch

Perovskite materials are currently the playground of choice of condensed matter scientists. Although much is known of their bulk structures and electronic properties, the study of their surfaces and interfaces is just beginning. The majority of perovskite thin films are produced using Pulsed Laser Deposition, and the unchallenged experimental method for precise structure solution is Glancing-Incidence Surface X-Ray Diffraction. At the Materials Science Beamline of the Swiss Light Source, we have married these two techniques, allowing the growth of perovskite materials and *in-situ* determination of their surface atomic coordinates. Among the beneficiaries of this marriage will be thin-film devices, photoelectron spectroscopy and correlated electron theory.

Observation of the ferroelectric stripe domains in thin $PbTiO_3$ films by using a standard x-ray diffraction

Thomas TYBELL
NTNU Nanolab, Department of Electronics and Telecommunications Norwegian University of Science and Technology, Trondheim, Norway
E-mail: thomas.tybell@iet.ntnu.no

We report on the observation of the ferroelectric stripe domains in thin $PbTiO_3$ films by using standard x-ray diffraction equipment at room temperature. High-quality c-axis oriented $PbTiO_3$ films, with thickness varying between 16 and 200 unit cells, were grown on buffered NH4-HF treated $SrTiO_3$ and Nb-doped $SrTiO_3$(001) substrates using off-axis radio-frequency magnetron sputtering. All films showed atomically smooth surfaces with a step and terrace structures of 1 unit-cell height. High resolution measurements along the Q_x direction show satellite peaks around the 00l specular peaks due to an in-plane aligned super structure. One possible interpretation, taking into account the thickness dependence of the satellites, is that the origin is due to a ferroelectric stripe domain structure. Miss-fit dislocations as cause to the observed signal will also be addressed. In this presentation, we will also discuss possible in-plane alignment of the domains.

Diffraction studies of ferroic materials under an electric field

Frode MO
Dept. of Physics, NTNU, N-7491 Trondheim, Norway
E-mail: Frode.Mo@ntnu.no

In previous studies of a hydrated glucose complex with an alleged ferroelastic phase transition we observed a deterioration of the crystals which appeared to be strongly enhanced by X-rays. In fact, crystals of many organic hydrates are unstable and may denature easily, either by efflorescence or deliquescence, depending on the relative humidity and temperature of the environment. This process, involving a partial change in structure, is detrimental to accurate structure studies which are required in order to gain insight in the often subtle structural changes accompanying a phase transition.

In order to eliminate or at least slow down the denaturation of such crystals we have constructed a gas-flow thermostat (Peltier elements) single-crystal sample cell with control of relative humidity. A unique additional feature of the cell is a transparent, rotatable capacitor allowing an electric DC-field to be applied to the crystal in a fixed crystallographic direction during the experiment. With this novel cell we have studied the ferroelectric compound Rochelle salt, another organic hydrate, which is extremely sensitive to X-rays in an unconditioned environment. Diffraction data of unprecedented quality have been collected for the HT paraelectric phase of Rochelle salt, more recently also for its ferroelectric phase, and as well for one of the phases of the hydrated glucose complex.

The capacitor geometry has now been modified to accomodate plate-shaped samples of thickness ~ 500 μm carrying epitaxial ferroelectric thin films. First tests have given very promising results showing angular shifts of diffraction maxima, and changes in intensity reflecting the response of both film and substrate structure to the impact of DC fields up to 2000 V/cm.

Micro-Raman spectroscopy of ferroelectric thin films

Yury.I. YUZYUK*
Centre de Recherche sur les Matériaux à Haute Température, Université Orléans Orléans, France
E-mail: yuzyuk@rambler.ru

Epitaxially grown ferroelectric thin films are usually highly constrained because the fabrication of heterostroctures is accompanied by several strain factors such as misfit strain due to lattice mismatch between the film and the underlying substrate, thermoelastic strain generated by the difference between the thermal expansion coefficients of the film and the substrate, and transformation strain, which usually appears at ferroelectric phase transition. The two-dimensional (2D) stresses imposed by the substrate increase remarkably the Curie temperature and even change the entire phase transition sequence in epitaxial ferroelctric thin films, creating new phases that are not present in bulk materials.

Micro-Raman spectroscopy was employed to study the lattice dynamics at phase transitions in $(Ba,Sr)TiO_3$ (BST) thin films and $BaTiO_3/SrTiO_3$ (BT/ST) superlattices deposited on (001)MgO substrates. We observed significant transformation of the *E*(TO) soft mode due to two-dimensional (2D) stress imposed by the substrate. In fact, the soft mode frequency in these films can be used as very sensitive internal probe of the 2D clamping. The upward shift of the Curie temperature due to the 2D stress was systematically studied in several BST/(001)MgO thin films by means of x-ray diffraction and Raman spectroscopy. Low-temperature Raman studies showed that rhombohedral phase is unstable in BST/MgO thin films and in contrast to the bulk material the phase transition from tetragonal to monoclinic phase was observed. To clarify the factors determining stress formation we have studied stress relaxation in partially unsupported and completely free-standing areas of the epitaxial BST film.

Due to in-plane compressive stresses generated by the lattice mismatch of the constituting layers in BT/ST superlattices the *E*(TO) soft-mode was found to be underdamped and markedly shifted to higher frequencies with respect to its analogs in the bulk. As a result of perfect periodic modulation the folding of the transverse acoustic branch along the direction perpendicular to the layers was observed in the low-frequency Raman spectra.

Polarized Raman spectra of BST/MgO films as a function of film thickness (10-1000 nm) were systematically studied. Significant transformation of the E(TO) soft mode was found in the thickness-dependent Raman spectra of BST/MgO films at around 100 nm. Temperature dependence of the soft mode in nanoscale ferroelectic films is discussed.

**On leave from the Faculty of Physics, Rostov State University (Russia)*

Nanocrystallography

Walter STEURER
Laboratory of Crystallography, Department of Materials
ETH Zurich, Zurich, Switzerland
E-mail: walter.steurer@mat.ethz.ch

What is the critical size of a nanocrystal when structural changes become observable by diffraction methods? What is the influence of temperature, pressure or other external fields on the structure? What happens to incommensurately modulated structures when the crystals get smaller and smaller? When incommensurability does disappear? How does the structure of quasicrystals change with particle size? I will ask many questions of this kind in my lecture and try to review what is known about nanocrystallography and where the white spots are.

Synthesis and Characterization of Nano-Sized WO_3

Vladimir DMITRIEV
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: dmitriev@esrf.fr
Elizabeth DJURADO, Guy LUCAZEAU
Laboratoire d'Electrochimie et de Physico-Chimie des Matériaux et des Interfaces, INP Grenoble, France

Nanometric tungsten trioxide has very high impact due to its efficiency in different electrochemical applications, showing excellent sensoring, electrochromic and catalytic properties. The present paper reports on experimental study of the size effect, in the mesoscopic range, on the stability of crystal phases of the tungsten trioxide compound.

WO_3 powder samples were synthesized for the first time by the spray-pyrolysis technique using an ultrasonic atomiser. The gaseous mixture carried the aerosol of a precursor solution through a tubular furnace heated at different selected temperatures from 400 to 900°C by 10°C steps. The samples of resultant material were fully characterized with synchrotron radiation diffraction technique. The phase content, phase structures, crystallite size, and grain size distribution have been found for every sample. High-resolution transmission electron microscopy observations were carried out for a complementary characterization of individual nanograins.

The existence of several polymorph modifications known for microcrystalline WO_3 (monoclinic $P2_1/n$, and high-temperature tetragonal $P4/nmm$ and cubic $Pm3m$) was evidenced in its nanocrystalline state at ambient conditions. However, stability of different structures depends on the synthesis conditions. We have managed to synthesize even a hexagonal structure, which have never been obtained from the known forms but only as result of a special chemical treatment.

The thermal stability of all structures grown in nanocristalline WO_3 was studied in a wide temperature range.

XRD characterization of iron-oxide nanoparticles for ferrofluids

A. VOROBIEV[1], D. CHERNYSHOV[2], G. GORDEEV[3], D. ORLOVA[3]
[1]*ESRF, Grenoble, France*
[2]*SNBL, Grenoble, France,*
[3]*PNPI, Gatchina, Russia*
E-mail: alexei.vorobiev@esrf.fr

Ferrofluids – also known as magnetic colloids – are textbook examples of a fluid material with properties tailored on the nanometer level. They consist of single domain magnetic particles with a typical size of 10 nm dispersed in a liquid carrier. Because of their superparamagnetic susceptibility, they can conventionally be manipulated by external magnetic fields which gives rise to extremely wide range of technical applications. From more fundamental perspective, ferrofluids are scientifically very attractive examples of disordered materials: a combination of magnetic and nonmagnetic interactions results in various local interpartical correlations that, in turn, changes macroscopic properties of the whole system. Therefore, any additional information about the particle ensemble simplifies significantly understanding of results obtained in different experiments on ferrofluids. Here we show how such important parameters as particle mean size and dispersion as well as crystal structure can be easily obtained in very fast experiment on synchrotron light diffraction.

Instrumentation for investigating nanoscale materials on SNBL (BM01A) illustrated with some recent examples

D. CHERNYSHOV and P. PATTISON
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: dmitry.chernyshov@esrf.fr

Station BM01A on SNBL offers the user community a wide range of options for single crystal and powder diffraction experiments. The KM6 multi-axis diffractometer is equipped with a point detector for high angular resolution measurements of individual reflections, while the CCD area detector mounted on the same arm provides the option of rapid data collection. The six rotation axes of the KM6 diffractometer allow a wide choice of scattering geometries (vertical plane, horizontal plane, grazing incidence etc). The mar345 image plate detector on a standard MarResearch base provides a single phi rotation axis together with a large area detector. For more rapid data collection, the image plate can be exchanged for a marCCD with a 4 second readout cycle. The station has access to a wide range of ancillary equipment such as heaters, cryostats and pressure cells. Examples will be given of recent research projects related to nanoscience. Topics include powder diffraction measurements of mesoporous silica, single crystal study of nano-domains in a relaxor ferroelectric, diffuse scattering in Prussian Blue analogue, reconstruction of reciprocal space for a boron-doped diamond single crystal, and the investigation of nanometer sized precipitates embedded in a aluminium single crystal matrix.

Structure defines the nano-world: Investigation of very small semiconductor nanoparticles

Christian KUMPF
Experimentelle Physik II, Universität Würzburg
Würzburg, Germany
E-mail: christian.kumpf@physik.uni-wuerzburg.de

Semiconductor nanoparticles are of increasing interest for both, applied and fundamental research. Besides applications in material science, they are used as markers in biology and for cancer treatment. Nanoparticles in the diameter range from 1-5 nm are of particular interest in fundamental research since they represent a size scale between solid state and molecular physics which is difficult to investigate.

The structural, electronic, optical, and magnetic properties of particles in this size range are very often not known and understood. Even a precise determination of basic geometrical parameters like the size and shape is difficult. Potentially, diffraction methods are able to provide complete structural information, but common analysis methods do not yield sufficiently precise results in the particle range below 5 nm. We present a new approach for the analysis of synchrotron radiation diffraction data (XRD) obtained from small particles. The experiments were performed at HASYLAB, Hamburg. The entire particle is modeled, and its diffraction pattern is computed using the Debye formula. This allows us to address not only fundamental parameters like size and crystal structure, but also shape, stress, relaxation effects, and stacking faults. In contrast to common analysis methods these essential structural features are explicitly taken into account as intrinsic parameters of the nanoparticle model. An ensemble-averaging is performed and hence the parameter distributions, most prominent the size distribution of the particles, can be determined. This is enabled by using a stochastic fit algorithm.

Furthermore, we report on photoelectron spectroscopy experiments (PES) performed at BESSY, Berlin. The use of synchrotron radiation at different wavelength allows to vary the surface sensitivity of the measurement. Additionally core level shifts are utilized to identify different atomic species, for example atoms with different chemical bonds and in different coordinations. The combination of a quantitative analysis of chemically different species with that of their bulk- vs. surface sensitivity is utilized to determine the location of various atoms within the nanoparticle. This approach has been applied in detail to CdS particles resulting in an atomic model, which is consistent with the XRD results.

We believe that our two approaches enable a new access to detailed structural parameters of small nanoparticles and improve the knowledge about growth mechanism and particle formation.

Local atomic and electronic structures at nanoscale level: advanced analysis by XANES spectroscopy

Alexander V. SOLDATOV
Laboratory for Nanoscale Atomic Local Structure Analysis[*)]*, Faculty of Physics, Rostov State University, Rostov-Don, Russia*
E-mail: soldatov@rsu.ru

The status of modern theoretical analysis of the experimental x-ray absorption spectra to extract structural parameters will be presented. Novel method for extracting of 3D structural information on the basis of advanced quantitative analysis of X-ray absorption near edge structure (XANES) realized in "FitIt" software will be described [1]. The approach is based on the fitting of experimental XANES data using multidimensional interpolation of spectra as a function of structural parameters and advanced "*ab-initio*" XANES simulations. Small number of required *ab-initio* calculations is the main advantage of the approach, which allows one to use computationally time-expensive non-muffin-tin methods. The possibility to extract information on bond angles in addition to bond-lengths accessible to standard EXAFS is demonstrated and it opens new perspectives of quantitative XANES analysis as a 3D local structure probe. As XANES peaks have much higher intensity then EXAFS signal, one can use XANES to study the local structure also in these cases when the EXAFS cannot be registered: for example in time-dependent experiments of for low Z materials.

Advanced theoretical analysis based either on self-consistent muffin-tin model or full potential (non-muffin-tin) theory, coupled with DFT geometry optimization have been applied to extract structural information from experimental XANES data. The status of modern research shows that XANES spectroscopy and its "*ab initio*" theoretical analysis can be a useful tool for the investigation of both local structure and electronic subsystem of many advanced materials without long range order. The present approach can provide a subatomic level (i.e., 0.01- 0.03 Å) of accuracy in the determination of the interatomic distances and several of degrees in the determination of the bonding angles at specific atomic site of nanomaterials.

In the framework of this approach, results of recent studies of local atomic structure for several types of nanostructures (nanoclusters, nanotubes etc.), polymers, catalysts, and defects in semiconductors will be reported. Funding by Russian Ministry for Education and Science (project 2.1.1.1038) is acknowledged.

[*)] http://www.phys.rsu.ru/~XANES/

[1] Smolentsev G., Soldatov A. (2006) J. Synchrotron Rad. **13,** 19.

List of Participants

Dr. Beukes, Jon Are
Dept. of Physics, NTNU, N-7491 Trondheim, Norway
E-mail: brukes@phys.ntnu.no

Dr. Bras, Wim
Dutch-Belgium Beam Lines at ESRF, France
E-mail: wim.bras@esrf.fr

Dr. Chernyshov, Dmitry
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: dmitry.chernyshov@esrf.fr

Dr. Dmitriev, Vladimir
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: dmitriev@esrf.fr

Mr. Emerich, Herman
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: ermano@esrf.fr

Prof. Feidenhans'l, Robert
Niels Bohr Institute, Copenhagen University, Denmark
E-mail: robert@fys.ku.dk

Prof. Kildemo, Morten
Dept. of Physics, NTNU, N-7491 Trondheim, Norway
E-mail: Morten.Kildemo@phys.ntnu.no

Dr. Kumpf, Christian
Experimentelle Physik II, Universität Würzburg, Würzburg, Germany
E-mail: christian.kumpf@physik.uni-wuerzburg.de

Dr. Kvashnina, Kristina
Dutch-Belgium Beam Lines at ESRF, France
E-mail: kristina.kvashnina@esrf.fr

Dr. Leon Aline
Institute for Nanotechnology, Research Center Karlsruhe, Germany
E-mail: Aline.Leon@int.fzk.de

Dr. Lund Ramstad, Astrid
Department of Chemistry, NTNU, N-7491 Trondheim, Norway
E-mail: astrid.lund.ramstad@chem.ntnu.no

Dr. Maehlen, Jan Petter
Institute for Energy Technology, Kjeller, NO 2027, Norway
E-mail: jepe@ife.no

Dr. Mathisen, Karina
Department of Chemistry, NTNU, N-7491 Trondheim, Norway
E-mail: Karina.Mathisen@nt.ntnu.no

Prof. Mo, Frode
Dept. of Physics, NTNU, N-7491 Trondheim, Norway
E-mail: Frode.Mo@ntnu.no

Prof. Nicholson, David G.
Department of Chemistry, NTNU, N-7491 Trondheim, Norway
E-mail: david.nicholson@chem.ntnu.no

Prof. Norby, Poul
Department of Chemistry and Centre for Materials Science and Nanotechnology University of Oslo, Norway
E-mail: p.a.norby@kjemi.uio.no

Prof. Patterson, Bruce D.
Swiss Light Source, Paul Scherrer Institute Villigen, Switzerland
E-mail: bruce.patterson@psi.ch

Dr. Pattison, Philip
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: pattison@esrf.fr

Prof. Petoukhov, Andrei
van ’t Hoff laboratory for physical and colloid chemistry, Utrecht University, The Netherlands
E-mail: a.v.petukhov@chem.uu.nl

Dr. Pitt, Mark
Institute for Energy Technology, Kjeller, NO 2027, Norway
E-mail: mark.pitt@ife.no

Dr. Safonova, Olga
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: safonova@esrf.fr

Prof. Soldatov, Alexander
Laboratory for Nanoscale Atomic Local Structure Analysis, Faculty of Physics, Rostov State University, Rostov-Don, Russia
E-mail: soldatov@rsu.ru

Prof. Steurer, Walter
Laboratory of Crystallography, Department of Materials, ETH Zurich, Zurich, Switzerland
E-mail: walter.steurer@mat.ethz.ch

Prof. Törnroos, Karl Wilhelm
Department of Chemistry, University of Bergen, 5007 Bergen, Norway
E-mail: karl.tornroos@kj.uib.no

Prof. Tybell, Thomas
NTNU Nanolab, Department of Electronics and Telecommunications, Norwegian University of Science and Technology, Trondheim, Norway
E-mail: thomas.tybell@iet.ntnu.no

Mr. Van Beek, Wouter
Swiss-Norwegian Beam Lines at ESRF, France
E-mail: wouter@esrf.fr

Dr. Vorobiev, Alexei
ESRF, Grenoble, France
E-mail: alexei.vorobiev@esrf.fr

Dr. Yartys, Volodymyr
Institute for Energy Technology, Kjeller, NO 2027, Norway
E-mail: volodymyr.yartys@ife.no

Dr. Yuzyuk, Yury
Faculty of Physics, Rostov State Universit, Russia
E-mail: yuzyuk@rambler.ru