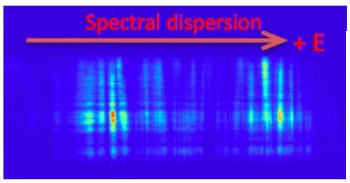
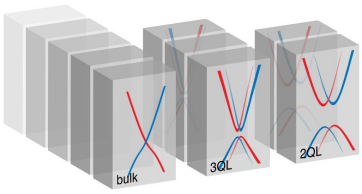
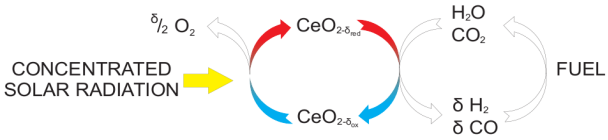
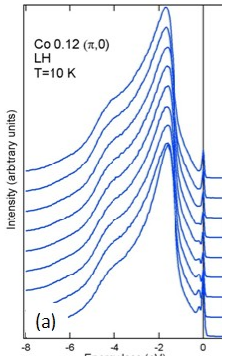








SLS Symposium on

Spectroscopy

Tuesday, April 1, 2014

10:00 to 12:15, WBGB/019

10:00 High resolution single-shot spectral monitoring of hard XFEL radiation
Mikako Makita, P. Karvinen, D. Zhu, J. Grünert, S. Cartier, Y. Feng, J.H. Jungmann, P. Juranic, H.T. Lemke, A. Mozzanica, S. Nelson, L. Patthey, M. Sikorski, S. Song, and Ch. David

10:30 *In situ* XAS of CeO2 -based materials for two-step solar thermo-chemical H_2O and CO_2 splitting
Matthäus Rothensteiner, H. Emerich and J.A. van Bokhoven

11:00 Coffee

11:15 Resonant Inelastic X-ray Scattering (RIXS) studies on the high energy spin-excitations of electron doped 122-type iron-based superconductor
Yao Bo Huang, J. Pelliciari, V. Bisogni, P. O. Velasco, K. J. Zhou, M. Dantz, G. F. Chen, V. Strokov, H. Ding and T. Schmitt

11:45 Spin texture of topological insulator thin films in the quantum tunneling limit
Gabriel Landolt, S. Schreyeck, S.V. Eremeev, B. Slomski, S. Muff, J. Osterwalder, E.V. Chulkov, C. Gould, G. Karczewski, K. Brunner, H. Buhmann, L.W. Molenkamp, and J.H. Dil

High resolution single-shot spectral monitoring of hard XFEL radiation

Mikako Makita[1], Petri Karvinen[1], Dilling Zhu[2], Jan Grünert[3], Sebastian Cartier[1], Yiping Feng[2], Julia H. Jungmann[1], Pavle Juranic[1], Henrik T. Lemke[2], Aldo Mozzanica[1], Silke Nelson[2], Luc Patthey[1], Marcin Sikorski[2], Sanghoon Song[2], and Christian David[1]

[1] *Paul Scherrer Institut, Villigen PSI, CH5232, Switzerland*

[2] *National Accelerator Laboratory, Menlo Park, California, 94025, USA*

[3] *European XFEL GmbH, 22607, Hamburg, Germany*

The self-amplified spontaneous emission (SASE) of X-Ray Free-Electron Lasers (XFELs) leads to a fluctuating spiky spectrum, which by its stochastic nature cannot be predicted. In order to eliminate the effects of these fluctuations from the data collected by experimenters, XFEL facilities face the challenge to provide spectral measurements on each individual pulse, with sufficient resolution, and without interfering with the experiment itself. So far, no method has been established that fulfils all these requirements.

Within the collaboration of several research institutions, we have developed and demonstrated a novel type of noninvasive, single-shot hard x-ray spectral monitor. The instrument is based on nanostructured diamond diffraction gratings to diffract a fraction of the beam onto a dispersive bent Bragg crystal, and to record the Bragg reflection with a fast-framing strip detector. This geometry combines the high resolution of a crystal-based analyzer [1] with the robustness and low interference of a grating spectrometer [2].

We have established the properties of this scheme regarding the X-ray energy range from 4.4 keV up to 8.4 keV, and its stability under 120 Hz LCLS full beam intensity. The energy resolution observed had achieved 0.1 eV-0.2 eV on the detector. This successful result further suggests the possibility to permanently implement this set-up in the tunnel of XFEL sources to provide single-shot spectra as a reference required in user experiments. Moreover, this single shot spectral monitoring provides information required to optimize the accelerator operation parameters, for instance for the commissioning of seeding schemes or as the sensor for feedback-loops to stabilize the emission.

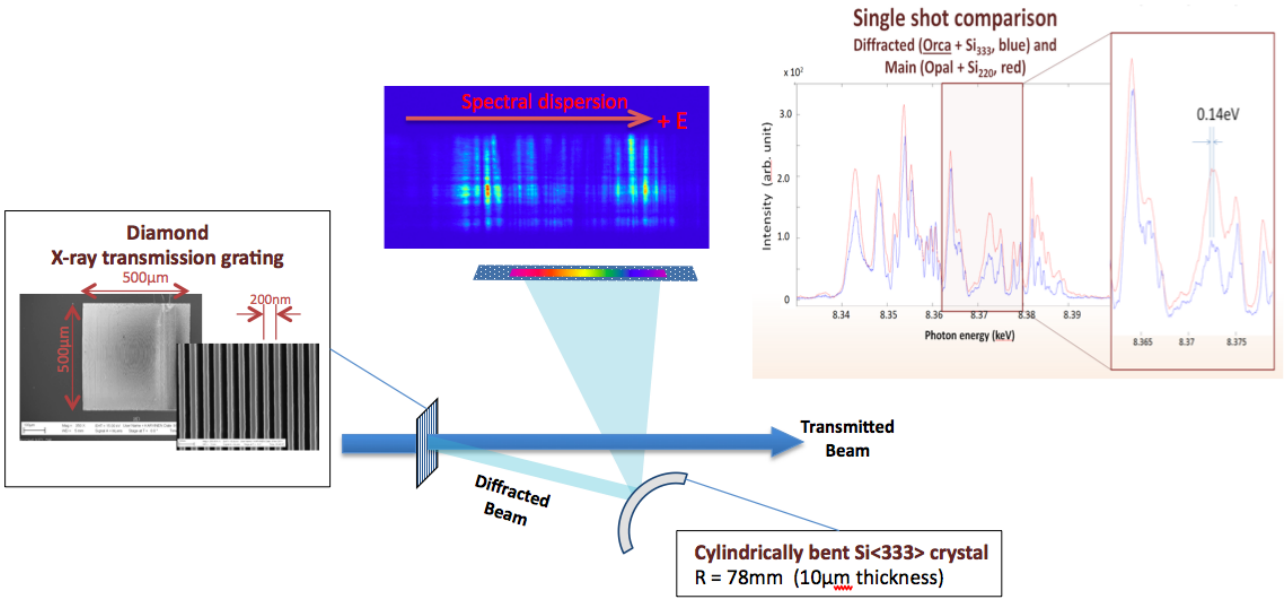
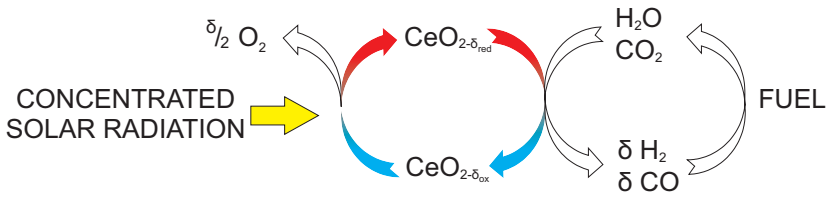


Figure 1: The schematic diagram of the setup and the resultant single-shot spectra plot (top-right). The Diamond grating transmits ~95% of the beam, and the bent crystal receives one of the diffracted beams (~1% of the beam), which will spectrally diffract onto the detector. The frame-rate of the detector is set to ~120Hz to capture LCLS single shots. The spectra plot compares the diffraction from two bent crystals – one with diffracted beam and one with transmitted beam. It confirms that the beam spectra and distribution stays same between the transmitted and the diffracted beam, and hence the non-intrusive nature of the Diamond grating. The highest spectra resolution observed on the detector was ~0.14 ±0.3 eV.

[1] D.Zhu et al, APL 101, 2012

[2] P.Karvinen et al, Optics Letters 37, 2012



In situ XAS of CeO_2-based materials for two-step solar thermochemical H_2O and CO_2 splitting

Matthäus Rothensteiner[1], Hermann Emerich[2] and Jeroen Anton van Bokhoven[1]

[1]ETH Zurich/Paul Scherrer Institut, 5232 Villigen PSI, Switzerland
[2]European Synchrotron Radiation Facility, 6 Rue Jules Horowitz BP 220, 38043 Grenoble Cedex 9, France

Thermochemical redox cycles driven by concentrated solar radiation present a viable pathway to efficiencies of 20 % in the conversion and storage of solar energy [1]. Ceria-based non-stoichiometric oxides are of great interest as reactive intermediates for the production of H_2 from H_2O (and CO from CO_2) in a two-step process. In a solar reactor, reactions (1) and (2) are carried out at low O_2 concentrations and temperatures of typically 1773 K.

$$CeO_{2-\delta_{ox}} \longrightarrow CeO_{2-\delta_{red}} + \frac{\delta}{2} O_2 \tag{1}$$

$$CeO_{2-\delta_{red}} + \delta\ H_2O \longrightarrow CeO_{2-\delta_{ox}} + \delta H_2 \tag{2}$$

The introduction of dopants such as Zr or Hf into the fluorite-type $CeO_{2-\delta_i}$ lattice strongly affects the non-stoichiometry δ_i, which is pivotal for the efficiency of the process. In order to study structural changes under relevant conditions, a high temperature *in situ* cell for XAFS has been built. Measurements at the Ce K edge have been carried out under relevant conditions at temperatures up to 1773 K to determine the electronic structure of Ce (Ce^{III}/Ce^{IV}-ratio) and local geometric distortions.

In the light of these extreme conditions, the opportunities and limitations of *in situ* XAFS for establishing structure-property relationships (such as oxygen storage capacity, reaction kinetics and stability) are discussed.

[1] Roeb, M., Sattler, C. *Science*, 2013, 341, 470
[2] Chueh, W. C., Falter, C., Abbott, M., Scipio, D., Furler, P., Haile, S. M., Steinfeld, A. *Science*, 2010, 330, 1797

Resonant Inelastic X-ray Scattering (RIXS) studies on the high energy spin-excitations of electron doped 122-type iron-based superconductor

Y. B. Huang[1, 2], *J. Pelliciari*[1], *V. Bisogni*[1], *P. O. Velasco*[1], *K. J. Zhou*[3], *M. Dantz*[1], *G. F. Chen*[2], *V. Strokov*[1], *H. Ding*[2] *and T. Schmitt*[1]

[1] *Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland*

[2] *Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

[3] *Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK.*

Since the discovery of the iron-based superconductors, great interest has been attracted on studying the relationship between their magnetic properties and the novel superconductivity. Our previous RIXS studies reveal robust high energy spin modes on the parent compound $BaFe_2As_2$ *(BFA)* and the optimally hole-doped superconductor $Ba_{0.6}K_{0.4}Fe_2As_2$ (*BKFA*), which indicates a correlated spin state originated spin fluctuations in these materials, suggesting a close link between magnetism with superconductivity [1]. In order to extend our understanding of the magnetic properties in iron-based superconductors, we investigate the high energy spin-excitations in the electron-doped iron-based superconductor $Ba(Fe_{1-x}Co_x)_2As_2$ (*BFCA*) with Fe-L_3 edge RIXS. From a systematic measurement on the under-, nearly optimal- and over-doped samples we observed well defined dispersive high spin-excitations up to 200 meV (Fig.1) which persist into the superconducting phase, similar as found in the hole-doped superconductor *BKFA*, thereby demonstrating the existence of an universal correlated spin state responsible for the spin fluctuations in these materials. High energy spin-excitations in *BFCA* are nearly independent of electron doping, in contrast to *BKFA* that softened relative to the parent *BFA*[1] This shows that electron doping *BFA* seems not affect significantly the high energy spin-excitations, which is consistent with the INS result[2]. The result indicates a close relation of high energy spin-excitation to the electron correlation in these materials.

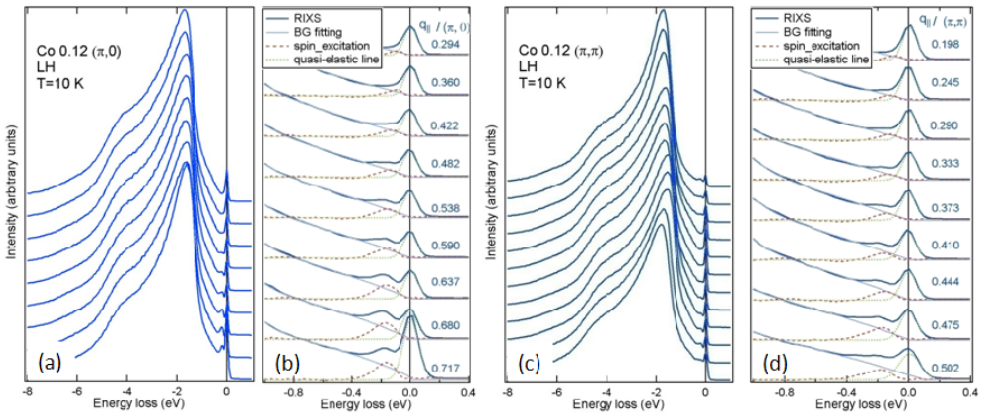


Fig.1 (a) and (b) the RIXS result of *BFCA* along (0,0)–>(π,0) in the Brillouin zone for Co doping x=0.12;(c) and (d) the same as (a) and (b) but along (0,0) –>(π, π) direction.

References

[1] K. J. Zhou, *.et.al., Nat. Commun.* **4**1470(2013)

[2] M. S. Liu, *et.al., Nat. Phys.* **8** 376–381 (2012)

Spin texture of topological insulator thin films in the quantum tunneling limit

Gabriel Landolt[1,2], Steffen Schreyeck[3], Sergey V. Eremeev[4,5], Bartosz Slomski[1,2], Stefan Muff[1,2,6], Jürg Osterwalder[1], Evgueni V. Chulkov[5,7], Charles Gould[3], Grzegorz Karczewski[3,8], Karl Brunner[3], Hartmut Buhmann[3], Laurens W. Molenkamp[3], and J. Hugo Dil[1,2,6]

[1] *Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*
[2] *Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen, Switzerland*
[3] *Physikalisches Institut, Experimentelle Physik III, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany*
[4] *Institute of Strength Physics and Materials Science, Russian Academy of Sciences, Siberian Branch, Akademicheskiy pr. 2/4, Tomsk, 634021 Russia*
[5] *Tomsk State University, Tomsk, 634050 Russia*
[6] *Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*
[7] *Donostia International Physics Center (DIPC) and CFM - MPC, Centro Mixto CSIC-UPV/EHU, Departamento de Fisica de Materiales, UPV/EHU, 20080 San Sebastian, Spain*
[8] *Institute of Physics, Polish Academy of Sciences, Al. Lotnikov 32/46, 02-668 Warsaw, Poland*

By means of spin- and angle-resolved photoelectron spectroscopy we studied [1] the spin structure of thin films of the topological insulator Bi_2Se_3 grown on InP(111). For thicknesses below six quintuple layers the spin-polarized metallic topological surface states interact with each other via quantum tunneling and a gap opens. Our measurements show that the resulting surface states can be described by massive Dirac cones which are split in a Rashba-like manner due to the substrate induced inversion asymmetry. The inner and the outer Rashba branches have distinct localization in the top and the bottom part of the film, whereas the band apices are delocalized throughout the entire film. Supported by ab-initio calculations our observations help understand the evolution of the surface states at the topological phase transition.

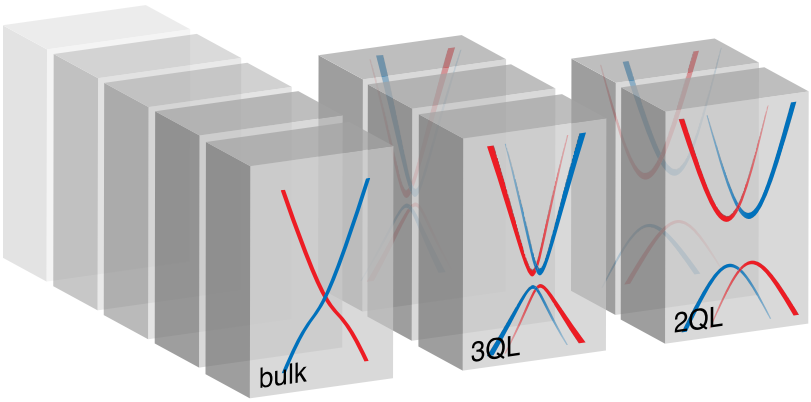


Figure 1: Schematic illustration of the evolution of the surface states upon reduction of the Bi_2Se_3 film thickness.

[1] G. Landolt *et al.*, Phys. Rev. Lett. 112, 057601 (2014)