HAXPES 2011

4th International Workshop on Hard X-ray Photoelectron Spectroscopy

14-16 September 2011
DESY, Hamburg, Germany

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Program and Abstracts

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Deutsches Elektronen-Synchrotron
A Research Centre of the Helmholtz Association

DESY

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WELCOME TO HAXPES 2011

Photoelectron spectroscopy with hard X-ray excitation (HAXPES, HIKE, HXPS or whatever acronym you may prefer) has gone a long way over many years until its great potential for electronic structure analysis of "real" materials had been recognized by the community on a broader scale. When our activities started here in Hamburg back in the mid 1990s no one was really interested in this exotic undertaking. Also, we were struggling with instrumental problems quite a bit, notably with the electron spectrometer which was not at all optimized for higher kinetic energies. Fortunately, this is history and things have improved considerably since then. The real boost was initiated by the activities of our Japanese colleagues at SPring-8 where significant progress was made in improving the HAXPES instrumentation and a number of very impressive scientific results were obtained with this new technique.

Meanwhile, several electron spectrometers that perform well in the 10 keV range are commercially available and their use in combination with high-brilliance X-ray undulator sources have demonstrated the potential and wide applicability of HAXPES in many areas of materials science, both basic and applied. In most applications, the key ingredient that HAXPES provides in addition is "bulk" sensitivity which is an order of magnitude larger compared to standard XPS techniques. This enables extending the unique and well-established capabilities of electron spectroscopy for surface analysis to applications where the composition and electronic structure of buried interfaces, complex correlated bulk materials or technologically relevant multi-layered functional materials are at the focus of interest.

Today, quite a number of HAXPES instruments are at work at synchrotron facilities, mainly in Japan and Europe, and others are being planned or commissioned. We were nevertheless overwhelmed by the strong interest in this workshop which was not anticipated at the beginning. The number of registered participants is 137 (see statistics at the end of this booklet) which implies that this event is more resembling a conference rather than a workshop. Not unexpectedly, the largest share of participants comes from Germany as the host country. However, we are very happy to welcome 77 colleagues from all over the world which demonstrates the worldwide interest in this technique. Clearly, our Japanese colleagues lead the international group of participants, reflecting the impressive HAXPES activities in Japan, mainly at Spring-8. The broad diversity and high quality of the contributions to this workshop document the strength of the method in many areas and also provide an excellent overview of emerging new activities.

It is a great pleasure to welcome you all to this 4th international HAXPES workshop held at DESY and I am confident that it will be a very interesting, lively and successful meeting. I wish you a very pleasant stay in Hamburg.

Wolfgang Drube
Conference Chair

Agenda HAXPES 2011

Tuesday, Sep. 13

17:00 - 20:00	**Registration** (canteen annex building)
18:00 - 20:30	**Get together** (canteen annex building)

Wednesday, Sep. 14

08:30 - 09:00	**Registration** (lobby auditorium)
09:00 - 09:15	***Welcome*** **E. Weckert**
09:15 - 10:00	***Introduction: Research with photons at DESY*** **W. Drube**
10:00 - 10:45	***Hard X-ray photoemission: a brief status report, some recent applications, and some future directions*** **C.S. Fadley** (invited)
10:45 - 11:15	**Coffee break**
Session 1 **Chair: C.M. Schneider**	**Theory and New Directions**
11:15 - 11:40	***One step model description of HAXPES: correlation, matrix elements and temperature effects*** **J. Minar** (invited)
11:40 - 12:05	***Band gap states and magnetism studied by photoelectron diffraction and HAXPES*** **P. Krüger**, A. X. Gray, C. S. Fadley (invited)
12:05 - 12:30	***Hard X-ray photoelectron spectroscopy using synchrotron radiation and free electron laser*** **Y. Takata**, A. Chainani (invited)
12:30 - 12:55	***Hard X-ray photoelectron spectroscopy with variable photon polarisation: linear and circular dichroism*** **G. H. Fecher** (invited)
12:55 - 13:10	***Quantitative interpretation of (HAX)PES using SESSA (simulation of electron spectra for surface analysis)*** **W.S.M. Werner**, W. Smekal, F. Salvat-Pujol, Th. Hisch, C.J. Powell
13:10 - 14:20	**Lunch (and opt. poster setup)**
Session 2 **Chair: S. Suga**	**Correlated Materials & Oxide Heterostructures I**
14:20 - 14:45	***The electronic structure of a-site ordered perovskite $ACu_3Ru_4O_{12}$ (A=Ca, Na, La) by hard X-ray photoemission spectroscopy*** **M. Taguchi** (invited)
14:45 - 15:10	***Interface-sensitive photoelectron spectroscopy on oxide heterostructures*** **M. Sing,** G. Berner, A. Müller, F. Pfaff, M. Paul, S. Glawion, A. Ruff, M. Kamp, S. Thiel, C. Richter, J. Mannhart, S.A. Pauli, C.W. Schneider, P.R. Willmott, H. Boschker, G. Koster, G. Rijnders, D.H.A. Blank, A. Hloskovskyy, F. Schäfers, M. Gorgoi, S. Thiess, W. Drube, R. Claessen (invited)
15:10 - 15:25	***Mott Insulating State of Ultrathin Epitaxial $LaNiO_3$ Thin Films Detected by Hard X-ray Photoemission*** **A. Gray,** A. Janotti, J. Son, J. M. LeBeau, S. Ueda, Y. Yamashita, K. Kobayashi, A.M. Kaiser, R. Sutarto, H. Wadati, G. A. Sawatzky, C.G. Van de Walle, S. Stemmer, C.S. Fadley
15:25 - 15:40	***Coherent Metallic Screening in Strongly Correlated Oxides: Experiment and Theory*** **S. Ueda**, H. Takami, T. Kanki, K. Kobayashi, H. Tanaka
15:40 - 16:10	**Coffee break**
Session 3 **Chair: P. Lysaght**	**Functional Interfaces**
16:10 - 16:35	***HAXPES to investigate advanced devices for microelectronic applications*** **E. Martinez,** B. Detlefs, P. Calka, R. Boujamaa, C. Guedj, M. Gros-Jean, V. Jousseaume, F. Bertin, J. Roy, J. Zegenhagen, O. Renault (invited)
16:35 - 16:50	***Bias application HX-PES study of metal/oxide interface: oxide based RERAM application*** **T. Nagata**, Y. Yamashita, H. Yoshikawa, M. Haemori, K. Kobayashi, T. Chikyow
16:50 - 17:05	***Electronic and electrical properties of functional interfaces studied by hard X-ray photoemission*** **A. Zenkevich,** Y. Lebedinskii, Y. Matveyev, S. Thiess, W. Drube
17:05 - 17:20	***Electronic structure of EuO magnetic oxide "spin filter" contacts on silicon*** **M. Müller**, C. Caspers, A.X. Gray, A.M. Kaiser, A. Gloskovskii, C.S. Fadley, W. Drube, C.M. Schneider
17:20 - 18:00	walk to FLASH hall & poster setup
18:00 - 21:00	**Poster Session** food & drinks (FLASH hall)
~21:00	opt. transfer to hotels

Thursday Sep. 15

Session 4 **Chair: J. Zegenhagen**	**Energy Research**
08:30 - 08:55	***Activation of erbium films for hydrogen storage*** **M. Brumbach**, J. Ohlhausen, K. Zavadil, C. Snow, J. Woicik (invited)
08:55 - 09:20	***HAXPES investigation of nanostructured PEM fuel cell catalysts*** **V. Matolin,** I. Matolinova, H. Yoshikawa, K. Kobayashi, B. Detlefs (invited)
09:20 - 09:45	***Probing the buried Si/ZnO thin-film solar cell interface by HAXPES*** **M. Bär** (invited)
09:45 - 10:10	***Understanding molecular interfaces used for energy conversion*** **H. Rensmo** (invited)
10:10 - 10:25	***High energy photoemission spectroscopy as tool for thin film solar cell characterisation*** **I. Lauermann**, H. Mönig, N. Allsop, P. Pistor, A. Grimm, B. Johnson, R. Caballero, C.A. Kaufmann, M. Gorgoi, F. Schäfers, W. Braun, M. Lux-Steiner, C.-H. Fischer
10:25 - 11:00	**Coffee break**
Session 5 **Chair: R. Claessen**	**Correlated Materials & Oxide Heterostructures II**
11:00 - 11:25	***Core level spectroscopy of thin film oxide heterointerfaces and bilayer CMR manganites*** **M.S. Golden**, E. Slooten, E. van Heumen, F. Massee, Y.K. Huang, D. Prabhakaran, A.T. Boothroyd, S. de Jong, H. Dürr, M. Gorgoi, Z. Zhong, H. Molegraaf, M. Huijben, G. Rijnders, G.-J. Koster, A. Brinkman, D. Blank, P. Kelly, H. Hilgenkamp (invited)
11:25 - 11:50	***HAXPES studies of phase separations in perovskite Mn–oxide superlattices*** **H. Wadati**, E. Sakai, M. Tamamitsu, K. Horiba, H. Kumigashira, M. Oshima, T. Sugiyama, E. Ikenaga, M. Nakamura, M. Kawasaki, Y. Tokura (invited)
11:50 - 12:15	***Many-body effects in strongly correlated materials: coupling DFT calculations of K edge absorption to experimental 1s photoemission*** **J.-P. Rueff,** M. Calandra, D. Céolin, A. Shukla and D. Chandesris (invited)
12:15 - 12:30	***Valence band analysis of $LaAlO_3$/$SrTiO_3$ oxide heterostructures using hard X-ray photoelectron spectroscopy*** **G. Berner**, F. Pfaff, A. Müller, S. Paetel, C. Richter, J. Mannhart, A. Hloskovskyy, W. Drube, M. Sing and R. Claessen
12:30 - 12:45	***Electronic structure of Pt based topological Heusler compounds with C1b structure explored by hard X-ray photoelectron spectroscopy*** **S. Ouardi**, G. H. Fecher, C. Shekhar, X. Kozina, G. Stryganyuk, C. Felser, E. Ikenaga, S. Ueda, and K. Kobayashi
12:45 - 13:00	Group photo
13:00 - 14:00	**Lunch**
Session 6 **Chair: S. Svensson**	**Atoms & Molecules**
14:00 - 14:25	***X-ray photoionization of free and confined atoms*** **S.T. Manson** (invited)
14:25 - 14:50	***Complex decay patterns in Ar following K-edge photoexcitation or photoionization disentangled by ion recoil experiments*** R. Guillemin, C. Bomme, T. Marin, L. Journel, T. Marchenko, R. K. Kushawaha, M.N. Piancastelli, **M. Simon** (invited)
14:50 - 15:15	***Resonant inelastic X-ray scattering on atoms and simple molecules in the tender X-ray region*** **M. Kavčič** (invited)
15:15 - 15:30	***Photoelectron time-of-flight spectroscopy in a hard X-ray regime*** **M. Ilchen**, M. Braune, J. Buck, S. Deinert, L. Glaser, F. Krasnqi, D. Rolles, F. Scholz, J. Seltmann, P. Walter, J. Viefhaus
15:30 - 16:00	**Coffee break**
Session 7 **Chair: W. Eberhardt**	**HAXPES & Diffraction Phenomena**
16:00 - 16:25	***Graphene on Ir(111) studied by X-ray standing waves*** **C. Busse** (invited)
16:25 - 16:40	***XSW imaging of thin lanthanum aluminate films on strontium titanate*** **C. Schlüter**, T-L. Lee, C. Aruta, J. Zegenhagen
16:40 - 16:55	***Site-specific electron diffraction resolved via nuclear recoil*** **A. Winkelmann**, M. Vos
17:00 - 18:30	transfer to hotels & Hamburg harbor
19:00 - 22:00	**Banquet on the river**
22:00 -	transfer to hotels & guest houses

Friday Sep. 16

Session 8 **Chair: G. Panaccione**	**Facilities & New Applications**
08:40 - 09:05	***Probing orbital symmetry in the valence bands of solids by polarization-dependent hard X-ray photoemission*** **A. Sekiyama**, A. Higashiya, S. Imada, S. Suga, M. Y. Kimura, Y. Tomida, H. Fujiwara, K. Tamasaku, M. Yabashi, T. Ishikawa (invited)
09:05 - 09:30	***Recent development of HAXPES instrumentations at BL47XU/SPring-8*** **E. Ikenaga**, M. Kobata, H. Matsuda, T. Sugiyama, H. Daimon, K. Kobayashi (invited)
09:30 - 09:45	***X-ray spectroscopy at NIST NSLS beamlines: recent upgrades, scientific results, and future plans*** **J.C. Woicik**
09:45 - 10:00	***Electronic structure of high temperature phase of strongly correlated oxides and of interface between oxide insulators*** **Ku-Ding Tsuei**, J. Weinen, S. Agrestini, M. Rotter, T. Willers, C. Schüßler-Langeheine, L. H. Tjeng, Y. F. Liao, Y.-Y. Chu, W.-C. Liu, D.-J. Huang
10:00 - 10:15	***HAXPEEM - spectroscopic imaging with hard X-rays*** **C. Wiemann**, M.C. Patt, A. Gloskovskii S. Thiess, W. Drube, M. Merkel, M. Escher, C.M. Schneider
10:15 - 10:30	***Magnetometry of buried layers by means of hard X-ray photoelectron spectroscopy*** **A. Gloskovskii**, G. Stryganyuk, G.H. Fecher, C. Felser, S. Thiess, H. Schulz-Ritter, W. Drube, M. Yamamoto
10:30 - 11:00	**Coffee break**
Session 9 **Chair: T.-L. Lee**	**Techniques & Instrumentation**
11:00 - 11:25	***Development of laboratory HXPS system and its applications*** **K. Kobayashi**, M. Kobata, H. Iwai, H. Matsuda, H. Daimon, H. Yamazui, H. Takahashi, M. Suzuki (invited)
11:25 - 11:40	***Development of ambient pressure hard X-ray photoelectron spectroscopy*** **M. Kobata**, T. Masuda, H. Yoshikawa, T. Miura, T. Kawasaki, K. Uosaki, and K. Kobayashi
11:40 - 11:55	***FOCUS GmbH: all about electrons...*** **M. Merkel** (FOCUS GmbH)
11:55 - 12:10	***HAXPES analyser MBS A1HE and high voltage electronics 2011*** **P. Baltzer,** M. Matsuki (MB Scientific AB)
12:10 - 12:25	***Angle-resolved and high-pressure hard X-ray photoelectron spectroscopy instrument development*** **R. Moberg** (VG Scienta AB)
12:25 - 12:40	***The PHOIBOS analyzer series: electron spectrometers for hard X-ray photoemission spectroscopy*** S. Mähl, O. Schaff, **Th.U. Kampen** (SPECS GmbH)
12:40 - 13:50	**Lunch**
Session 10 **Chair: D. Chandesris**	**Oxides & Materials Science**
13:50 - 14:15	***Probing s electron states in metal oxides with hard X-ray photoemission*** D.J. Payne, K.H.L Zhang, G. Panaccione, **R.G. Egdell** (invited)
14:15 - 14:40	***HAXPES studies of oxides and electronic interfaces at NIST beamline X24A*** **A. Rumaiz** (invited)
14:40 - 14:55	***HAXPES of novel charge transfer compounds*** **K. Medjanik**, A. Gloskovskii, D. Chercka, M. Baumgarten, K. Müllen , G. Schönhense
14:55 - 15:10	***Alloying and interface properties of Fe/V multilayers*** **S. Granroth**, R. Knut, M. Gorgoi, S. Svensson, O. Karis
15:10 - 15:25	***Direct observation of Al doping induced electronic states in the valence band of ZnO films*** M. Gabás, P. Torelli, N.T. Barrett, **M. Sacchi,** F. Bruneval, Y. Cui, L. Simonelli P. Díaz-Carrasco, J.R. Ramos Barrado
15:25 - 15:50	**Summary & conclusion**
15:50 - 16:00	**Closing**
16:00 - 18:00	**Optional lab visit** (PETRA III and FLASH)

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SPEAKERS' ABSTRACTS

RESEARCH WITH PHOTONS AT DESY

W. Drube

Deutsches Elektronen-Synchrotron DESY
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DESY is one of the world's leading accelerator centers and develops, builds and operates large particle accelerators to investigate the structure of matter. The laboratory is one of the pioneers of synchrotron radiation - first experiments were done in the mid 1960s - although the main focus was on particle physics until a few years ago. However, the 2nd generation source DORIS had been at the forefront of utilizing intense wiggler beams for SR experiments in the early 1990s and has been serving as a productive "workhorse" machine since then.

On the basis of new superconducting accelerator technologies developed by DESY and its international partners, the free-electron laser FLASH, which is operated for user experiments since 2005, was the first VUV-FEL light source worldwide pioneering the field of the rapidly emerging X-ray FEL activities. DESY also is the major partner within the European XFEL project. This X-ray laser with its 2 km long superconducting accelerator starting at the DESY site is currently being built and is expected to go into operation in 2015.

The conversion of the large accelerator PETRA into the 3rd generation X-ray source PETRA III has further boosted the photon science activities at DESY. This low emittance 6 GeV storage ring has been operating for user experiments since 2009 and is currently delivering the most brilliant photon beams in the hard X-ray regime among the storage-ring-based sources. It provides excellent conditions for coherence applications and high-resolution experiments on nano-structured materials. A total of 14 undulator beamlines are located in the new PETRA III experimental hall adjacent to the FLASH hall. Ten additional beamlines will be built in the course of a major PETRA extension project starting 2013.

There are also activities relating to this HAXPES 2011 workshop. First hard X-ray photoelectron spectroscopy experiments began at DORIS III in the mid 1990s utilizing the high photon flux from an X-ray wiggler at beamline BW2. However, the low source brilliance was not suitable for high energy resolution studies. This option became available recently with a new HAXPES instrument implemented at PETRA III undulator beamline P09. This station is now being operated for users and is starting to become a very productive and powerful instrument.

HARD X-RAY PHOTOEMISSION: A BRIEF STATUS REPORT, SOME RECENT APPLICATIONS, AND SOME FUTURE DIRECTIONS

C.S. Fadley (1,2) ***(invited)***

(1) Department of Physics, University of California Davis
(2) Materials Sciences Division, Lawrence Berkeley National Laboratory

In this talk, I will briefly summarize the status of hard x-ray photoemission (HAXPES, HXPS), as an introduction to the exciting and varied program of this Fourth International Workshop. I will also discuss some recent studies by my group and its several collaborators [1-9], including experiments at BESSY, SPring8, and PETRA III. These involve the bulk electronic structure of some spintronic materials [2,5,8]; buried layers and interfaces in magnetic and transition-metal oxide multilayers [3,4,8,9], including band-offset measurements [9]; the use of standing waves from multilayer mirrors to enhance depth contrast [3,4]; and the prospects for carrying out bulk sensitive hard x-ray ARPES (HARPES) [7] and hard x-ray photoelectron diffraction (HXPD) [1].

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1. "High energy photoelectron diffraction: model calculations and future possibilities", A. Winkelmann, J. Garcia de Abajo and C.S. Fadley, New J. Phys. 10, 113002 (2008); plus presentation by A. Winkelmann in this Workshop.
2. "Band Gap and Electronic Structure of an Epitaxial, Semiconducting $Cr_{0.80}Al_{0.20}$ Thin Film", Z. Boekelheide, A. X. Gray, C. Papp, B. Balke, D. A. Stewart, S. Ueda, K. Kobayashi, F. Hellman, and C. S. Fadley, Phys. Rev. Letters 105, 236404 (2010)
3. "Interface properties of magnetic tunnel junction $La_{0.7}$ $Sr_{0.3}MnO_3/SrTiO_3$ superlattices studied by standing-wave excited photoemission spectroscopy", A. X. Gray, C. Papp, B. Balke, S.-H. Yang, M. Huijben, E. Rotenberg, A. Bostwick, S. Ueda, Y. Yamashita, K. Kobayashi, E. M. Gullikson, J. B. Kortright, F. M. F. de Groot, G. Rijnders, D. H. A. Blank, R. Ramesh, and C. S. Fadley, Phys. Rev. B 82, 205116 (2010).
4. "Hard X-ray photoemission study using standing-wave excitation applied to the MgO/Fe interface", S. Döring, F. Schönbohm, U. Berges, R. Schreiber, D. E. Bürgler, C. M. Schneider, M. Gorgoi, F. Schäfers, C. Papp, B. Balke, C. S. Fadley, C. Westphal, Phys. Rev. B 83, 165444 (2011), plus presentation by S. Döring in this Workshop.
5. "Hard X-ray Photoemission Study of Near-Heusler Fe_xSi_{1-x} Alloys", A. X. Gray,J. Karel, J. Minar, C. Bordel, H. Ebert, J. Braun, S. Ueda, Y. Yamashita, L. Ouyang, D. J. Smith, K. Kobayashi, F. Hellman, and C. S. Fadley, Phys. Rev. B 83, 195112 (2011).
6. "Insulating state of ultrathin epitaxial $LaNiO_3$ thin films detected by hard x-ray photoemission", A. X. Gray, A. Janotti, J. Son, J. M. LeBeau, S. Ueda, Y. Yamashita, K. Kobayashi, A. M. Kaiser, R. Sutarto, H. Wadati, G. A. Sawatzky, C. G. Van de Walle, S. Stemmer, C. S. Fadley, Phys. Rev. B 84, 075104 (2011); plus presentation by A.X. Gray in this Workshop.
7. "Hard X-ray angle-resolved photoemission in the 3-6 keV regime: first experimental data and theory for W(110) and GaAs(100)", C. Papp, A. Gray, B. Balke, S. Ueda, K. Kobayashi, S. Sakai, H. Yoshikawa, Y. Yamashita, S. L. He, E. Yylvisaker, L. Plucinski, C. Schneider, J. Minar, J. Braun, H. Ebert , W.E. Pickett, C. S. Fadley: Nature Materials, to appear, August, 2011; plus theory presentations by J. Minar, J. Braun and L. Plucinski in this Workshop.
8. "Chemical state of the magnetic oxide EuO on silicon investigated by HAXPES", C. Caspers, M. Müller, A. X. Gray, A. Gloskovskij, A. M. Kaiser, C. S. Fadley, W. Drube, C. M. Schneider, Phys. Rev. B, submitted, plus presentation by C. Caspers in this Workshop.
9. "Determination of Band Offsets in Complex Oxide Thin-Film Heterostructures by Hard X-Ray Photoelectron Spectroscopy", G. Conti, A. X. Gray, A. M. Kaiser, A. Greer, J.Karel, S. Ueda, Y. Yamashita, A. Gloskovskii, A. Jannotti, C. G. Van de Walle, K. Kobayashi, W. Drube, S. Stemmer, and C.S. Fadley, plus presentation by G. Conti in this Workshop.

ONE STEP MODEL DESCRIPTION OF HAXPES: CORRELATION, MATRIX ELEMENTS, AND TEMPERATURE EFFECTS

Jan Minar ***(invited)***

(1) Department. Chemie, University of Munich, Munich, Germany

Angle resolved as well as angle integrated photoemission in the soft and hard X-ray regime became a very important tool to investigate the bulk properties of various materials [1]. Contrary, bulk sensitivity can be achieved by so called threshold photoemisison, e.g. by using for example laser light at 405 nm [2].

The increased bulk sensitivity might lead to the impression that the LSDA band structure or density of states can be directly compared to the measured spectra. However, various important effects, like matrix elements, the photon momentum or phonon excitations, are in this way neglected. Here, we present a generalization of the state of the art description of the photoemisison process, the so called one-step model that describes excitation, transport to the surface and escape into the vacuum in a coherent way. A short introduction to the main features of the one-step model implementation within the Munich SPR-KKR program package will be given. Special emphasis will be put on the spin-polarised relativistic mode that allows to deal with magnetic dichroism. Also, the possibility to account for correlation effects and chemical disorder using the LSDA+DMFT (dynamical mean field theory) scheme in combination with the Coherent Potential Approximation (CPA) method [3] will be demonstrated by various examples.

Furthermore, the impact of the photon momentum and of a small sample tilt within high energy angle resolved PES will be discussed showing results from W(110) and Fe-pnictides as examples [4]. The effect of correlation, matrix elements effects and chemical disorder will be discussed on the examples of Au(111), FeSi and the diluted magnetic semiconductor GaMnAs [5]. For photon energies, even in the soft-x-ray regime, a considerable effect of lattice vibrations is present [4]. Here, we discuss a theoretical description of lattice vibrations which is based on the CPA. In particular this allows a coherent description of the direct and indirect (density of states like) transitions which reflect the breakdown of the dipole selection rules. Finally, our recent developments allows us to describe the layer-dependent and angle resolved photoemission that is measured by the x-ray standing waves method. A first example of a LSDA+DMFT calculation on the $SrTiO_3$/$LaSrMnO_3$ multilayer system will be presented.

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4. L. Pluczinski, J. Minar et al., Phys. Rev. B, accepted (2011), Phys. Rev. B 78, 035108 (2008)
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**Wed.
11:40**

BAND GAP STATES AND MAGNETISM STUDIED BY PHOTOELECTRON DIFFRACTION AND HAXPES

P. Krüger (1), A. X. Gray (2), C. S. Fadley (2) ***(invited)***

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Valence band photoelectron diffraction (VBPED) provides combined structural and electronic information of materials. We have used VBPED at the 2p-3d resonance to gain spatial information on selected electronic states in TiO_2 and Fe_3O_4. In TiO_2, a band gap state appears upon reduction which is believed to play a crucial role in the chemical and photocatalytic properties of TiO_2. Using VBPED we have studied the charge distribution of the band gap state at an oxygen-defective [1] and at a sodium covered TiO_2(110) surface. The gap state charge distribution is found to be very similar in the two cases, suggesting that it is an intrinsic property of weakly reduced TiO_2(110), independent of the origin of the excess electrons. In Fe_3O_4, VBPED has been used to identify the crystallographic site of Fe^{2+} ions. In agreement with previous studies, we find that Fe^{2+} occupies octahedral sites [2]. We have developed a computational method for VBPED based on real space multiple scattering. Through the results obtained for Cu(111) we discuss the relationship between angle-resolved photoemission, VBPED and core-level PED [3].

In the second part, an experimental and theoretical study on the electronic structure of FeRh is presented [4]. FeRh undergoes an antiferromagnetic to ferromagnetic transition around 350 K. The valence band and Fe-2p level have been studied using hard x-ray photoemission spectroscopy (HAXPES). Both the valence band spectra and the Fe-2p line display small but clear differences between the two phases. The valence band spectra are calculated using first principles density functional theory. The changes in lineshape across the transition are very well reproduced in the calculations. They mainly reflect changes of the spin-polarization of the Rh-4d density of states which is induced by Fe-Rh hybridization. The Fe-2p spectra have been calculated using an Anderson impurity model and good lineshapes have been obtained. The small changes observed across the magnetic transition are related to the opening of a new screening channel from coherent Fe-Fe hopping in the ferromagnetic phase.

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Wed. 12:05

HARD X-RAY PHOTOELECTRON SPECTROSCOPY USING SYNCHROTRON RADIATION AND FREE ELECTRON LASER

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Photoelectron Spectroscopy (PES) is a powerful method to investigate electronic structure of materials, and is widely used in solid state physics and chemistry. Over the last 10 years, high-brilliance synchrotron radiation (SR) at SPring-8 has allowed Hard X-ray Photoelectron Spectroscopy (HAXPES) for bulk-sensitive PES. Important results include the recoil effect in core level and valence band PES, surface versus bulk electronic structure of correlated materials, as well as depth-dependent and buried layer measurements. Given the development of low and high energy lasers using a variety of techniques over the last few years, the next challenge is to carry out Time-resolved PES using the free-electron lasers (FELs). We discuss our HAXPES experiments with SR (hv = 6 – 8 KeV) and recent attempts to measure PES with the low energy FEL (hν =62 eV) at the SCSS Test Accelerator. These experiments provide us with the conditions and requirements for carrying out PES with the XFEL named SACLA, presently being commissioned at SPring-8 site. Time-resolved PES is expected to provide element selective real-time dynamics of electronic excitations and phase transitions in solids. A few possible experiments will be discussed.

Wed.
12:30

HARD X-RAY PHOTOELECTRON SPECTROSCOPY WITH VARIABLE PHOTON POLARISATION: LINEAR AND CIRCULAR DICHROISM

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This work reports on photoemission experiments using hard X-rays (8 keV) with variable polarisation for excitation. The polarisation of the hard X-rays is changed using an in-vacuum diamond phase retarder. The initial linear *p* polarisation can be changed to linear *s* or circular (σ+, σ-). The variation of the polarisation enables to measure linear as well as circular dichroism in the angular distribution of the photoelectrons. The set-up of the experiment is sketched in Figure 1.

The high bulk sensitivity of HAXPES is suitable to determine the magnetism in magnetic multilayers making use of the magnetic dichroism from core-levels and valence band. Linear dichroism experiments were performed on Au(111), NiTiSn and NiMnSb bulk samples [1]. The change from *p* to *s* polarisation results in pronounced changes of the valence band spectra. The observed changes are explained by differences in the β-parameters of the contributing s and d initial states that result in a dichroism already without magnetic effects.

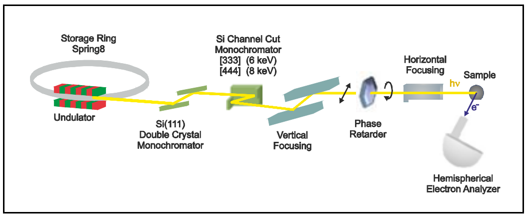

Fig1. Experimental set-up of the variable polarisation HAXPES experiment.

The magnetic circular dichroism experiments were performed on exchange biased magnetic layers [2]. Two types of structures were used with the MnIr (10 nm) exchange bias layer either on top or below the ferromagnetic layer. The latter were CoFe (3 nm) on-top or Co_2FeAl (30 nm) on-bottom. A pronounced magnetic dichroism of up to 50% is found at the Co and Fe 2p states of both materials. This demonstrates the feasibility of the method for the study of magnetism in deeply buried layers.

The financial support by the DFG (P 1.3-A in FOR 1464 ASPIMATT), DfG-JST (FE633/6-1), and BMBF (05KS7UM1) is gratefully acknowledged. The measurements were performed at beamline P09 of PETRA III in Hamburg and BL-47XU of SPring8 in Hyogo (Proposal No. 2009B0017).

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**Wed.
12:55**

QUANTITATIVE INTERPRETATION OF (HAX)PES USING SESSA (SIMULATION OF ELECTRON SPECTRA FOR SURFACE ANALYSIS)

Wolfgang S.M. Werner (1), Werner Smekal (1,2), Francesc Salvat-Pujol (1), Thomas Hisch (1), and Cedric J. Powell (3)

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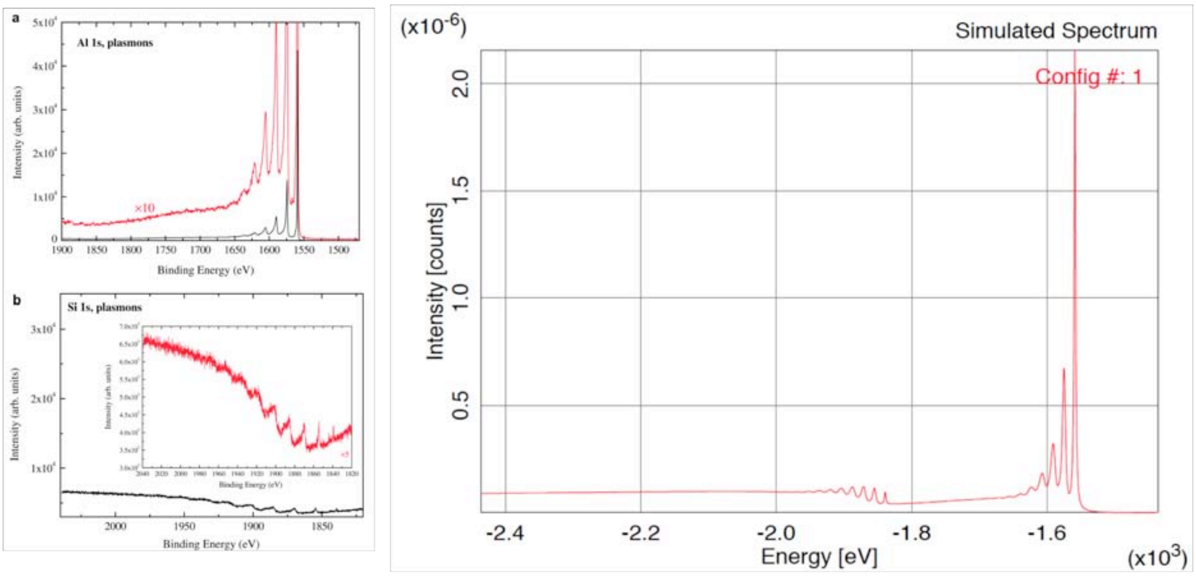
Predicting peak intensities and the shape of the inelastic background in photoelectron spectroscopy is generally a difficult task due to the combined influence of the anisotropy of the photoelectric cross section, elastic and inelastic scattering of the photoelectrons inside the solid, the experimental geometry, and the structure of the studied specimen. In the case of HAXPES, the situation becomes even more complex since one also has to account for the influence of non-dipole effects and the polarization state of the incoming beam. Predicting peak intensities and spectral shape is then greatly facilitated by the NIST database SRD100-"SESSA" (Simulation of Electron Spectra for Surface Analysis) that contains extensive databases for all parameters relevant for quantitative spectrum interpretation, as well as an expert system and simulation module that allows a user to perform such calculations with very little effort [1,2]. In our presentation, we discuss the influence of various physical phenomena on peak intensities and spectral shape for HAXPES by comparing SESSA simulations with HAXPES data found in the literature. The example given below, taken from Ref. [3], shows the HAXPES of a 70 nm Al film on Si. The simulated spectrum from SESSA agrees well with the measured spectrum.



Comparison of SESSA simulations (right panel) with experimental HAXPES data of a 70 nm Al Film on Si [2] (left panels).

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THE ELECTRONIC STRUCTURE OF A-SITE ORDERED PEROVSKITE $ACu_3Ru_4O_{12}$ (A=Ca, Na, La) BY HARD X-RAY PHOTOEMISSION SPECTROSCOPY

M. Taguchi ***(invited)***

Harima Institute, RIKEN/SPring-8, Hyogo 679-5148, Japan

Perovskite oxides containing transition metal (TM) ions at the A site of the ABO_3 structure are quite rare. An example of such an A-site ordered perovskite is $AA'_3B_4O_{12}$, in which 3/4 of the A sites in an ABO_3 perovskite (denoted as A') are occupied by TM ions such as Cu^{2+} and Mn^{3+}. Recently, various A-site ordered perovskite oxides $ACu_3B_4O_{12}$ have been synthesized and their physical properties have been attracting great interest, because of the rich electronic/magnetic properties with changing the combinations of A and B ions [1]. In particular, $ACu_3Ru_4O_{12}$ (A=Na, Ca and La) has attracted much attention, because of its metallic conductivity with heavy effective mass [2,3]. In $CaCu_3Ru_4O_{12}$, Kobayashi *et al.* found that the magnetic behavior is ascribable to the lattice Kondo effect between Cu^{2+} ion and Ru 4d orbital. Krimmel *et al.* reported the possibility of non-Fermi-liquid behavior below 2K [4]. However, systematic understanding of their electronic structures is still lacking.

In the present study, we have performed bulk-sensitive hard x-ray photoemission spectroscopy (HAXPES) on Cu 2p core-level of A-site ordered perovskite $ACu_3Ru_4O_{12}$ (A=Ca, Na, and La). Comparison of conventional Cu 2p core-level spectra with soft x-ray PES [5], our HAXPES results show clear additional well-screened features at low binding energy side, clarifying the difference of the electronic state of $ACu_3Ru_4O_{12}$ with A=Ca, Na, La.

The author is grateful to M. Mizumaki, T. Sudayama, T, Mizokawa, A. Chainani, Y. Takata, M. Matsunami, R. Eguchi, M. Yabashi, K. Tamasaku, Y. Nishino, T. Ishikawa, S. Tanaka, H. Takatsu, S. Yonezawa, Y. Maeno and S. Shin.

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INTERFACE-SENSITIVE PHOTOELECTRON SPECTROSCOPY ON OXIDE HETEROSTRUCTURES

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Transition metal oxides display a huge variety of intrinsic functionalities such as ferroelectricity, magnetism, superconductivity, or multiferroic behavior. With the developments of thin film deposition techniques such as pulsed laser deposition during the last decade it is nowadays possible to epitaxially grow heterostructures from this materials with atomic precision. At their interfaces new phases emerge due to the rearrangement of charge, spins, orbitals, and lattice and the resulting re-balancing of their mutual interactions. Cases in point are the quasi-twodimensional electron gas (q2-DEG) at the interface of $LaAlO_3/SrTiO_3$ (LAO/STO) [1], which even becomes superconducting below about 200mK [2], or the system $LaVO_3/SrTiO_3$, which involves a Mott insulator instead of a semiconductor [3]. The great appeal of these new material systems lies in the possibility to electrostatically modify the interfaces either by varying the thickness of the polar layers, exploiting the mechanism of electronic reconstruction [4], or by applying a gate voltage [4,5]. While thus being of enormous interest from both the fundamental and the applicational point of view, such kind of structures pose huge challenges to spectroscopy since the method of choice at the same time has to provide a sufficiently large probing depth and the required contrast to access and probe the physical properties of the buried interfaces. Referring to the above examples, it will be shown what kind of information can be obtained from hard x-ray photoelectron spectroscopy (HAXPES) on the electronic and chemical structure of buried interfaces in oxide heterostructures (see Fig. 1).

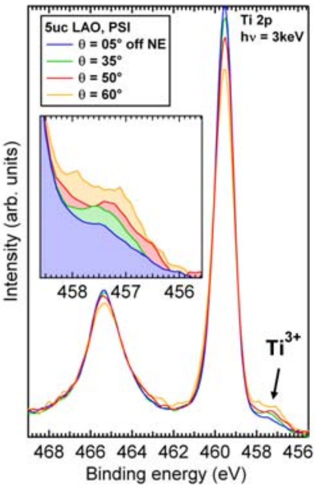

Fig1. Ti 2p HAXPES spectra of LAO/STO. The Ti^{3+} weight is direct evidence of the q2-DEG [6].

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Wed.
15:10

MOTT INSULATING STATE OF ULTRATHIN EPITAXIAL LaNiO$_3$ THIN FILMS DETECTED BY HARD X-RAY PHOTOEMISSION

A. X. Gray (1,2), A. Janotti (3), J. Son (3), J. M. LeBeau (3), S. Ueda (4), Y. Yamashita (4), K. Kobayashi (4), A. M. Kaiser (1,2), R. Sutarto (5,6), H. Wadati (5), G. A. Sawatzky (5), C. G. Van de Walle (3), S. Stemmer (3), and C. S. Fadley (1,2)

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In order to understand the influence of strain and film thickness on the electronic structure of thin films of strongly correlated oxides, we have applied hard x-ray photoemission (HAXPES) at 6 keV, soft x-ray photoemission (XPS) at 1.5 keV, and transmission electron microscopy to epitaxial LaNiO$_3$ films deposited on two substrates: LaAlO$_3$ (compressive strain) and (LaAlO$_3$)$_{0.3}$(Sr$_2$AlTaO$_6$)$_{0.7}$ (tensile strain). Using inelastic attenuation lengths in LaNiO$_3$ determined from the HAXPES data, we have decomposed valence-band spectra into layer-specific contributions. This decomposition is validated by comparing with the results of first-principles calculations using a hybrid functional. The resultant thin-film LaNiO$_3$ densities of states exhibit significant differences in spectral weights for the thinnest LaNiO$_3$ films. A gap opening consistent with a metal-to-insulator transition is observed for the thinnest 2.7 nm LaNiO$_3$ film on an (LaAlO$_3$)$_{0.3}$(Sr$_2$AlTaO$_6$)$_{0.7}$ substrate, with a similar gap opening also being observed in complementary soft x-ray photoemission at 1.5 keV for a thinner 1.4 nm film on an LaAlO$_3$ substrate. A metal-to-insulator transition in very thin nm-scale films of LaNiO$_3$ is thus suggested as a general phenomenon.

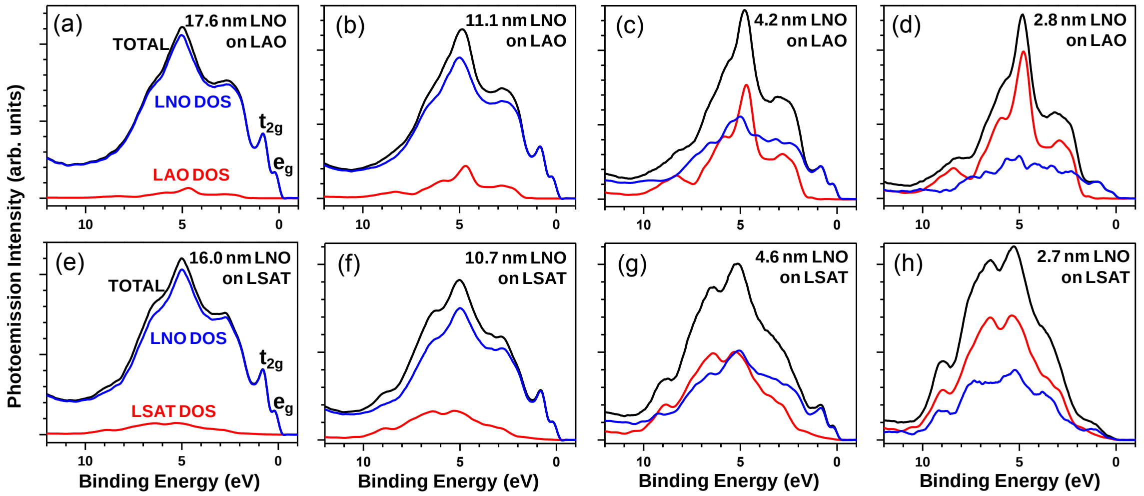

Fig. 1. Isolated substrate- and thin-film DOS components for LNO on an LAO substrate (a) 17.6 nm of LNO, (b) 11.1 nm of LNO, (c) 4.2 nm of LNO, and (d) 2.8 nm of LNO. Isolated substrate- and thin-film DOS components for LNO on an LSAT substrate (e) 16.0 nm of LNO, (f) 10.7 nm of LNO, (g) 4.6 nm of LNO, and (h) 2.7 nm of LNO.

COHERENT METALLIC SCREENING IN STRONGLY CORRELATED OXIDES: EXPERIMENT AND THEORY

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Strongly correlated transition metal oxides, which show a satellite structure due to a coherent metallic screening process in core-level photoemission, were studied by hard x-ray photoemission spectroscopy (HAXPES) and configuration interaction theory based on a cluster model. In the cluster model calculation, we take the hybridization between transition metal 3***d*** states and metallic coherent states (V*) into account [1]. As reported by Tanaka ***et al.***, the intensity of the satellite structure ($\boldsymbol{I_s}$) due to coherent metallic screening in the Mn 2***p*** core-level spectra of $La_{1-x}Ba_xMnO_3$ (LBMO) thin films shows strong temperature dependence [2, 3] and is proportional to $(V^*)^2$ [2]. To clarify this linear relationship between $\boldsymbol{I_s}$ and $(V^*)^2$, we have carried out a series of cluster model calculations, in which the multiplet states were neglected for simplicity. These calculations give us the spectral weight in the final states for various V* values and $\boldsymbol{I_s}$ as a function of $(V^*)^2$, and are plotted in Fig. 1. The linearity between $\boldsymbol{I_s}$ and $(V^*)^2$ was found when the charge transfer energy (Δ and Δ*), the Coulomb interactions ($\boldsymbol{U_{dc}}$ and $\boldsymbol{U_{dd}}$) and the Mn 3***d*** - O 2***p*** hybridization strength (V_{eff}) were treated as fixed parameters.

To further explore the relationship between $\boldsymbol{I_s}$ and $(V^*)^2$, we have performed V 2***p*** core-level and valence band HAXPES measurements for $V_{1-x}W_xO_2$ thin films [4] at BL15XU [5] of SPring-8. In this system, the W-doping increases metallic behavior. With increased W-doping, the $\boldsymbol{I_s}$ of the V 2p core-level spectra steeply increases. To estimate V*, we used the electronic structure parameter set for VO_2 in Ref.[6], and calculated $\boldsymbol{I_s}$ as a function of V*, where Δ, Δ*, V_{eff}, $\boldsymbol{U_{dc}}$, and $\boldsymbol{U_{dd}}$ were again treated as fixed parameters. From these calculations (not shown), we found that $\boldsymbol{I_s}$ is neither proportional to V* nor to $(V^*)^2$ for $V_{1-x}W_xO_2$ thin films. On the other hand, $(V^*)^2$ determined from the experimental $\boldsymbol{I_s}$ showed that the intensity observed at the Fermi level was proportional to $(V^*)^2$. This relationship is also expected from the impurity Anderson model [7]. We will present the experimental and theoretical results for both LBMO and $V_{1-x}W_xO_2$ thin films in detail.

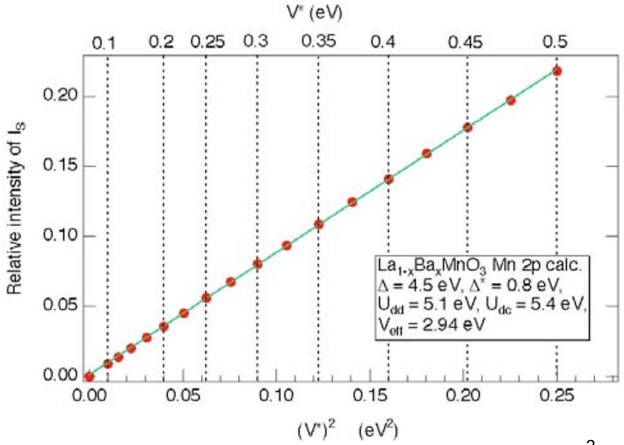

Fig.1. Calculated $\boldsymbol{I_s}$ for LBMO as a function of $(V^*)^2$.

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Wed. 16:10

HAXPES TO INVESTIGATE ADVANCED DEVICES FOR MICROELECTRONIC APPLICATIONS

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M. Gros-Jean (3), V. Jousseaume (1), F. Bertin (1), J. Roy (2), J. Zegenhagen (2)
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There is a huge need to obtain in-depth chemical information non-destructively to help to develop and optimize new advanced devices for microelectronic applications. We present recent HAXPES results obtained for innovative Oxide Resistive Random Access Memories (OxRRAM) and Complementary Metal Oxide Semiconductor (CMOS) devices. Experiments were performed at the ID32 beamline of the European Synchrotron Radiation Facility (ESRF) to investigate the chemical composition of buried layers and interfaces.

Resistive memories are candidates for future non volatile random access memories. Data storage is based on switching the resistance of a transition metal oxide between high and low states under bias voltage. However, the switching mechanism is still poorly understood. HAXPES was carried out on the NiO(20 nm)/Pt system after *ex-situ* resistive switching. Analysis of Ni2p, O1s and valence band spectra highlight similar energy shifts as well as band gap states after switching (see figure 1). These results suggest that oxygen vacancies are created in the low resistive state, thus pointing out the major role of oxygen diffusion across the structure [1]. This is a key point since oxygen vacancies are particularly unstable and difficult to identify with other techniques.

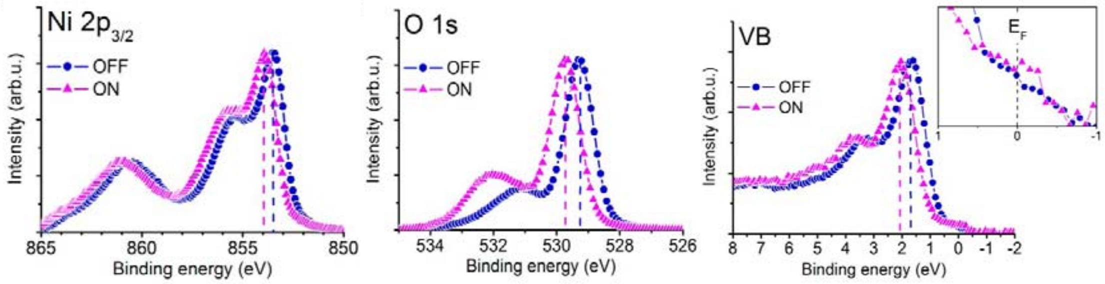

Figure 1: Ni2p$_{3/2}$, O1s and valence band spectra measured by HAXPES at 2.1 keV for the high (OFF) and low (ON) resistance states.

Downscaling of CMOS transistors requires the use of new materials and complex structures such as high-k / metal gate stacks with thin LaO capping layers. HAXPES measurements were performed without removing the metal gate, thus preserving the underlying layers. Results highlight La diffusion through the entire stack towards the bottom high-k/Si interface as well as formation of La-silicate [2]. The energy shifts measured for Hf4f, O1s and Ti2p core levels are directly assigned to a modification of the energy band diagram. They are in good agreement with electrical C(V) measurements, thus indicating a dipole-like behavior at the high-k/Si interface [3]. Other techniques, in particular destructive ones, require partial removal of the gate or backside preparation with possible related artifacts.

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BIAS APPLICATION HX-PES STUDY OF METAL/OXIDE INTERFACE: OXIDE BASED RERAM APPLICATION

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K. Kobayashi (2) and T. Chikyow (1)

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Resistive random access memory (ReRAM) has been proposed as a new application for oxide materials. An oxide sandwiched between two metal electrodes shows reversible electric field–induced resistance switching behaviors. Recently, hafnium oxide (HfO_2), which is used as a high-k gate insulator, has shown resistance switching phenomena and been increased interest in the use of HfO_2 and related oxides as potential ReRAM materials. For the oxide based ReRAM, two mechanisms of resistance switching have been proposed. One is the filament model, which comprises the generation and rupture of a metal filament using a metal such as Cu acting as a fast mobile ion in oxides. The other model is that of oxygen vacancy nucleation at the metal/oxide interface. To put the oxide based ReRAM on practical applications, understanding on controls of metal/oxide interface is essentially important. Here, we employed hard x-ray photoelectron spectroscopy (HX-PES) under bias operation, which enabled us to observe bias-induced compositional changes around the metal/oxide interface and the oxide film region, to examine the electronic structure of Pt or Cu/HfO_2 interface in an operating device.

A HfO_2 layer was deposited on a Pt bottom electrode by pulsed laser deposition. 10-nm-thick Pt or Cu top electrodes were formed on the HfO_2 film by DC sputtering. The interface electronic states were measured with HX-PES in the SPring-8 BL15XU undulator beamline. The incident X-ray energy was 5.95 keV and the total energy resolution was 240 meV.

In the case of the Pt/HfO_2 interface, applying a forward bias increased the Pt–O bonding peak as shown in Fig 1, indicating evidence of Pt electrode oxidization and oxygen vacancy formation around the interface. In contrast, the application of a bias to the Cu/HfO_2 interface reduced the copper oxide bonding state, providing evidence of oxygen reduction and Cu diffusion into the HfO_2 layer. We achieved direct observation of oxygen migration at the metal/HfO_2 interface under device operation, which is the key to controlling the electrical properties of oxide based ReRAM. The relationship between the interface structure and the electrical properties will be discussed in detail.

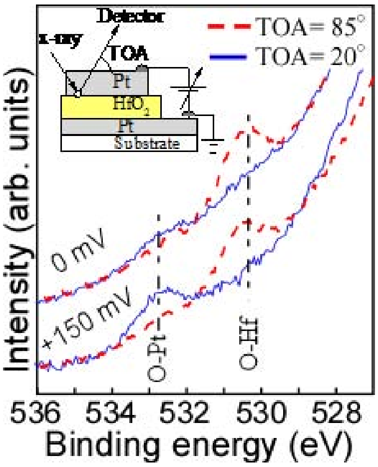

Fig. 1. HX-PES of O 1*s* as a function of bias at TOAs of 20° (interface sensitive) and 85° (bulk sensitive). The inset shows measurement setup.

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**Wed.
16:50**

ELECTRONIC AND ELECTRICAL PROPERTIES OF FUNCTIONAL INTERFACES STUDIED BY HARD X-RAY PHOTOEMISSION

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As the device downscaling in nanoelectronics has reached the 10 nm range, the functionality of materials employed in multi-layered structures to be used in future logic and memory devices is largely determined by their interface properties. The functional properties of multi-layered stacks such as metal-oxide-semiconductors with novel high-k dielectrics and metal gates, metal/isolator/metal structures with resistive switching properties, metal/ferroelectric/metal or ferromagnetic/tunnel isolator/ferromagnetic stacks exhibiting tunneling electro-resistance are related to their band alignment which is affected by the electric dipoles building up at the interface(s). Due to the high (3-12 keV) kinetic energies of photoelectrons in hard X-ray photoelectron spectroscopy (HAXPES), the technique is capable of non-destructively probing the detailed electronic structure including the electronic conditions at the interface(s) of (multi)layered structures at 10-30 nm depths. The latter advantage provides an opportunity to study the band alignment in the whole stacks consisting of layers with thicknesses modeling real world applications. In addition, HAXPES provides an opportunity to monitor the spatial redistribution of charges upon *ex situ* or *in situ* biasing thus modeling the device functional structure under operation. In this work, we report on the application of HAXPES (at DORIS III and PETRA III instruments) to investigate the electronic and electrical properties at the interfaces of several relevant multilayered functional structures.

In particular, the cyclic biasing of $Pt/HfO_2/Si$ stacks at elevated temperature monitored by HAXPES has been shown to result in reversible energy shifts of core level lines in HfO_2, eventual growth respectively dissolution of the SiO_x layer at the bottom interface and consistent changes of the flatband voltage. The obtained data are described in terms of positively charged oxygen vacancy migration in HfO_2 under biasing [1].

In another example, we systematically investigate the effect of the ferromagnetic Gd marker interlayer thickness on the “effective” work function of Fe in contact with the tunnel Al_2O_3 isolator. Fe(6 nm)/Gd(0.2-2 nm)/Al_2O_3(10 nm)/Si structures were analyzed by HAXPES at E=4.5 keV which provides the depth sensitivity to probe the entire stack down to the Si substrate. The band alignment at the Gd/Al_2O_3 interface is clearly visible in the Al 2s peak shift and depends on the Gd thickness (see Fig.1).

Finally, we provide for the first time the electronic band alignment at the metal/ferroelectric interface (metal=Fe, Pt; ferroelectric= $BaTiO_3$) as determined by HAXPES.

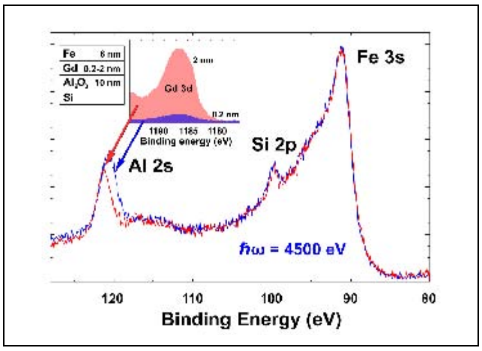

Fig1. HAXPES data measured on $Fe/Gd/Al_2O_3/Si$ heterostructures: the band alignment at the Fe/Al_2O_3 interface is clearly affected by the thickness of Gd marker layer.

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ELECTRONIC STRUCTURE OF EuO MAGNETIC OXIDE "SPIN FILTER" CONTACTS ON SILICON

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Accenting semiconductor electronics with spin functionality is a major thrust of current spintronics research. At present, considerable efforts are being made to replace conventional ferromagnet/semiconductor (FM/SC) or FM/oxide/SC contacts - which have hitherto been underlying many key experiments - with functional magnetic contact materials that could substantially alter the efficiency of spin injection and detection in semiconductor-based spintronics devices. In this talk, we present a comprehensive electronic structure study of a magnetic oxide/semiconductor model system, EuO on Silicon [1], which is dedicated for efficient spin injection and spin detection in novel silicon-based spintronics devices .

In particular, we demonstrate the successful chemical stabilization of stoichiometric EuO thin films grown directly on Si with no buffer layer. We present hard x-ray photoemission spectroscopy experiments of EuO compounds with different chemical ground states, i.e. stoichiometric EuO and O-rich EuO. A combined quantitative electronic structure analysis of Eu *4s*, *4d* and *3d* core levels and Eu *4f* valence bands was performed via hard x-ray photoemission spectroscopy at beamline P09 at PETRAIII. We carefully determined the initial oxidation state of Eu cations via a quantitative peak analysis of core-level and valence spectra [2]. Furthermore, we performed depth-sensitive measurements and extracted the Eu valency in the bulk and interface regions, confirming that nearly ideal, homogeneous and stoichiometric thin films of the magnetic oxide EuO can be grown directly on Si. Moreover, we could verify the absence of any silicon oxide at the EuO/Si interface [3]. Our results provide evidence for the successful integration of a magnetic oxide tunnel barrier silicon, paving the way for the future integration of magnetic oxides into functional spintronics devices.

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Thu.
8:30

ACTIVATION OF ERBIUM FILMS FOR HYDROGEN STORAGE

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Hydriding of metals can be routinely performed at high temperature in a rich hydrogen atmosphere. Prior to the hydrogen loading process, a thermal activation procedure is required to promote facile hydrogen sorption into the metal. Despite the wide spread utilization of this activation procedure, little is known about the chemical and electronic changes that occur during activation. This study utilized variable kinetic energy X-ray photoelectron spectroscopy to interrogate the changes during *in situ* thermal annealing of erbium films.

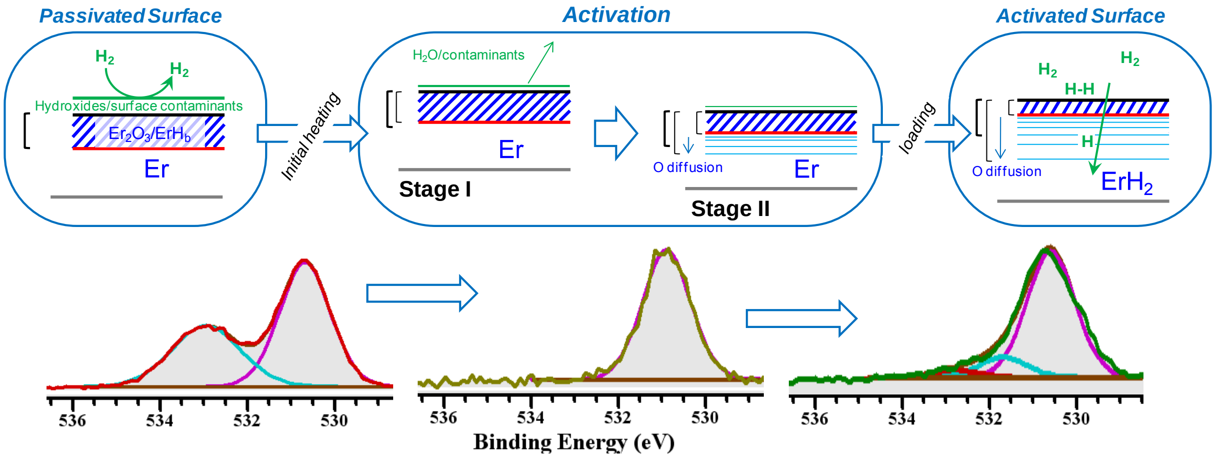

Fig1. Thermal activation of erbium leads to desorption of surface contaminants and oxygen diffusion of the passive surface oxide into the bulk. Activation is observed to occur through a two stage mechanism. The O(1s) shows changes in the surface oxide as a function of *in situ* thermal annealing indicative of defect state formation as the oxide/metal boundary moves towards the surface.

Activation can be identified by a large increase in photoemission between the valence band edge and the Fermi level. The increases in photoemission develop over two distinct stages. XPS shows that the first stage involves desorption of contaminants and recrystallization of the oxide, initially impeding hydrogen loading. Further heating overcomes the first stage and leads to degradation of the passive surface oxide leading to a bulk film more accessible for hydrogen loading. XPS results are supported by depth profiles from time-of-flight secondary ion mass spectrometry and low energy ion scattering.

[§]Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

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HAXPES INVESTIGATION OF NANOSTRUCTURED PEM FUEL CELL CATALYSTS

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Powering of electronic devices by microfabricated power sources, including micro-proton exchange membrane fuel cells (μ-PEMFC), are being actually investigated in laboratories world-wide. The possibility of co-fabricating of a power source on the same substrate as the electric circuit offers many advantages, including a reduction in size and weight, increased processing efficiency, and lower cost. The important issue of planar type fuel cells is a preparation of large specific surface area catalysts grown by thin film deposition techniques which are compatible with planar technology.

Recently we showed by fuel cell activity and electron microscopy measurements the possibility of preparation of porous large surface and high activity nanostructured thin film catalysts by depositing the catalysts in form of Pt-Ce-O [1] solid solutions on carbon nanotubes (CNTs), grown on Si wafers, by magnetron sputtering. The catalysts reveal nanoporous columnar structure and high specific power when used in the reference hydrogen-fed PEMFC. Figure 1 shows the CNTs coated by the porous Pt-CeO_2 catalyst film.

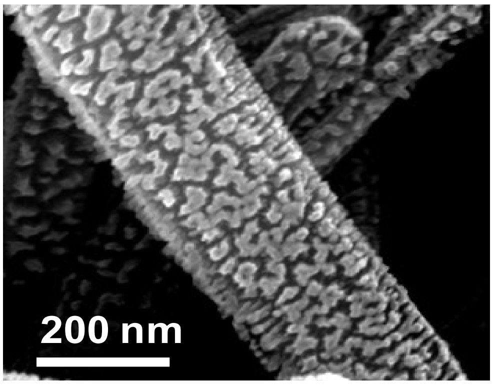

Fig1. CNTs coated by the catalyst film

Chemical composition of the films was investigated by hard x-ray synchrotron radiation photoelectron spectroscopy (HAXPES) at Spring-8 (BL15XU) [1] and recently at the ESRF (ID 32) by taking advantage of high brilliance and high resolution of the beamlines. The Pt-doped sputtered cerium oxide films contained high concentration of cationic platinum Pt^{2+} and Pt^{4+} which were highly active species for hydrogen dissociation to protonic hydrogen H^+. Because of porous structure of the catalyst films with active sites at the surface and boundaries of grains inside the pores and the formation of multiple chemical states of dopants and Ce atoms ($Ce^{3+,4+}$), HAXPES was a suitable technique for such studies due to combination of high resolution and high information depth. The experiment showed that Pt^{2+}/Pt^{4+} and Ce^{3+}/Ce^{4+} ratio, which were key parameters of the catalyst activity, changed with HAXPES photon energy, i.e. with HAXPES probing depth.

HX resonant PES has been performed by measuring resonant profiles Ce $3d_{5/2}$ f^2, f^1 and Ce $3d_{3/2}$ f^0 of both Ce^{4+} and Ce^{3+} states.

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PROBING THE BURIED Si/ZnO THIN-FILM SOLAR CELL INTERFACE BY HAXPES

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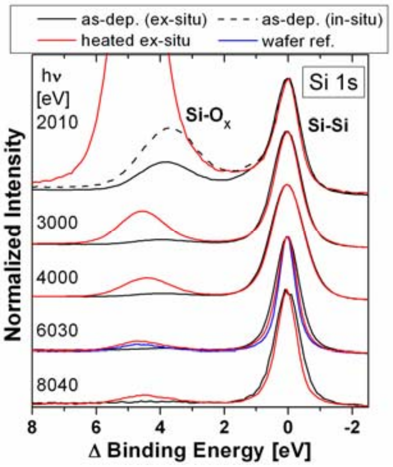
State-of-the-art thin-film solar cells are complex multilayer devices. One promising thin-film photovoltaic technology combines the advantages of a high-quality absorber layer and low-cost processing by depositing amorphous silicon (a-Si), which is subsequently solid-phase crystallized (SPC) via an annealing process at 600 – 650 °C[1] (a-Si → polycrystalline silicon, "poly-Si"). One major challenge of this superstrate solar cell concept is the implementation of a transparent conductive oxide window layer, which would allow electric contacts and light trapping schemes to be easily implemented.[2] So far the proposed Al/a-Si:H(p$^+$)/poly-Si(p)/poly-Si(n$^+$)/ZnO:Al/glass device structure yields lower efficiencies than the standard device without ZnO:Al. This suggests that the Si(n$^+$)/ZnO:Al ("Si/ZnO") interface is not properly designed and/or its properties deteriorate during the annealing processes.

In this contribution, it will be demonstrated how hard x-ray photoelectron spectroscopy (HAXPES) is used to study the buried Si/ZnO interface elucidating the chemical changes induced by SPC. The HAXPES measurements were conducted at the KMC-1 beamline[3] of the BESSY II synchrotron facility using the HIKE endstation.[4] By varying the excitation energy (hν) between 2010 and 8040 eV, it was possible to probe the Si/ZnO interface buried below 12 nm Si.



Si 1s photoemission spectra of as-deposited (black) and SPC heated (red) Si/ZnO thin-film stacks recorded at different hν. For comparison, the 6030 eV spectrum of an oxidized Si wafer is presented (blue) is shown.

The figure shows the Si 1s photoemission spectra of the as-deposited and heated Si/ZnO samples for different hν. The Si 1s spectra are dominated by two main contributions, attributable to Si in Si-Si ("Si 1s$^{\text{Si-Si}}$") and Si-O$_X$ ("Si 1s$^{\text{Si-Ox}}$") bonding environments. After annealing, a slight narrowing of the Si 1s$^{\text{Si-Si}}$ signal can be observed. This narrowing is characteristic of the SPC-induced conversion of a-Si into poly-Si, as is confirmed by comparison with the (even narrower) 6030 eV Si 1s spectrum of a single-crystalline Si wafer reference (blue spectrum). Note that the narrowing can in particular be observed for the measurements in the high-resolution energy range of the experimental setup.[4] After SPC the Si 1s$^{\text{Si-Ox}}$ signal increases strongly, which clearly indicates that the sample further oxidizes during SPC. With increasing hν the Si 1s$^{\text{Si-Ox}}$ photoemission signal decreases. Although this finding suggests that surface oxidation predominates, it will be shown how an optimized experiment design and sophisticated data analysis result in evidence for an SPC-induced silicon oxidation also at the Si/ZnO interface, taking place at the expense of Zn-O bonds.

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UNDERSTANDING MOLECULAR INTERFACES USED FOR ENERGY CONVERSION

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This presentation focus on the use of hard X-ray photoelectron spectroscopy for the understanding of molecular interfaces in mesoscopic materials used for energy conversion. Such materials systems have been subject of substantial academic and commercial research over the last decades, in particular with the development of molecular solar cells and Li-ion batteries. The efficiency of the conversion process in these systems is largely dependent on the properties of the interfacial region including molecular organization as well as on energy matching between the molecules, the inorganic materials and electrolytes. Insight into the molecular and electronic structure of the dye at the interface is therefore crucial in order to understand and optimize the function. X-ray based techniques such as photoelectron spectroscopy (PES) are powerful for obtaining such information at a molecular level due to the possibility for element specificity. This contribution review some of our recent synchrotron based PES results and developments for understanding the interactions between the molecular materials, inorganic materials, and electrolyte in such environments.

For example, we obtain insight into the molecular surface organization and energy matching between the different materials. Specifically it will be shown how hard X-ray photoelectron spectroscopy can be used to experimentally understand the molecular orbital structure in molecular materials [1,2]. The talk will also discuss the use of new solid molecular materials for conversion between light energy and electrical energy [3].

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HIGH ENERGY PHOTOEMISSION SPECTROSCOPY AS TOOL FOR THIN FILM SOLAR CELL CHARACTERISATION

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Fig.1: Cross section SEM of a chalcopyrite solar cell

Solar cells based on the material system $Cu(In_{1-x}Ga_x)(S_ySe_{1-y})_2$ consist of a layer stack as shown in Fig 1. Since each layer has a different chemical and electronic structure, interfaces between them have a complex composition, yet determine the device properties. Thus, an exact knowledge of the interface composition is necessary. The use of HAXPES allows material analysis up to a depth of around 30 nm [1], depending on excitation energy and electron mean free path. This allows the non-destructive depth profiling of chemical and electronic properties of the near-surface bulk regions, which are crucial for the device operation and which are not accessible by standard, surface sensitive PES. Here we present results regarding three different topics:

- Evidence for a very thin, completely Cu-depleted surface in Cu-poor grown $Cu(In,Ga)Se_2$ absorbers obtained by energy-dependent HAXPES measurements [1]. A fit of photoemission peak ratios from Cu, Ga, and In recorded at different photon energies suggests a very thin (0.6 - 0.8 nm), completely Cu-free surface on Cu-poor chalcopyrite absorbers.
- The direct measurement of a voltage drop in a semiconductor (i.e. band bending) near the interface between semiconductor and metal in a GaAs/gold model system by analysis of the width of respective photoemission peaks excited by high energy photons. (Fig. 2)
- The in-situ observation of Cu-diffusion from a chalcopyrite absorber into an In_2S_3 buffer layer [2]. A Cu $2p_{3/2}$ peak from an In_2S_3/CIGSe stack excited by 4 keV photons was recorded as a function of sample temperature. A strong increase in peak intensity starting at a sample temperature of about 200°C points towards diffusion of Cu through the In_2S_3 layer.

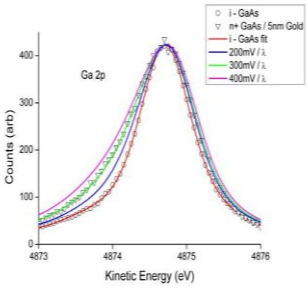

Fig.2: Ga $2p_{3/2}$ signal from i-GaAs and n^+-GaAs/ Au with calculated peaks for different band bending

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CORE LEVEL SPECTROSCOPY OF THIN FILM OXIDE HETEROINTERFACES AND BILAYER CMR MANGANITES

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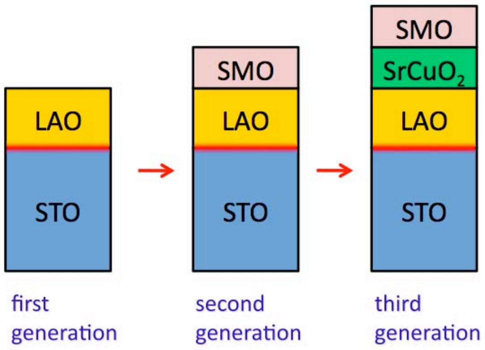
HAXPES is freeing us of the chains of surface sensitivity, enabling measurements on samples simply transferred in from air without further surface preparation. In addition, buried interfaces are finally becoming accessible for scrutiny, with the elemental and electrostatic sensitivity inherent to core level spectroscopies. The use of high kinetic energies in photoemission also allows us to study whether the surface or near surface (VUV, soft X-ray) electronic structure of important drosophila systems for unconventional quantum electronic matter such as the high T_c cuprates and bilayer colossal magnetoresistance manganites - which have been so widely studied using ARPES and scanning probe-based techniques - are representative of their bulk properties as studies by our colleagues doing optical, transport and thermodynamic measurements.

In this contribution I will present recent HAXPES data from three generations of oxide heterointerface systems (see sketch), in which $LaAlO_3$ is grown using PLD on TiO_2-terminated STO substrates and subsequently capped with either nothing, $SrTiO_3$, with $SrMnO_3$ or with $SrCuO_2$ and then $SrMnO_3$. I will discuss the data both in terms of the potential build-up as the LAO layer thickness increases as well as the spectroscopic signature of Ti3d occupancy seen in the $Ti2p_{3/2}$ core level, comparing with the transport data recorded on the same samples.



In a second part, new HAXPES data from cleaved single crystals of $(La,Sr)_3Mn_2O_7$ will be presented. In this system, the ferromagnetism at the surface is weakened [1,2] and the electronic states at the surface show increased signs of localised behaviour [3]. Thus, we use bulk-sensitive HAXPES to underpin measurements of core level energies at temperatures around T_{Curie} as a tracker for the chemical potential, searching for signs of electronic phase separation close to the paramagnetic-ferromagnetic transition that is so central to the physics of the colossal magnetoresistance effect.

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HAXPES STUDIES OF PHASE SEPARATIONS IN PEROVSKITE Mn–OXIDE SUPERLATTICES

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Phase competition between ordered phases is one of the most interesting phenomena in condensed-matter physics, and is often observed in perovskite Mn-oxides $R_{1-x}A_xMnO_3$, where *R* is a rare-earth (*R* = La, Nd, Pr) and *A* is an alkaline-earth atom (*A* = Sr, Ba, Ca). Around x = 0.5, $La_{0.5}Sr_{0.5}MnO_3$ (LSMO) has a ferromagnetic-metallic ground state and $Pr_{0.5}Ca_{0.5}MnO_3$ (PCMO) has a charge-orbital ordered ground state, which result from the subtle difference in the electronic bandwidth. Recently, the superlattice (SL) of LSMO and PCMO was successfully grown on $(LaAlO_3)_{0.3}$-$(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}$ (LSAT) (011) substrates [1]. On LSAT (011) substrates, charge-orbital ordering is realized in PCMO layers, which forms phase separation between ferromagnetic-metallic states and charge-orbital ordered states along the film stacking direction.

Hard x-ray photoemission spectroscopy (HAXPES) is extremely suitable for studying the electronic structures of such SL structures. We performed HAXPES measurements of the $[PCMO(5)/LSMO(5)]_{15}$ SL on LSAT (011) in BL-47XU in SPring-8. The photon energy was 7.94 keV, and the mean free path of photoelectrons is > 6 nm in the valence-band and Mn 2*p* core level, which can cover at least 2-3 periods in the SL.

Figure 1 shows the Mn $2p_{3/2}$ core-level spectra for the $[PCMO(5)/LSMO(5)]_{15}$ SL during the heating cycle. Well screened structures are observed at lower binding-energy sides at all temperatures. This structure was reported to be present in the pure $La_{1-x}Sr_xMnO_3$ and $La_{1-x}Ba_xMnO_3$ thin films [2, 3], and to be in good agreement with the behaviour of magnetization [3]. In Fig1, this structure is most pronounced at 200 K, and is weak at 25 K. This result is not in agreement with the magnetization of this SL [3], indicating that the intensity of well screened feature reflects electronic coherence rather than magnetization. At lower temperatures, PCMO turns into charge-orbital ordered states, and electronic coherence is lost in such ordered structures. We also observed hysteresis behaviour in the heating and cooling cycles, reflecting the complex phase transitions and consequent phase separations in the SL. Such temperature dependence was also observed in the valence-band spectra.

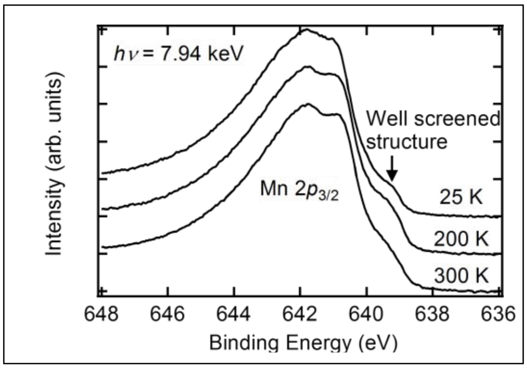

Fig1. Temperature dependence of the Mn $2p_{3/2}$ core-level spectra for the $[PCMO(5)/LSMO(5)]_{15}$ superlattice during the heating cycle.

This work is supported by JSPS through its FIRST Program.

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MANY-BODY EFFECTS IN STRONGLY CORRELATED MATERIALS: COUPLING DFT CALCULATIONS OF K EDGE ABSORPTION TO EXPERIMENTAL 1S PHOTOEMISSION

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The understanding of electronic correlations is one of the challenging issues of condensed matter physics. The K-edge x-ray absorption spectroscopy (XAS) of transition metals is well suited to probe correlation effects in materials, with wider applicability in mineralogy or catalysis. Yet the understanding of the K-edge XAS remains a formidable task because of the many body nature of electronic states. We have recently carried out measurements and density functional theory (DFT) calculations of the K-edge absorption spectra (XAS) in correlated transition metal compounds [1]. Despite the fair agreement between theory and experiments, we find that some of the near-edge features are systematically not described by DFT – cf. peak F in Fig1. As previously argued [2], these additional structures could be due to many body, charge-transfer like excitations. But their treatment at the moment exceeds DFT capacities. On the other hand, many-body effects can be introduced "by hand" in the calculations through convolution of the XAS and 1s photoemission spectra [3]. To that aim, we have performed recently 1s hard x-ray photoemission spectroscopy (HAXPES) on NiO, a model compound for correlated materials. The measurements were carried out at the KMC 1 beamline at BESSY on a NiO thin film grown on a silver Ag(001) substrate. The convolution of the experimental 1s HAXPES spectra with theoretical calculations clearly improves the agreement with the experimental XAS. This confirms the assignment of the F feature as due to many-body screening effects. We believe our result allows us to address the long-standing issue of the occurrence of near-edge charge transfer excitations in K-edge XAS.

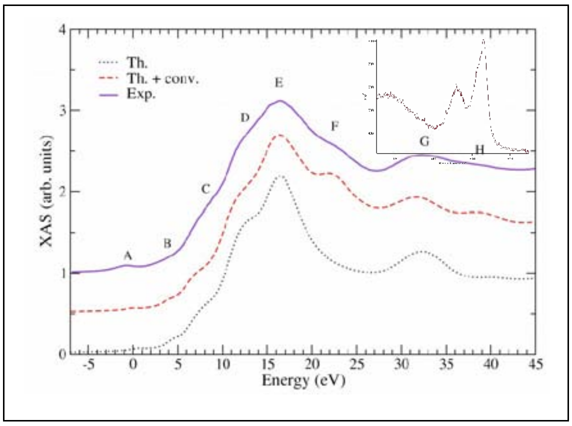

Fig1.: Ni K-edge XAS in NiO : Measured spectrum (solid line) and calculations with (dashed lined) and without (dotted line) convolution by the Ni 1s HAXPES (inset).

Finally, we will review the possibilities offered at SOLEIL synchrotron for HAXPES on the GALAXIES beamline.

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**Thu.
12:15**

VALENCE BAND ANALYSIS OF LaAlO$_3$/SrTiO$_3$ OXIDE HETEROSTRUCTURES USING HARD X-RAY PHOTOELECTRON SPECTROSCOPY

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The origin of the two-dimensional electron gas (2DEG) at the interface of the LaAlO$_3$/SrTiO$_3$ oxide heterostructure (LAO/STO) is a heavily discussed topic in both theory and experiment [1, 2, 3, 4]. Apart from possible influences of oxygen defects recent experimental and theoretical works suggest electronic reconstruction as the driving mechanism for the high conductivity of the interface. In this simplified picture half an electron is transferred from the surface to the interface due to an electric potential gradient across the polar LAO overlayer. Such a gradient is also consistently found in density functional calculations (DFT) [5]. Using hard x-ray photoelectron spectroscopy (HAXPES) the potential gradient should be observable as a significant broadening of the Al 1*s* core level. In addition, due to the electron transfer the valence band of the topmost LAO layer should cross the chemical potential.

We performed HAXPES measurements at beamline P09 of PETRA III on several samples with different overlayer thicknesses. The samples were grown by pulsed laser deposition as described in Ref. [3]. As reference samples we used Nb doped STO and a 50nm thick LAO film. In our data none of the predicted signatures are observed, which indicates a flat band behavior in the LAO overlayer.

Furthermore, the DFT calculations give an estimation for the band offset between both band insulators LAO and STO, where the valence band maximum (VBM) of STO is above the VBM of LAO. We determined the band offsets of LAO and STO at the interface analyzing the valence band spectra. For that, we measured the valence band of both bulk components for reference. These spectra were then shifted and weighted in such a way, that the superposition of both spectra fits the measured data. Figure 1 shows such a valence band analysis for a 4uc sample. It can be seen - at variance with the DFT calculations - that the VBM of LAO is actually *above* the VBM of STO. The resulting value for the band offset is about 0.35eV. From our data the valence band offset is independent of the LAO overlayer thickness.

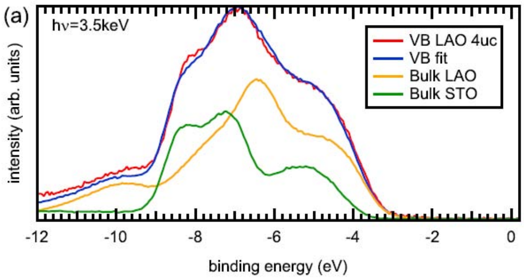

Fig 1. Valence band analysis of a LAO/STO sample with 4uc overlayer thickness.

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ELECTRONIC STRUCTURE OF Pt BASED TOPOLOGICAL HEUSLER COMPOUNDS WITH $C1_b$ STRUCTURE EXPLORED BY HARD-X-RAY PHOTOELECTRON SPECTROSCOPY

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Besides of their well-known wide range of properties it was recently shown that many of the heavy Heusler semiconductors with 1:1:1 composition and C1b structure exhibit a zero band gap behavior and are topological insulators induced by their inverted band structure [1]. Based on topologically protected electronic surface states, this class of materials is supposed to open up innovative directions for future technological applications in spintronics, quantum computing and thermoelectrics.

In the present study, the electronic structure of the Heusler compounds PtMSb (with M= Y, La, Gd, and Lu) were investigated by bulk sensitive hard x-ray photoelectron spectroscopy HAXPES. The measured valence band spectra are clearly resolved and in well agreement to the first-principles calculations of the electronic structure of the compounds [Fig.1]. The comparison of the experimental results to first principles calculations gives clear evidence for the zero band gap state of the compounds. Valence band spectra close to the Fermi energy ε_F exhibit a nearly linear behavior, as is expected for a Dirac-cone type density appearing for linear dispersing bands.

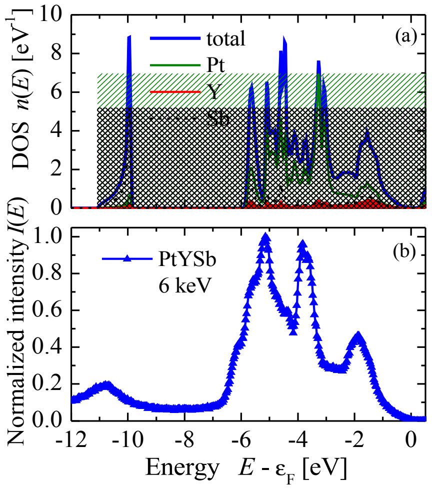

Fig1. Electronic structure of PtYSb.
(a) Total and partial density of states (DOS).
(b) Valence band spectra measured with excitation energy of 5.95 keV.

The authors gratefully acknowledge the financial support by the DFG (P 1.3-A in FOR 1464 ASPIMATT) and the Forschungszentrum Komplexe Materialien (COMATT, JGU Mainz). The synchrotron radiation measurements were performed at BL15XU with the approval of NIMS (Nanonet Support Proposal No. 2010B4903).

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X-RAY PHOTOIONIZATION OF FREE AND CONFINED ATOMS

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Atoms are of interest in themselves, but they are the elementary particles of molecules, clusters, liquids and solids, i.e., the building blocks of the macroscopic world. Thus, the properties of atoms are often reflected in much more complex formations. For example, inner-shell photoionization cross sections in solids, away from threshold, are quite similar to the corresponding atomic cross section [1].

X-ray photoionization differs from its UV counterpart in that electron ejection can come from both inner and outer shells, while in the UV case, only outer (valence) electrons can be ejected. In addition, electron ejection from inner shells results in very significant relaxation processes, *via* processes such as x-ray emission and Auger electron emission. Furthermore, when both inner and outer shells can be photoionized by the same photon, the wave functions corresponding to these processes interact, which is known as interchannel coupling, which can produce significant effects. Thus, the phenomenology of inner-shell photoionization is significantly more complex, and richer, than low-energy valence-shell photoionization.

In this report, several examples of photoionization of atoms by energetic x-rays will be discussed, examples which apply, at least qualitatively, to photoabsorption by other states of matter as well. Among these examples are:

- The asymptotic high-energy form of atomic cross sections which, through the action of interchannel coupling, are very different than the prediction of the single-particle model, i.e., contrary to popular belief, the single-particle approximation is often very wrong at really high energies [2].
- The effects of inner-shell cross sections on valence-shell cross sections, again due to the breakdown of the single-particle model *via* interchannel coupling [3].
- Nondipole effects on the photoelectron angular distribution in the x-ray range which must be taken into account if ARPES measurements are to be correctly interpreted [4]. These nondipole effects are known to increase with photon energy; even below 1 keV however, the effect of quadrupole and even octupole transitions are seen.
- Inner-shell photoionization of atoms confined in fullerenes, and how the confinement alters the atomic properties [5].

This work was supported by NSF and DOE, Office of Chemical Sciences.

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COMPLEX DECAY PATTERNS IN Ar FOLLOWING K-EDGE PHOTOEXCITATION OR PHOTOIONIZATION DISENTANGLED BY ION RECOIL EXPERIMENTS

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The creation of an inner-shell deep hole by photoexcitation or photoionization in an isolated many-electron atom and the subsequent relaxation phenomena involving a multi-step vacancy cascade constitute a complex process, leading to multiply charged ions which can be produced in a variety of pathways. We have studied the relaxation (radiative and non radiative) of the K shell vacancy on the prototypical exemple of Argon.

We performed the measurements on beamline LUCIA at SOLEIL using a newly developed setup, CELIMENE, that belongs to the extended family of cold target recoil momentum spectroscopy (COLTRIMS) apparatuses [1, 2, 3]. The instrument is based on the double-velocity spectrometer. The photon beam crossed a cold supersonic jet of argon at right angle. Electrons and ions are accelerated towards facing time-of-flight (TOF) spectrometers, perpendicularly to the photon beam and atomic jet. The particles were detected with position sensitive microchannel plates detectors. Time of flight and impact positions of the ions and electrons detected in coincidence were recorded, allowing thus to determine the full momentum vector of all particles for each ionization event. The overall energy resolution was found to be 8 meV for the ions and 0.8 eV for the electrons.

Recoil measurements and conservation momentum law allowed to reconstruct the different relaxation pathways. To our knowledge, this method is unique in providing direct information on the branching in ion production between radiative and non radiative decay.

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RESONANT INELASTIC X-RAY SCATTERING ON ATOMS AND SIMPLE MOLECULES IN THE TENDER X-RAY REGION

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We present the results of our recent work on single photon two-electron atomic excitations and nuclear dynamics in core excited molecules employing a high resolution resonant inelastic X-ray scattering (RIXS) spectroscopy. A Johansson type crystal spectrometer coupled to the ID26 beamline of the European Synchrotron Radiation Facility (ESRF) was employed to record a comprehensive series of high resolution KL, KM RIXS spectra of Ar in the [1s2p,3p] near-threshold region and KL, KV RIXS spectra of some simple Cl containing molecules (HCl, CH_3Cl) around the Cl K edge. In case of Ar we have successfully separated spectral features pertaining to different two-electron atomic processes (shake-off, up, and resonant excitations) and extract the [1s2p,3p]***nln'l'*** excitation spectra [1]. RIXS measurements on HCl molecules revealed electronic state interference in the region between the main resonances resulting from the coherent excitation to sigma* and Rydberg states [2]. A complete breakdown of characteristic linear dispersion law is observed for the $1s^{-1}$ sigma* core-excited molecular state revealing an interplay between the fast dissociation and the radiative relaxation.

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PHOTOELECTRON TIME-OF-FLIGHT SPECTROSCOPY IN A HARD X-RAY REGIME

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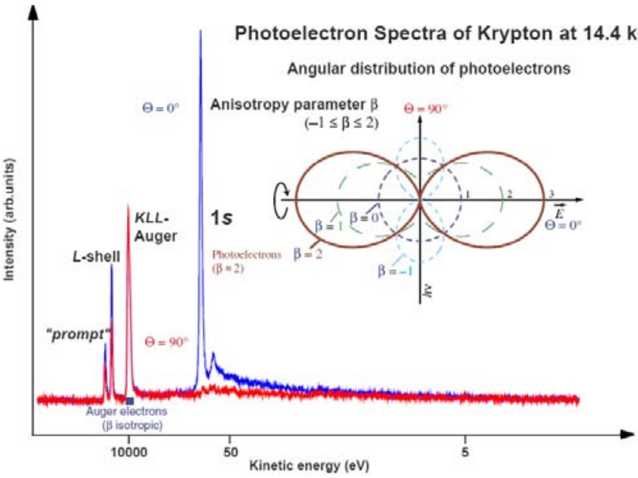
(3) Advanced Study Group of CFEL, Notkestraße 85, 22609 Hamburg

Using photoelectron time-of-flight spectroscopy for the determination of several Synchrotron and FEL beam properties is a well characterized method for the soft X-ray regime. Upcoming and already working XFEL facilities as well as hard X-ray photon beamlines at Synchrotron Radiation facilities like PETRA III at DESY are also highly interested in online beam diagnostics in terms of beam positioning, energy, flux and the degree of polarization.

The energy range in which this method is successfully tested was increased from the soft X-ray regime up to 15 keV. Not only diagnosis but also angle resolved photoelectron spectroscopy of rare gases like Argon, Krypton and Xenon were performed in that energy range at the P09 beamline at PETRA III. Beside these gaseous targets first investigations on a solid state target were realized during our recent beamtime in July 2011 at P09 showing the capability of our spectrometer of measuring electron signatures from solids.

The actual status of the developed spectrometer, the latest measurements for polarization determination and scientific insights in angular distribution studies of rare gases with hard X-rays will be presented. Furthermore the latest analysis of our solid state investigations will be highlighted and the adaptability to XFELs in terms of shot to shot polarization analysis and relevant technical issues will be discussed.



. Fig1. Angle resolved photoelectron spectra
of Kr at 14,4 keV for 0° and 90° detectors as
a basic example for polarization determination.

Thu.
16:00

GRAPHENE ON Ir(111) STUDIED BY X-RAY STANDING WAVES

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Epitaxial growth on metal surfaces is an established method to produce highly ordered, extended graphene sheets. Ir(111) stands out from other substrates as the graphene grown on it is of extraordinary structural quality [1], shows an electronic structure almost equivalent to the one of free graphene [2], and can serve as a template for the growth of ordered superlattices of metal clusters [3]. Here I report measurements of the structure of graphene / Ir(111) based on X-ray standing waves (XSW), density functional theory (DFT) and scanning tunneling microscopy (STM).

XSW reveals a bonding distance of (3.42 ± 0.02) Å between graphene and the substrate. This height can be accurately confirmed in DFT when the van-der-Waals-interaction is taken into account. STM experiments show that due to the mismatch of graphene and Ir(111) an incommensurate moiré pattern is formed. The chemical interaction between C and Ir as determined by DFT is attractive only in some regions of the superstructure, whereas it is even repulsive for other parts. This is the reason for the significant corrugation of the graphene. Using Bragg-reflexes of higher orders makes it possible to derive further information on the height distribution of the C atoms in this strongly buckled layer. Deposition of clusters broadens the height distribution in the underlying graphene, in agreement with the proposed rehybridisation model for cluster binding.

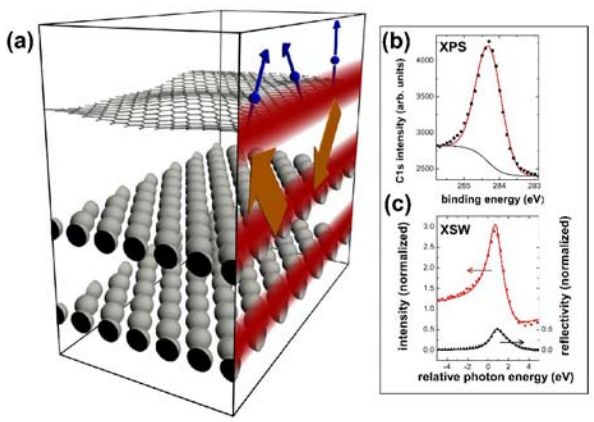

Fig1. (a) Schematic representation of the X-ray standing wave experiments. Depicted is a corrugated honeycomb mesh of graphene on top of two Ir(111) lattice planes. Orange arrows: Interfering incoming and outgoing X-ray beam. Red stripes: Standing wave pattern. Blue spheres and arrows: Emitted photoelectrons. (b) Squares: X-ray photoemission intensity of the C1s-peak. Thin line: Shirley-type background, Thick line: Gaussian fit. (c) X-ray reflectivity (triangles) and C1s photoemission yield during an XSW energy scan.

Contributions from N. Atodiresei, R. Brako, S. Blügel, V. Caciuc, V.-V. Chi, J. Coraux, R. Djemour, T. Gerber, P. Lazić, T. Michely, A. T. N'Diaye, S. Runte, J. Zegenhagen and the staff at ESRF ID32 are gratefully acknowledged.

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XSW IMAGING OF THIN LANTHANUM ALUMINATE FILMS ON STRONTIUM TITANATE

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Conductive interfaces formed between insulating oxides such as $LaAlO_3$ grown on $SrTiO_3$ (001) surfaces have generated significant interest. Since the first report [1], research is still ongoing and these efforts have revealed a multitude of unexpected properties, such as high electron mobility, superconductivity, large magnetoresistance and Seebeck effect [1-4]. It is expected that lattice mismatch and the build up of the diverging electrostatic potential at the interface, both increasing with increasing film thickness, manifest themselves in subtle structural changes in the interface region. Density functional calculation predicted a polar distortion of the AlO_2 and LaO planes [5]. A buckling of Δz=0.15 Å was calculated for the interfacial AlO_2 planes and a relative displacement of Δz=0.36 Å for the LaO planes. The distortion seems to be dominated by a substantial outwards movement of the La by up to 0.26 Å. Recent X-ray diffraction results appear to confirm the calculations [6]. The strongest distortion was found for 2uc thick LAO films.

It is the goal of the experiments presented herein to verify theses theoretical and experimental findings. The X-ray standing waves (XSW) technique is a *model-free* approach which adds chemical specificity to X-ray diffraction. It allows to experimentally measure the *amplitude and phase* of the atomic distribution function. The relatively big displacements of up to 9% of the lattice constant should be readily detectable by the highly sensitive X-ray standing wave imaging technique. It was shown that valuable information on the initial stages of growth which is not easily accessible by diffraction techniques can be obtained by XSW real space imaging. For example the mixed perovskite precursor phase for ultra thin films of YBCO on $SrTiO_3$ (0.5uc) was confirmed by this method.

For the imaging of a 2uc thick LAO film the XSW modulated core level photo electron yield was recorded for the 5 elements present in film and substrate for 7 different Bragg reflections. Subsequent analysis provided for each reflection and for each element the amplitude *and phase* of one Fourier coefficient of the elemental atomic distribution function. Application of the 4-fold symmetry of the $SrTiO_3$ film yielded 29 Fourier coefficients. By direct Fourier inversion one can reconstruct the three dimensional real space image of the atomic distribution for each of the elements. The results of the analysis will be discussed in detail.

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SITE-SPECIFIC ELECTRON DIFFRACTION RESOLVED VIA NUCLEAR RECOIL

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Many of the phenomena observed in high-energy photoemission can also be studied in ‘simple’ electron scattering experiments, even at higher energies than is currently possible in HAXPES. Two such phenomena are the recoil effect [1], and the formation of Kikuchi patterns [2]. Here we present a study of sapphire (Al_2O_3), combining both phenomena in a scattering experiment using 35 keV electrons [3].

For sapphire, the difference in recoil energy allows us to determine if an incident electron backscattered from an aluminium or from an oxygen atom. The angular electron distributions obtained in such measurements are expected to be a strong function of the recoiling lattice site, as shown below for the calculated element-resolved (11-20) Kikuchi bands. These element-specific recoil diffraction features, based on dynamical theory of high energy electron diffraction, are confirmed by the experiment.

This observation opens up new possibilities for local, element-resolved crystallographic analysis using high-energy electrons. Moreover, our results shed light on the processes by which, with increasing recoil energy, quasi-elastically backscattered electron waves are effectively decoupled from an incident beam with respect to their phase. While the incident and the outgoing pathways are still largely governed by coherent forward scattering, we show here that an experimentally identifiable source of dephasing is introduced by nuclear recoil.

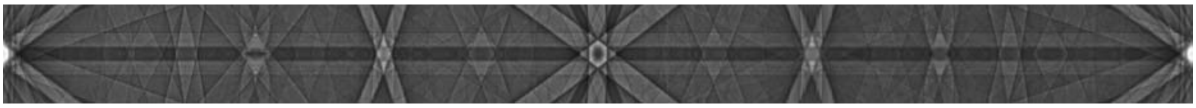
Fig. 1: Sapphire: Oxygen (11-20) Kikuchi Band 35kV, based on Dynamical Simulation

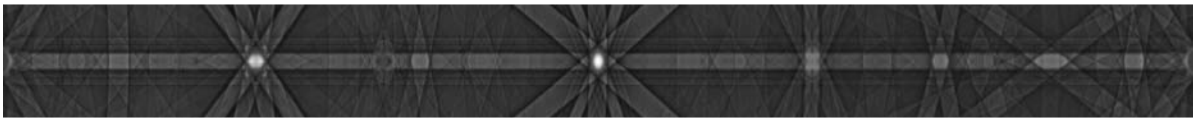
Fig. 2: Sapphire : Aluminium (11-20) Kikuchi Band 35kV, based on Dynamical Simulation

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3. A. Winkelmann, M.Vos, ***Physical Review Letters* 106**, 085503 (2011)

Fri. 8:40

PROBING ORBITAL SYMMETRY IN THE VALENCE BANDS OF SOLIDS BY POLARIZATION-DEPENDENT HARD X-RAY PHOTOEMISSION

A. Sekiyama (1,2), A. Higashiya (2,3), S. Imada (4), S. Suga (1,2), M. Y. Kimura (1), Y. Tomida (1), H. Fujiwara (1), K. Tamasaku (2), M. Yabashi (2,5) and T. Ishikawa (2)
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For hard x-ray photoemission spectroscopy (HAXPES) of solids at hν = 5-10 keV, there are other characteristics than the high bulk sensitivity as follows [1]: (1) The photoionization cross sections for the ***s*** and ***p*** states per electrons are rather comparable with those for the ***d*** and ***f*** states. (2) When a linearly polarized light is used for HAXPES, the photoelectron angular distribution with respect to the angle θ between the two directions of photoelectron detection and the electric field has strong orbital dependence. As an overall tendency, the calculation [1] predicts that the photoelectron intensity for the s and ***ip*** (***i*** > 4) states is strongly suppressed along the direction perpendicular to the polarization vector (θ = 90˚, s-polarization configuration) compared to that along or near the vector (θ~0-30˚, p-polarization configuration) while the angular dependence of photoelectron intensity is relatively weak for the ***d*** and ***f*** states. Therefore, the orbital symmetry in the bulk valence bands can be probed by the polarization-dependent HAXPES.

We have developed the polarization-dependent HAXPES system with switching incident-light polarization at BL19LXU in SPring-8 [2]. An indecent x-ray of ~8 keV is further monochromatized by a channel-cut crystal (Si 444, 440 or 551 reflection) after the primal Si 111 double-crystal monochromator with linear polarization along the horizontal direction (the so-called degree of linear polarization P_L > +0.98). In order to switch the linear polarization from the horizontal to vertical directions, a (100) single-crystalline diamond with the thickness of 0.7-mm was used as a phase retarder with the 220 reflection. The transmittance of the x-ray at ~8 keV for the diamond was confirmed to be ~35%. P_L of the x-ray downstream from the phase retarder was estimated to be better than -0.8 (nearer to -1), which corresponds to the linear polarization components along the horizontal and vertical directions of <10 and >90%, respectively. An MBS A1-HE hemispherical photoelectron spectrometer has been used for the experiment. The energy resolution can be selected from ~65 meV [3] depending on the channel-cut crystal.

We have applied this technique to gold, silver, and several strongly correlated electron systems, from which it is found that the orbital symmetry of the conduction electrons is qualitatively different between gold and silver [2], and that the electric conduction seems to be rather independent of the magnetism for the multiferroic system $CuFe_{1-x}Ni_xO_2$.

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RECENT DEVELOPMENT OF HAXPES INSTRUMENTATIONS AT BL47XU/ SPring-8

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We have developed a high-spatial resolution, high-throughput hard X-ray photoelectron spectroscopy (HAXPES) technique at BL47XU/SPring-8. As one of efforts, a phase retarder of (111) diamond crystal was installed as optics in the framework of the DFG-JST program. The phase retarder manipulates the beam polarization by varying the relative phase between the circular and linear wave fields, which has realized the MCD-HAXPES. On the other hand, a 3D chemical analysis combining sample sannning (in-plane 2D) and take-off angle resolving (depth profile) has been conducted as a 5-years project in the framework of the JST Sentan program. The system consists of the Kirkpatrick-Baez focusing mirrors to achieve a beam size of 1.0 μm (H) x 0.98 μm (V) at the photon energy of 7.94 keV, and a wide-acceptance-angle objective lens installed in front of the VG Scienta R4000 analyzer. The objective lens system has been developed originally and achieved the total acceptance angle of ±30 degree with better than the resolution of 0.5 degree. The performance of this system was evaluated by applying the core spectra measurements of a typical multilayered sample of Ir(8 nm)/HfO_2 (2.2 nm)/ thickness-graded (TG) SiO_2 (0-10 nm) /Si (001) [2] schematically shown in Fig.1 (a). By scanning the position of the TG sample surface along the SiO_2 thickness varying direction, Si 1*s* and O 1*s* spectra found to exhibit features as shown in Fig.1(b) and (c). Si 1s from the SiO_2 layer loses intensity and shift towards lower binding energy as the thickness decreases. The substrate Si 1*s* peak is still clearly recognized even in the case it is buried under 20 nm thick over-layers in total, indicating the capability of a large probing depth. The intensity of O 1*s* from SiO_2 decreases relatively comparing with that from HfO_2 and their energy separation becomes smaller as SiO_2 thickness decreases. In addition, the depth profile of the structure has been mapped along the SiO_2 thickness varying direction with the take-off angle dependence of these core spectral intensities.

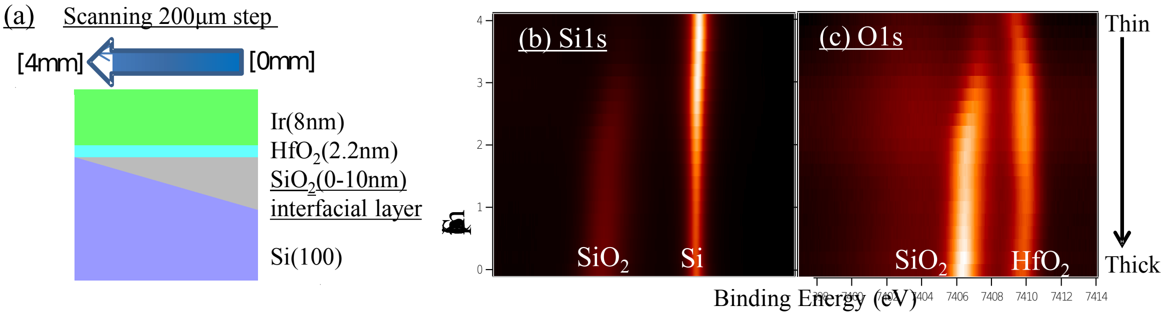

Fig. 1 (a) sample cross section. (b) and (c) position dependence of Si 1s and O 1s along TG direction, respectively.

Acknowlegements

This work is supported by DFG (Germany)-JST and Sentan-JST. We are thankful to Drs. Abe and Miyata of AIST for samples.

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X-RAY SPECTROSCOPY AT NIST NSLS BEAMLINES: RECENT UPGRADES, SCIENTIFIC RESULTS, AND FUTURE PLANS

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We will discuss recent upgrades and review the capabilities of the NIST HAXPES facility at beamline X24A at the National Synchrotron Light Source (NSLS). Results will include research in microelectronics, photocatalysis, hydrogen storage, magnetic tunnel junctions, and fundamental spectroscopy. An overview of NIST plans for the NIST NSLS-II spectroscopy suite will also be discussed.

ELECTRONIC STRUCTURE OF THE HIGH TEMPERATURE PHASE OF STRONGLY CORRELATED OXIDES AND OF THE INTERFACE BETWEEN OXIDE INSULATORS

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We have recently built a side line of Taiwan Beamline BL12XU at SPring-8 dedicated to HAXPES. It composes of a diamond pre-monochromator, a high resolution monochromator using channel cut and a KB mirror focusing system. The end station can be installed in two geometries with the photoemission direction either parallel or perpendicular to the horizontal polarization vector. The former geometry would enhance the contribution from 4*s* orbital of transition metals at high photon energies while the latter tends to suppress 4*s* with respect to 3*d* orbitals. This provides an opportunity to separate contributions from various orbitals particularly useful for these strongly correlated systems.

Two categories of recent experimental results will be presented. The first one is on the high temperature phase of strongly correlated systems such as $LaCoO_3$ and NiO. $LaCoO_3$ has attracted considerable interest because of its unconventional magnetic properties which are interpreted in terms of a thermally induced spin state transition from a non-magnetic low-spin (LS) ground state to a paramagnetic finite spin state. The nature (intermediate- (IS) versus high- (HS) spin state scenario) of the thermally excited spin state of the Co^{3+} ions have been heavily debated for many years. Here we present valence band and Co 2*p* core level spectra for a wide range of temperatures giving direct experimental evidence for a LS-to-HS transition. NiO is an antiferromagnetic insulator with T_N=523K and is considered a benchmark system in solid state physics. Its photoemission spectrum has been employed to critically test the accuracy of the different theoretical approaches used to describe the electronic properties of the system. Both Ni *2p* core level and valence band have a characteristic double peak structure which cannot be explained with a local picture. Even recent (single-site) DMFT calculations cannot reproduce the lineshape of valence band spectra. Here we report a clear change in the peak splitting in both Ni *2p* core level and valence band spectra across T_N indicating that the origin of the double peak is related to the antiferromagnetic order and thus indeed a non-local screening effect.

For the second category on the electronic structure at the interface we take $LaAlO_3/SrTiO_3$ as an example. It has been discovered that the interface of these two band insulators stays either insulating or becomes conductive depending upon the type of interface of the polar LAO slab and non-polar STO substrate. Applying a new concept of probing the interface near the critical angle of total external reflection our Ti 2*p* photoemission results show evidence of charge transfer at the TiO_2 interface. The resulting Ti^{3+} is distributed near the interfacial region with a depth ~ 48 Å or 12 unit cells of STO, and a total amount about half of the value predicted by the charge transfer model. Its implication will be discussed.

* Also in collaboration with A. Tanaka (Hiroshima University, Japan), and Y.-C. Yang, Y.-H. Chu (National Chiao-Tung University, Taiwan)

HAXPEEM - SPECTROSCOPIC IMAGING WITH HARD X-RAYS

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Photoelectron spectroscopy using hard x-rays as excitation (HAXPES) has proven to be a valuable tool to retrieve spectroscopic information from deep bulk regions and from buried layers (1). On the other hand, photoemission electron microscopy (PEEM) is a well-established technique for high-resolution imaging with soft x-rays already. A number of different contrast mechanisms has been exploited to gain valuable insight into electronic and magnetic properties of microstructured systems, among them elemental contrast due to absorption at element-specific absorption edges, magnetic contrast due to magnetic dichroism, and spectroscopic imaging using energy-selected photoelectrons from specific core levels (2). Combinig both methods into a spectroscopy tool that offers both high spatial and energy resolution together with the higher photoelectron escape depths at high kinetic energies seems a rewarding task. So far, PEEM has been employed in combination with hard x-rays as an imaging detector for local x-ray-absorption studies (NanoXAFS), using the low energy secondary electrons for image formation(3). Even in this operation mode, it was possible to obtain information from buried layers.

In this contribution, we present for the first time imaging spectroscopy at high kinetic energies using hard x-rays. The measurements were performed recently at beamline P09 at PETRA III (DESY, Hamburg), using a NanoEsca-type photoemission electron microscope with double hemisphere energy filter (4). To reach the higher retardation needed to operate at kinetic energies of several keV, the sample holder as well as the microscope's extractor lens had to be modified in close cooperation with the manufacturer to allow for higher voltages.

We will show the feasability of imaging at high kinetic energies at a reasonable spatial resolution as well as spatially resolved spectra from buried layers, demonstrating the power of this promising new experimental method.

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MAGNETOMETRY OF BURIED LAYERS BY MEANS OF HARD X-RAY PHOTOELECTRON SPECTROSCOPY

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A high resolution HAXPES instrument is in user operation since Fall 2010 at the undulator beamline P09 of PETRA III. The beamline is equipped with a high-heatload Si double-crystal primary monochromator providing two different reflections, Si(111) and Si(311). For very high resolution studies an additional channel-cut Si monochromator is used. Photoelectrons with kinetic energy up to 15 keV are analyzed in different experimental geometries by means of a SPECS Phoibos 225 HV analyser with a combined delayline and four channel micro-Mott spin detector.

We have studied linear magnetic dichroism (LMD) in the angular distribution of photoelectrons in buried exchange-biased MnIr/CoFe multilayers. In general, the intensity and the shape of the photoemission spectra depend on the relative orientation and/or direction of the sample magnetisation, X-ray polarisation and spectrometer axis (electron emission direction). The obtained dichroism is 5.5% for the Fe $2p_{3/2}$ line, 4.5% for Co $2p_{3/2}$ and -3.5% for Mn $2p_{3/2}$.

In addition, a spin resolved HAXPES experiment was performed (Fig. 1) using the micro-Mott detector. The integral Fe 2p spectrum taken with all four detector channels has an intensity above $5\times10^4 s^{-1}$.The asymmetry is due to the exchange splitting. A spin polarisation of 10% is determined for the Fe $2p_{3/2}$ core level. The majority component of the Fe $2p_{3/2}$ and Fe $2p_{1/2}$ states has a higher binding energy as the minority one. This result is consistent with magnetic circular dichroism experiments [1] and spin-resolved studies [2] of ferromagnetic Fe surfaces.

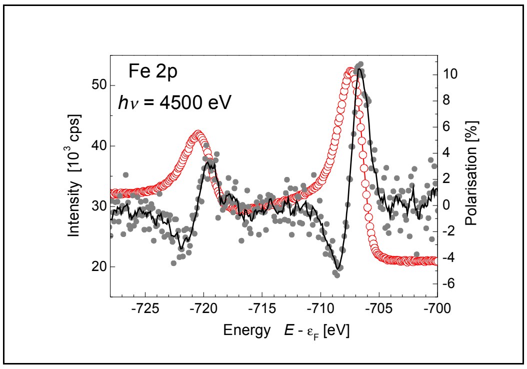

Fig 1. Fe 2p photoelectron spectra (open symbols) taken with 4 channel micro-Mott spin detector and measured spin polarisation (filled symbols). The solid line is a guide to the eye.

It is shown that HAXPES-LMD and spin resolved HAXPES allow performing element specific magnetometry of deeply buried layers that can not be accessed by conventional soft X-ray PES. In particular, HAXPES-LMD can give information about the relative orientation of the magnetisation with respect to the X-ray polarisation in different layers of a complex nano-structured sample.

Financial support by BMBF (05K10UMA) is gratefully acknowledged.

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DEVELOPMENT OF A LABORATORY HXPS SYSTEM AND ITS APPLICATIONS

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(3) Nara Advanced Institute of Science and technology
(4) Ulvac Phy Corporation

Since the first report of the hard x-ray photoelectron spectroscopy (HXPS) using synchrotron undulator radiation in 2003 [1], the application field of the HXPS has been rapidly widened to cover from the basic science to the industrial development, including physics, chemistry, materials sciences, device developments and analytical science and technology. Resources at the synchrotron radiation facilities for HXPS are apparently insufficient to cover the whole demands from the wide spread of the application fields. Consequently HXPS apparatus which are accessible on site of research and development are really needed. We have developed a High Energy Angle Resolved Photoelectron Spectrometer for Laboratory use (HEARP Lab) with practical throughput, and energy and angular resolutions [2]. The system is composed of a compact monochromatized CrKα (5.4 keV) X-ray source, an angle resolved wide acceptance objective lens, and a VG Scienta R4000 high energy analyzer, as schematically shown in Fig. 1. The basic performance of the system is summarized as follows. Energy resolution 0.55 eV, angular resolution 0.5 deg, angular acceptance ±35 deg, and X-ray focus size 10-200 μm. Aquisition time needed for angle integrated $Au4f_{7/2}$ spectrum is 2-3 min. The system has already been applied to bulk sensitive X-ray photoelectron difraction measurements [3], thickness determination of overlayers and buried layers [3, 4]. Mutilayered MOS structures have also been investigated [4]. Very recently, high pressure cells for HXPS observation is being developed using this laboratory system. All these verifies that HEARP Lab is a promising system for wide varieties of applications. HXPS with microfocused X-ray source is going to be inevitable for the studies of advanced materials, which are often prepared as microcrystals and thin films consist of micrometer size single crystal domains. The combination of HXPS and the combinatorial thin film synthesis [5] will provide a powerful tool in the new functional material developments. The HEARP Lab will be complementary to the microfocused HXPS with angle resolution at undulator beamline [6] to open up new application fields.

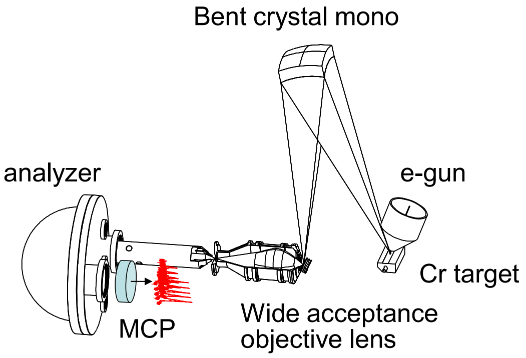

Fig. 1

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DEVELOPMENT OF AMBIENT PRESSURE HARD X-RAY PHOTOELECTRON SPECTROSCOPY

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Demands for the photoemission spectroscopy at higher pressures are rapidly increasing for the gas–solid interfaces studies. Differential pumping method has successfully been applied in the SX-region for this purpose; however, necessity of keeping large pressure differences requires considerably large scale instrumentations with a differential pumping system. Due to much longer photoelectron attenuation lengths, HXPES is expected enable us to realize the high pressure PES without the differential pumping system. We have developed environmental cells for HXPES as schematically shown in Fig. 1, modifying the cell for TEM observations developed by Kawasaki et al. [1]. An Au plate was irradiated by X-rays through a window at a side wall of the cell. Photoelectrons are emitted through an aperture with a 10-15nm thick amorphous membrane, which can bear pressure differences up to 1-2 atmospheric pressure. Figure 2 shows variation of the Au $3d_{5/2}$ spectrum measured by HEARP Lab (Cr Kα: 5.4 keV) laboratory HXPES system [2] with increasing air pressure inside the cell. The gap between Au plate and the aperture membrane was 2.5 mm in this measurement. This results suggests that HXPES using the environmental cell is expected to be applicable upto few hundreds Torr of the pressure inside the cell by decreasing the gap down to 10-100μm. One of the benefits of this method is that it realizes static pressure environment, which is not possible in case of the differential pumping methods. We will report results of feasibility test experiments of the cells developed in our group.

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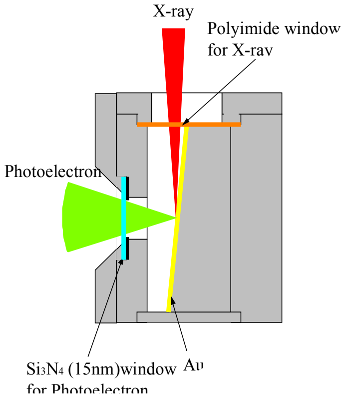

Fig.1

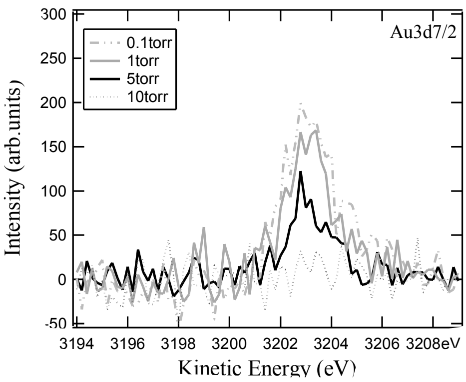

Fig.2

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FOCUS GmbH: ALL ABOUT ELECTRONS…

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Established in 1990, FOCUS has now been in existence for more than twenty years and has been engaged during this time in the field of electron beam evaporation, electron spectroscopy and electron microscopy, as well as in scientific apparatus construction generally.

With a sound foundation of long experience in the development and construction of electron beam reliant devices for surface analysis, FOCUS has recently also firmly established itself in the field of electron beam welding [1].

At the forthcoming HAXPES workshop 2011 we will give an update of our HAXPES instrumentation, our recent HAXPEEM activities as well as our recent steps towards a more efficient spin detection.

For HAXPES, we developed the HV CSA, a 15keV high energy and high transmission analyser equipped with a dedicated 2D event counting detector [2]. Test results, obtained by FOCUS at the hard x-ray beamline P09 of PETRA III in Hamburg, will be presented. We are currently preparing a version of the HV CSA that will be capable of working at ambient pressures (HP-HAXPEEM).

Quite recently, together with the group of C.M.Schneider (FZ Jülich) and the staff of W.Drube (DESY/PETRA III), we undertook first feasibility experiments in performing hard x-ray excited energy filtered PEEM (HAXPEEM), using a slightly modified NanoESCA instrument [3]. A dedicated scientific contribution on this issue and its results will be presented elsewhere at this workshop by the Julich group [4].

Furthermore, we will describe briefly our newly developed spin detector “FERRUM”, which is based on the exchange scattering of electrons on a magnetized and oxygen-passivated iron film [5]. In the near future, we expect a number of spin resolved experiments to take advantage of the new instrumental approach now available. Last but not least, spin resolved HAXPES experiments could take advantage of this approach, due to the essentially reduced acquisition time.

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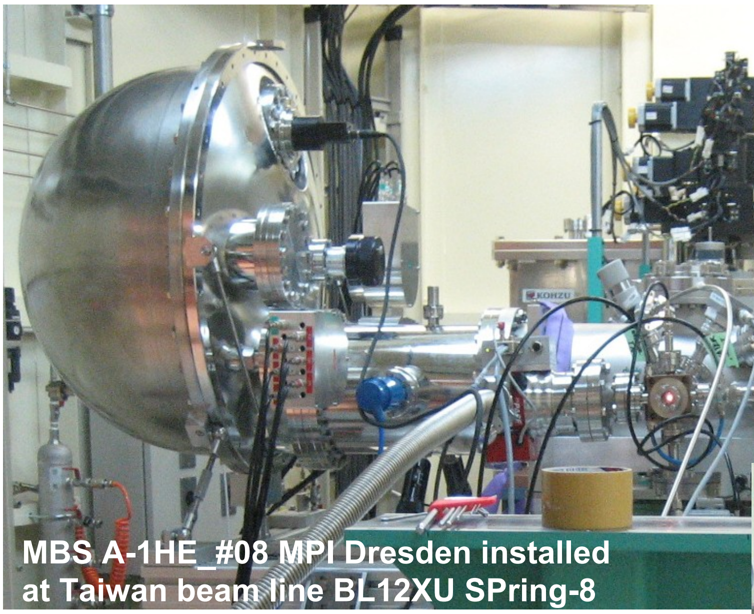
HAXPES ANALYSER MBS A1HE AND HIGH VOLTAGE ELECTRONICS 2011

P. Baltzer, M. Matsuki

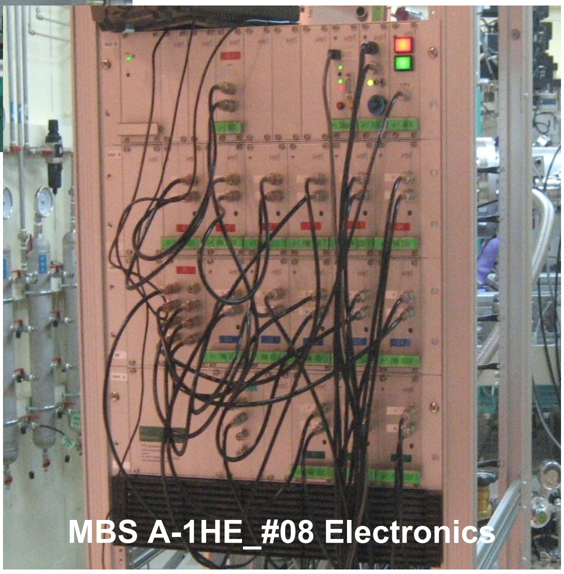
MB Scientific AB

MB Scientific AB manufactures the state of the art High Energy Photoelectron Analyser MBS A1-HE. The analyser and its associated electronics works above 12 keV safely and stably, less than 1 minute after switch-on.

The MBS A1-L2 high retardation lens can take 12keV electron to be analysed at 20eV pass energy which gives more than 1,000,000 resolving power using the standard 0.1 mm slit. Our fast, ultra-compact MBS A1HE electronics supplies the necessary voltages within specifications within 1 second. In the speech we will present our recent progress in this field, such as our new 20 kV high pressure system that is compatible with water at room temperature (15 Torr) .



MBS A-1HE_#08 MPI Dresden installed at Taiwan beam line BL12XU SPring-8



MBS A-1HE_#08 Electronics

MBS A-1HE_#19
being tested at BL P09 PETRAⅢ

ANGLE RESOLVED AND HIGH PRESSURE HARD X-RAY PHOTOELECTRON SPECTROSCOPY INSTRUMENT DEVELOPMENT

R. Moberg

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Traditionally the excitation energy of the Photoelectron Spectroscopy (PES) excitation sources has been up to about 1500 eV e.g. UV and soft x-ray sources. Later 3rd generation synchrotron facilities with higher energies (hard x-rays) have been applied to do PES forming the field of hard x-ray PES (HAXPES) [1]. This emerging field set new demands on PES instrumentation. In this talk we will present VG Scienta instrument development in the area of HAXPES.

The first challenge of HAXPES from an instrumental point of view is to be able to handle high retardation requirements in order to achieve high resolution and high transmission spectra recorded in a stable manner. Early models of VG Scienta analyzers was capable to measure up to 6 keV and in 2003 VG Scienta took a further step and developed a high energy (HE) version of the R4000 L1 analyzer, capable of recording spectra up to 10 keV. The novel angular resolved mode featured in the R4000 L1 analyzer can for example be used for x-ray diffraction measurements or for bulk band mapping [2].

In order to further increase transmission and angular range of the HE analyzers VG Scienta has now developed the EW4000 analyzer. This analyzer is capable of recording kinetic energies up to 10 keV with transmission and 60 degree parallel detection modes.

VG Scienta future plans for instrumental development includes combining the field of HAXPES with high pressure (HiPP) PES. The current VG Scienta R4000 HiPP analyzer is capable of measuring angular resolved spectra at elevated pressures in the soft x-ray regime. The goal is to produce a HiPP-HAXPES analyzer with an angle resolved mode for the hard x-ray regime (at least 7 keV kinetic energy) operating at 20 mbar.

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THE PHOIBOS ANALYZER SERIES: ELECTRON SPECTROMETERS FOR HARD X-RAY PHOTOEMISSION SPECTROSCOPY

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The PHOIBOS analyzers are electron spectrometers with unsurpassed transmission, energy and angular resolution. They come with a modular power supply and detector concept which makes them suitable for every aspect of electron spectroscopy: from laser based ARPES measurements at low kinetic energies starting at virtually zero kinetic energy, to quantitative XPS and high energy photoemission spectroscopy. The multi-element transfer lens of the hemispherical analyser PHOIBOS is optimized for ultimate energy resolution up to highest kinetic energies and can be operated in several different modes for angular or spatially resolved studies. The acceptance angle can be extended with additional pre-lenses up to +/- 30°. The PHOIBOS 150 is available for energies up to 7 kV, while the PHOIBOS 225 can work at energies up to 15 keV. Several detector options with high sensitivity and dynamic range are available: 2D-CCD detector with a Peltier cooled camera, 1D and 2D-delayline detectors, and combined 2D/SPIN detectors.

PROBING S ELECTRON STATES IN METAL OXIDES WITH HARD X-RAY PHOTOEMISSION

D. J. Payne(1) , K.H.L Zhang(1), G. Panaccione(2) and R.G. Egdell(1) *(invited)*

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The cross sections for ionization of highly penetrating 5s or 6s orbitals decrease with increasing photon energy much less rapidly that the O 2p cross section. This results in selective relative enhancement in the intensity of states with significant metal s character in valence band hard x-ray photoemission (HAXPES) of post transition metal oxides. Application of this simple principle will be illustrated by discussion of work on PbO_2 [1], In_2O_3[2-5], $In_4Sn_3O_{12}$ [6] and SnO_2.

Most attention will focus on In_2O_3 where comparison between HAXPES and conventional photoemission spectra led to the realization that the fundamental bandgap of this prototype transparent conducting oxide was almost 1 eV lower than the widely quoted value of 3.75 eV [2]. This in turn helped to establish that an electron accumulation layer presents itself on most In_2O_3 surfaces [3-5].

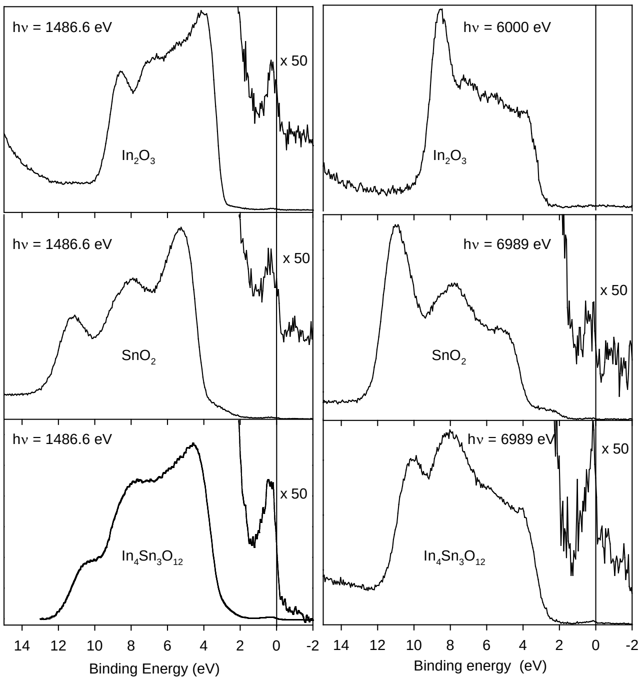

Figure 1.

Valence bands in conventional Al K alpha XPS and HAXPES of In_2O_3, SnO_2 and $In_4Sn_3O_{12}$.

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HAXPES STUDIES OF OXIDES AND ELECTRONIC INTERFACES AT NIST BEAMLINE X24A

Abdul Rumaiz **(invited)**

Brookhaven National Laboratory

Electronic structure of N doped TiO_2 using a combination of synchrotron based hard x-ray photoemission spectroscopy (HAXPES) and first principle density functional theory calculations will be presented. Our results demonstrate that N doping leads to the formation of oxygen vacancies, the electronic structure of which leads to the observed changes in the TiO_2 band gap. Recent results pertaining to B migration during rapid thermal annealing of CoFeB/MgO/CoFeB magnetic tunnel junctions and band offset limits in $Ge/HfO_2/TiO_2$ heterojunctions will also be discussed.

HAXPES OF NOVEL CHARGE TRANSFER COMPOUNDS

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Novel donor and acceptor molecules based on π-conjugated ring structures opened a lot of possibilities for the design of novel charge-transfer (CT) systems for future applications in development of organic electronics. Modelling new charge transfer systems is one of the main approaches for a designed control of the electronic structure of a special class of materials [1, 2]. Microcrystals of tetra- and hexamethoxypyrene as donors with the strong acceptor tetracyanoquinodimethane (TMP_x/HMP_x - $TCNQ_y$), grown from solution via vapour diffusion in stoichiometries x:y = 1:1, 1:2 and 2:1 and thin films of the same compounds co-deposited in-situ were studied at the P09 HAXPES endstation (PETRA III, Hamburg) at 6keV photon energy. Due to the large inelastic mean free path of the fast electrons the probing depth is of the order of 10-15 nm for 5-6 keV photoelectrons and thus surface contaminations play only a minor role.

Series of O 1s and N 1s spectra were taken for fractions of the solution-grown 3D crystallites. The O1s spectrum of HMP_x-$TCNQ_y$ microcrystal fractions is dramatically different from the signal (A) for pure HMP (Fig1.). Intense new signals on the low-binding-energy side are indicative of a changed electronic structure due to charge transfer in the complex. We interpret the narrow signal B as the O 1s main line in the complex and signals C and D, being shifted by 1.2eV and 2.6eV, respectively, from the main line B as shake-up satellites. Most likely these involve excitations across the strongly reduced HOMO-LUMO gap in the complex, as investigated for TMP-TCNQ by UPS and scanning tunnelling spectroscopy [2]. The shifts of N1s and O1s are an order of magnitude larger than the shifts in the K-edge NEXAFS spectra for the same samples [3].

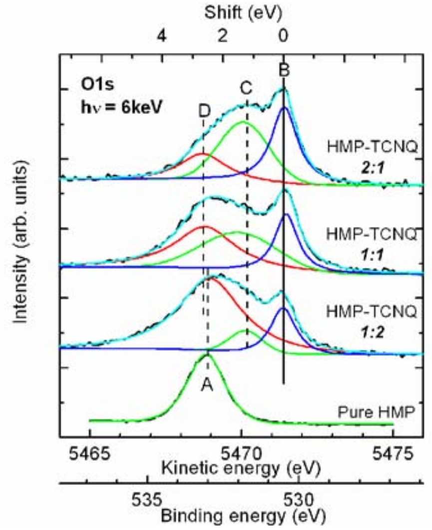

Fig1. Oxygen 1s HAXPES spectra for solution-grown microcrystals of the CT complexes HMP_x-$TCNQ_y$ with x:y = 2:1, 1:1, 1:2 and 1:0.

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ALLOYING AND INTERFACE PROPERTIES OF Fe/V MULTILAYERS

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As a comparison to bulk materials additional properties can be achieved by reducing the physical dimensions by combining thin layers with specific properties. Thin films, interfaces, multilayers and superlattices have highly important role in the development of different components in electronics nowadays. As the size of the components and thus also the thickness of the multilayers keeps decreasing the quality of thin layers and interfaces becomes a key factor in the functioning of the devices. This work reports on structural studies of Fe/V interfaces and their temperature dependent microstructure. High kinetic energy photoelectron spectroscopy (HIKE, also denoted as hard X-ray photoelectron spectroscopy, HAXPES) was used to study the intermixing of Fe and V layers and the effect of component concentration on the alloying process. In addition, our aim was to investigate the potential diffusion of capping material into the bulk.

The experiments were performed at HIKE end station which is placed at the bending magnet beamline KMC-1 at BESSY-II synchrotron at the Helmholtz-Zentrum Berlin. The samples were prepared by using UHV-based dc magnetron sputtering. The multilayer structures consisted of repeated Fe/V bilayers. The thickness of V was varied between 2 and 6 monolayers (ML) while the Fe layer thickness was kept constant being 6 ML. The samples were protected with Pt or Pd cap. To observe the interface roughening and alloying between Fe and V the samples were heated up to selected temperatures between room temperature and 500 ºC.

The processes related to intermixing, diffusion and alloying were investigated by analyzing the changes in the core-level spectra of V, Fe and cap materials as a function of heating temperature. The binding energies and peak intensities measured with selected photon energies were compared to each others. V *2p* spectra of all the samples broadens and shifts towards higher binding energies as the temperature increases and the alloying of interfaces proceeds. The binding energy change of the spectra between room temperature and 500 ºC is approximately +0.3 eV in Fe_6V_2/Pt and +0.4 eV in Fe_6V_6/Pt. The largest changes in binding energy seem to take place between 300 and 400 ºC in Fe_6V_6/Pt. The binding energy change in Fe_6V_2/Pt proceeds more gradually, which is expected when taking into account the initial structure where there are only interface, not bulk, V atoms. Much weaker changes were seen in Fe *2p* spectra but a small positive shift in the binding energy was resolved in all the samples. The behaviour of the Pt and Pd cap on Fe_6V_2 and Fe_6V_6 was observed by measuring the binding energy shifts in Pt *4f* spectra and the intensity ratios of Pt/Pd, Fe and V core-levels as a function of temperature.

The intensity changes and binding energy shifts show that the interface roughening has already started around 300 ºC and instead of sharp interface structure we are studying an alloy at temperatures higher than that [1]. Also strong signs of Pt diffusion and V segregation were observed.

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DIRECT OBSERVATION OF Al DOPING INDUCED ELECTRONIC STATES IN THE VALENCE BAND OF ZnO FILMS

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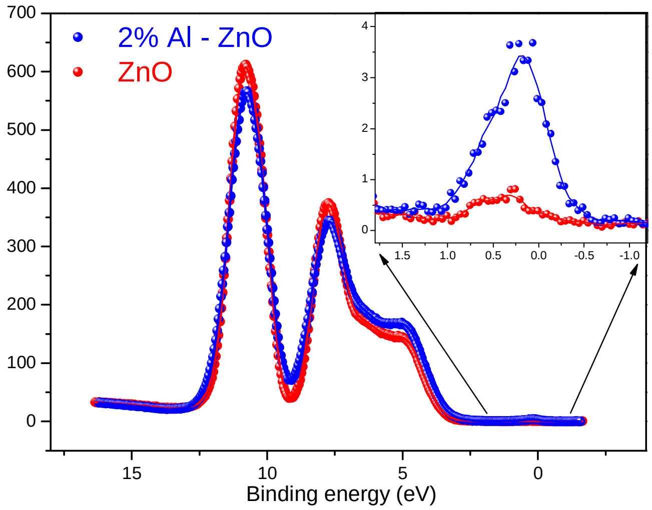
Al-doped ZnO (AZO) is regarded as a promising transparent conductive oxide for photovoltaic and optoelectronic applications[1]. To date, a realistic theoretical explanation of the effect of Al-doping on the electronic structure of ZnO has not been provided. The most accepted picture is that donor-doping shifts the chemical potential above the bottom of the conduction band (CB), making conduction carriers available at the Fermi level (FL) while preserving the transparency of the film[2]. X-ray photoemission spectroscopy was used to investigate the AZO valence band (VB) before[3]. However, its high surface sensitivity makes it difficult to obtain unquestionable results close to the FL in these sputter-deposited samples. HAXPES experiments on AZO samples were performed at ESRF using the VOLPE set-up on the ID16 beamline[4]. We present HAXPES results for ZnO and AZO films with different Al content, together with *ab initio* and model calculations of the DOS at the VB and FL regions, which conclusively show that Al doping of ZnO leads to impurity bands inside the band-gap region and in the valence band. The position of these impurity bands scarcely depends on doping, thus the FL is pinned. In Fig. 1, doping induced states appear between the Zn3d and O2p levels and in the band gap, just below the conduction band minimum (CBM). *Ab initio* calculations confirm the Al impurity origin of these induced states. Therefore, we conclude that the drop in the film resistivity with Al doping is not due to a progressive shift of the Fermi level above the CBM but rather to the filling of the Al impurity band states which pin the Fermi level just below the CBM. Conductivity changes with Al-doping should therefore be interpreted within the framework of these new results.



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P01

CHEMICAL STABILITY OF THE MAGNETIC OXIDE EuO ON SILICON INVESTIGATED BY HAXPES

C. Caspers (1), M. Müller (1), A. X. Gray (2), A. Gloskovskij (3), A. M. Kaiser (2),
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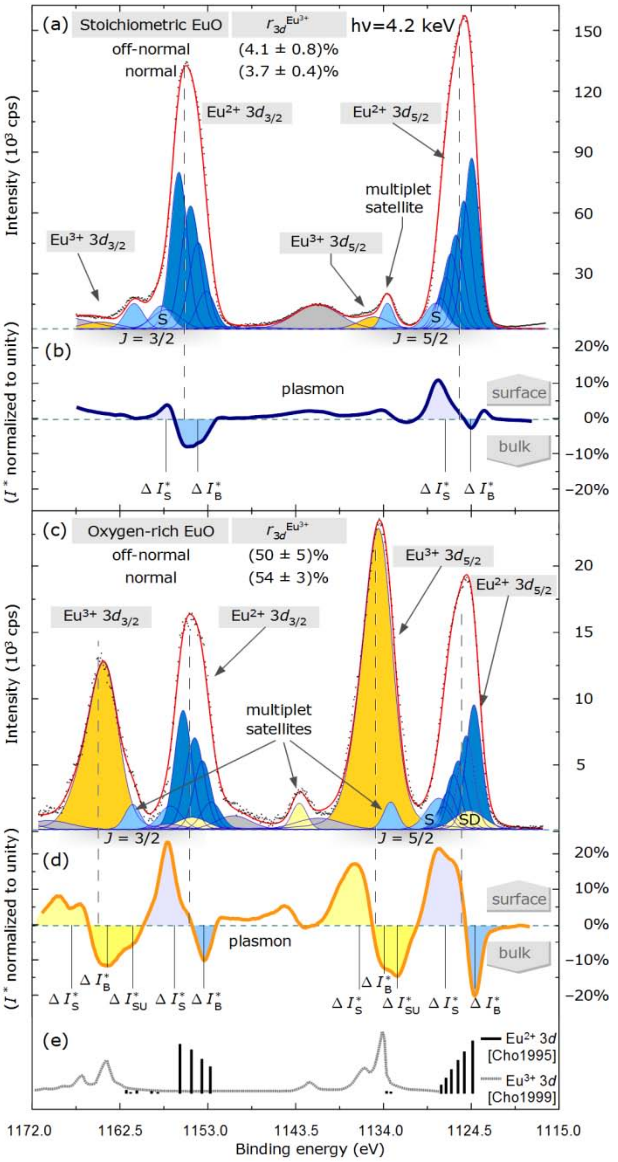
Magnetic oxides are interesting materials as they provide the combination of electrical insulation and ferromagnetism, which at the same time is desirable but rare in nature. Thin films of magnetic oxides are candidates for efficient spin filter tunnel barriers in spintronics devices[1].

Europium Oxide (EuO) is the only magnetic oxide predicted to be stable on silicon[2] which motivates its thin film synthesis for spintronics uses. Bulk and interface chemical properties of EuO films play a crucial role for a further development of functional heterostructures on silicon. A depth-sensitive study employing HAXPES[3] can provide valuable information about the chemical properties of EuO, which is buried under capping layers.



High quality EuO thin films were prepared under UHV in an oxide MBE system. We could show single-crystalline epitaxial growth on MgO and YSZ substrates. This successful growth method was transferred to EuO grown directly on silicon. For all substrates, i.e. MgO, YSZ, and Si, the EuO thin films show bulk-like magnetization curves. As an example of probing the chemical quality of EuO by photoemission, The figure compares the Eu 3d spectra of (a) an optimum sample with (b) an oxygen-rich Eu_1O_{1+x} layer on silicon recorded at a photon energy of hν=4.2 keV. The only variation between (a) and (c) is a step-up of oxygen pressure by 2×10^{-9} mbar during growth. The Eu 3d structure is spin-orbit split by 29.5 eV, and the Eu^{2+} contributions additionally exhibit asymmetric peak shapes. These can be explained by a complex multiplet-splitting, described e.g. by Cho et al.[4]

A quantitative analysis using the least squares fitting method reveals the ratios of Eu^{3+} and Eu^{2+} cations, which display the oxidation states of Eu_2O_3 and EuO, respectively, where Eu^{2+} is the desired valency. Our optimum sample (Fig. a) shows only 3.7% Eu^{3+} ions and can be labelled "stoichiometric", while the oxygen-rich sample (Fig. c) contains 54% Eu^{3+} ions. Concluding, we succeeded in the chemical stabilization of high quality EuO thin films on silicon, which have been grown in a special oxide MBE system—facing the pathway for the integration of functional magnetic oxide into silicon-based spintronics.

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P02

CHEMICAL PROFILING WITH PHOTOEMISSION: A COMPARISON BETWEEN ANGLE-RESOLVED XPS AND HIGH-ENERGY PHOTOEMISSION ON FULL GATE STACKS

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The replacement of poly-silicon by metallic compounds in the gate stack leads to the search for metals with suitable workfunctions. However, it is observed that the thermal budget has a large influence on the effective workfunctions of several metals. A possible origin is the modification of the high-k/metal interface. A precise analysis of the modification of buried interfaces is thus critical to the understanding of electrical changes.

A number of studies have been performed by angle-resolved XPS (ARXPS), which allows varying the information depth by changing effective mean free path. This approach is very successful for thin layer but rapidly reaches its limits when the full stack, including metal and cap layers is considered. An alternative to ARXPS is the use of high-energy photoemission in order to increase (and vary) the effective mean free path of the electrons.

In this study we investigated the effect of annealing on a stack composed of a $SiO_2/HfO_2/TiN/Si$ layers with varying TiN and Si-cap thickness. Both ARXPS with AlKα photons (angular range 20-80 degrees from the normal) and high-energy photoemission spectra with photon energies between ~2000 and 3000 eV were recorded.

This work shows that for thinner stack, ARXPS has the advantage to allow a large variation of the effective mean free path (~ factor 4 for angles between 20 and 80 degree) that is more difficult to achieve by varying the photon energy (~ factor 10 needed). However, as large angles cannot be used for thicker layer, high-energy photoemission is key to analyze buried layers.

We will also discuss the advantage to combine both approaches together.

DETERMINATION OF BAND OFFSETS IN COMPLEX OXIDE THIN-FILM HETEROSTRUCTURES BY HARD X-RAY PHOTOELECTRON SPECTROSCOPY

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Valence-band offsets in heterostructures with interfaces between band insulators, such as $SrTiO_3$ and $LaNiO_3$, and Mott-Hubbard insulators such as $GdTiO_3$ [1-2] are of great importance in connection with conductivity in such systems, and the possible electrostatic tuning of it. We have thus studied such heterostructures with hard and soft x-ray photoelectron spectroscopy.In the case of $SrTiO_3$ and $LaNiO_3$ heterojunction, both compounds are wide-gap semiconductors with the perovskite structure. However, it has been reported that metallic interface phases can be induced in such systems, even though the constituent materials are insulating. In addition, electrical transport measurements for epitaxial $GdTiO_3/SrTiO_3$ heterostructures show contributions from an interfacial conductive layer in $SrTiO_3$. Among the most important physical parameters for these heterojunction systems are the conduction-band and valence-band offsets. The quality and the practical feasibility of such hetero-junction devices depends crucially on the values of these band offsets, as has been known for some time in normal semiconductor heterostructures, where standard XPS has been used.

Accurate determination of such band offsets at the interfaces requires high-precision measurement of the core-level and valence-band-maximum (VBM) binding energies (should be accurate better than 0.025 eV) [3]. Such high precision has been very hard to achieve for oxide samples. The band offset determination in complex oxide heterostructures presents a challenge because of the charge accumulation at the surface when photoelectrons are emitted. These charges can cause the whole spectrum to shift. One way to correct from this shift is to choose a core level (e.g. C 1*s*) as reference. After the core-level peaks are properly aligned and the spectral shift caused by surface charging is corrected, the valence band offset can be determined. However, this method is very cumbersome and imprecise: shifting of spectra on the energy scale leads to difficulties in interpreting chemical states, different charging in different regions of the surface may cause a given peak to broaden or to split into more than one peak, etc. Owing to the detrimental effects mentioned above, it is important to avoid, or at least reduce charging by suitable experimental methods. Our approach is to use hard x-ray photoemission spectroscopy (HXPS) [4]. We present in this paper band offsets obtained using both XPS and HXPS for $[SrTiO_3/ LaNiO_3]\times 10$ and $[GdTiO_3/SrTiO_3]\times 20$ multilayers - results which demonstrate the advantage of using HAXPES.

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P04

HAXPES EXPERIMENTS WITH STANDING-WAVE EXCITATION ON THE TRI-LAYER SYSTEM MAGNESIUM OXIDE/GOLD/IRON

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The MgO/Fe interface plays an important role in magnetic tunnel junctions and was subject to many studies during the last years. Mainly the electronic states at the interface influence the tunnel magnetoresistance (TMR) ratio that can be employed in spintronic devices. It is well understood that oxidation of the iron layer at the interface disturbs the electronic band structure and thus reduces the TMR ratio. J. Mathon and A. Umerski suggested placing a gold monolayer at the interface to protect the iron from oxidation [1].

In our experiments we investigated the properties of an ultrathin gold layer located between an iron wedge and a magnesium oxide film on top. In order to obtain chemical sensitivity photoemission experiments were performed. The excitation energy was hν = 4 keV resulting in a sufficiently large probing-depth of a few nm inside the sample. A high depth-resolution was achieved by using x-ray standing-wave excitation [2]. Fig. 1 shows a schematic layout of the sample.

The tri-layer of interest was grown on top of a Si/MoSi$_2$ multilayer mirror with a high reflectivity for the incoming x-ray beam. The incoming and the reflected beams interfere above the multilayer mirror and thus create the standing-wave inside the tri-layer. By scanning the angle of incidence through the Bragg-angle a modulation of the XPS signals can be observed. This modulation is different for each element-specific signal and thus it contains information about the thickness and the intermixing or roughness of the layer that emits the measured photoelectrons.

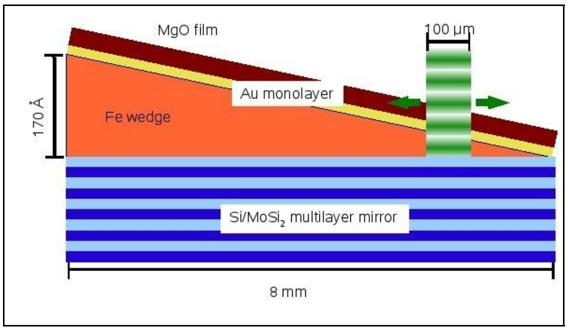

Fig.1: Schematic layout of the sample on top of the multilayer mirror, which is needed to create the x-ray standing-wave.

The iron layer was grown wedge-shaped for a special kind of standing-wave experiment, the so-called "swedge" scan, first described by S.-H. Yang [3]. In this experiment the angle of incidence is fixed at the first order Bragg condition while the sample is moved relative to the beam. Therefore, the gold and magnesium oxide layers on top of the iron wedge and their interfaces travel through the standing-wave, which has a fixed phase with respect to the mirror.

The analysis of the XPS signal modulations shows that the thin gold layer diffuses into the iron film below. The magnesium oxide layer shows no interaction with the layers below. No evidence for the formation of iron oxide at the interface was found.

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NON-DESTRUCTIVE CHARACTERIZATION OF INTERNAL STRUCTURE OF NANO-LAYERED SYSTEMS BY HIGH KINETIC ENERGY PHOTOELECTRON SPECTROSCOPY AND REFLECTOMETRY

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Nowadays nanometer-thin films and multilayer coatings find multiple applications ranging from gate oxide in microelectronic devices to X-ray reflective mirrors. The thickness of an individual film can be as small as a fraction of a nanometer, hence, the role of inter-layers (their extension and composition) generated at the interface between two different substances increases due to possible processes such as: inter-diffusion, chemical reactions and implantation during synthesis of films. It is obvious that one needs to develop analytical methods suitable for the analysis of both nanometer-thin films and interlayers formed at their interfaces. In this work we are focusing on the development of the mathematical analysis methods on the basis of high kinetic energy photoelectron spectroscopy (HXPES) and reflectometry (SXR) data. Both methods provide unique opportunities for the study of internal material structure including buried interfaces.

The in-depth chemical analysis of the samples by HXPES was realized through the variation of photoelectron emission angle at fixed photon energy that allowed us to modify systematically the probing depth. Taking into account the peak areas of all investigated core levels the individual thicknesses of the layer stacks were determined.

Atomic concentration profiles of all chemical elements composing the samples were reconstructed from analysis of the reflectivity curves measured versus the incidence angle at different SXR photon energies. The approach was based on the general philosophical principle of Ockham's Razor and implied step-by-step complication of the sample model until the desired accuracy between the experimental and the calculated reflectivity curves was achieved. The final refinement of the atomic concentration profiles was performed on the basis of the maximum entropy concept.

The developed methods were applied to investigate internal structure of TiO_2(Ti)/SiO_2/Si stacks. The sample parameters (variation of the chemical composition with depth, thicknesses of individual layers and their densities) extracted from HXPES and SXR measurements are in close agreement and correlate well with the HRTEM images.

This work was supported by the ISTC (Project No 3963).

P06

INTERFACTANT-MEDIATED GROWTH OF RARE-EARTH OXIDES ON SILICON

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The growth of high-quality, epitaxial thin oxide films on silicon is a long-standing goal in semiconductor technology. Among other multiple possible applications, rare-earth (RE) oxides are some of the most promising candidates for the realization of these so-called "high-k" dielectrics due to their predicted high thermodynamic stability and their almost vanishing lattice mismatch to silicon. However, growth of high-quality ultrathin films has so far been considerably impeded by RE-promoted Si oxidation at the interface, resulting in subsequent silicate formation. In this contribution, we present an extensive study of epitaxial ceria [1] and praseodymia [2] films grown on Cl-passivated Si(111) by molecular beam epitaxy.

X-ray photoemission spectroscopy is employed to investigate the stoichiometry of the as-prepared films, proving the sole existence of RE_2O_3 after the preparation as well as the formation of continuous RE oxide films. Truly ultrathin films of a few monolayer (ML) thickness were characterized by low-energy electron diffraction and X-ray standing waves (XSW) using Ce-L_α fluorescence and Ce(Pr)-3d photoelectrons as secondary signal. In all circumstances, the XSW results unanimously confirm the improved quality obtained by Cl pre-adsorption for both ceria and praseodymia (see, e.g., Fig. 1 for Ce_2O_3/Cl/Si(111)). Furthermore, the atomic structure and chemical composition of the interface were inferred from chemically-sensitive XSW measurements employing O1s photoelectrons, which allow to separately investigate the atomic structure of the different oxygen species in the interface region. Moreover, monitoring the Cl binding sites with XSW enabled us to draw conclusions on its role in the growth process. Finally, for praseodymia and ceria film thicknesses exceeding a few nanometers, their crystallinity, surface and interface roughness, and structure were characterized by grazing-incidence x-ray diffraction and high-resolution transmission electron microscopy.

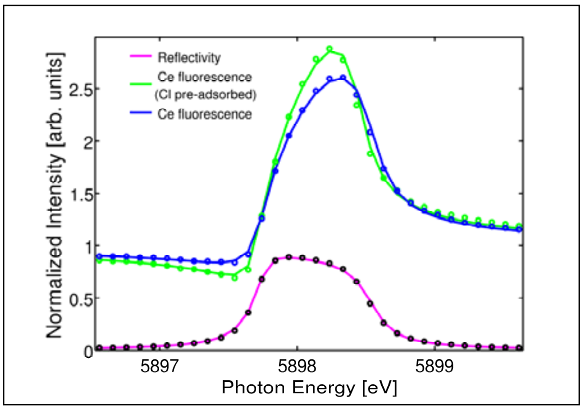

Figure 1: XSW data (circles) and theoretical fit (solid lines) for Ce L_α fluorescence obtained in (111) Bragg reflection for ~3 ML of Ce_2O_3/Si(111) with and without Cl pre-adsorption, yielding an enhanced (decreased) modulation of the fluorescence signal, directly reflecting the improved order of the film grown on the passivation layer.

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P07

X-RAY PHOTOELECTRON SPECTROSCOPY OF CERIUM OXIDE ON SILICON

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Cerium oxide is a promising candidate for a wide range of applications, e.g., as gate material for MOSFET applications because of its almost perfect lattice match to Si, its high stability, even at elevated temperatures, and because of a band gap of 2.4 eV in case of Ce_2O_3 and 6 eV for CeO_2 [1-2]. Yet, despite numerous attempts in the last decades, still no physically consistent fit for the Ce 3d photoemission spectrum from cerium oxide could be achieved. Essentially, the spectrum may be explained by the coexistence of two initial and two final states, which have traditionally been linked to the partial localization and occupation of the Ce 4f states, yielding 2 and 3 major spin-orbit-split components in the case of Ce_2O_3 and CeO_2, respectively. However, in this established and generally accepted approach, the occurrence of additional loss features as well as the possibility of a Ce 5d—O 2p hybridization are neglected [3-5]. However, these interactions could give rise to additional satellite features in the spectrum, adding to the complexity of the interpretation. Since a key point of this discussion is the purity of the oxide phase, it is essential to have a fingerprint for both oxide phases.

It is well known that when grown on Si(111), Ce_2O_3 is the dominant phase in the nanometer regime, while fully oxidized CeO_2 may be achieved for thicker deposits. Here, we investigated the phase transition from Ce_2O_3 to CeO_2 during stepwise cerium oxide growth on Si(111) after prior Cl passivation using synchrotron-based X-ray photoemission spectroscopy. The purpose of Cl passivation prior to oxide epitaxy is to saturate the Si dangling bonds to suppress silicon oxide growth, resulting in the formation of a well-defined Ce_2O_3 bixbyite phase [6-7]. For all subsequent stages of the phase transition from Ce_2O_3 to CeO_2 during cerium oxide growth, spectroscopic fingerprints of the mixed oxide phases were obtained by monitoring the O1s and Ce 3d spectra. As the total oxide thickness increases, the relative amount of CeO_2 increases as well. Using the intensity of the chemically shifted O1s components as an estimate for their relative concentration within the probing depth, a consistent correlation of the spectral features with existing oxide phases could be achieved. In this contribution, the finding of so far unexplained spectral features in the Ce 3d spectra (Fig. 1) and their possible origins will be discussed.

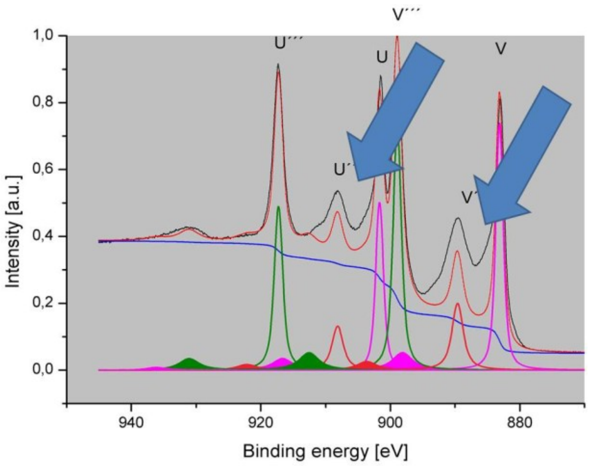

Fig. 1 : Ce 3d spectra of CeO_2, taken at 3000eV beam energy. In a first approximation, the spectrum is fitted, considering plasmons arising from every main line. Regions of unexplained peaks are indicated with arrows.

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P08

STUDY OF SEMICONDUCTOR BAND BENDING BY HARD X-RAY PHOTOELECTRON SPECTROSCOPY

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The electronic state of metal/semiconductor or insulator/semiconductor interface affects the properties of semiconductor devices. For example, in the case of GaN-based power devices, dry etching induced damage causes serious degradation of electronic properties, such as poor ohmic contacts to p-type GaN and reduction of channel mobility in field-effect transistors. Because information on the electronic state of the interface makes it possible to understand the device properties, it is important to study the electronic state of the interface.

We studied the semiconductor band bending by hard X-ray photoelectron spectroscopy (HAXPES). The band bending is expected to be determined by the core level shifts of photoelectron peak depending on take-off angle of photoelectrons. We evaluated the validity of this technique using well-controlled structure of Bi/Si(111)7x7.

Atomically flat 10 BL (bilayer) or 30 BL of thin Bi film was grown on Si(111)7x7 clean surface at ultra high vacuum condition. Various Si(111) substrates with different dopant concentration were used to change the band bending width. We consider that each sample has different band bending width depending on the dopant concentration, but the energy level of valence band maximum on the Fermi level basis is pinned at the same energy position due to the same interface structure. HAXPES measurements were carried out at SPring8 BL46XU using photon energy of 8keV.

Figure 1 shows Si 1s spectra of Bi/Si(111)7x7 samples with different substrates measured at different take-off angles. At all samples, the Si 1s peaks shifted to lower binding energy with lower take-off angle. Furthermore, with the exception of As doped 0.001Ωcm sample, the shift amount among the different tale-off angles increased with higher dopant concentration. These results can be explained by the upward band bending toward the Bi/Si interface and by the different band bending width determined by the dopant concentration. We suppose that the smaller shift amount of the As doped 0.001Ωcm sample was caused by the decrease As concentration near the interface due to desorption of As during flashing.

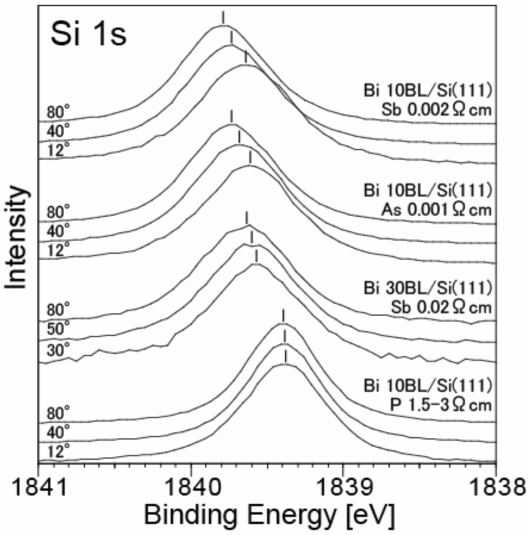

Fig1. Si 1s spectra of Bi/Si(111)7x7 smaples with different substrate measured at different take-off angles.

The binding energy of all Si 1s spectra were corrected with reference to Bi 4f7/2 spectra.

From the results, validity of this technique was experimentally evaluated. Moreover, as a practical application, we measured the band bending for GaN surface. As a result, the distinct differences in the shape of band bending were obtained at different device process. The evaluation of the band bending using HAXPES is quite helpful in explaining the device properties.

P09

A HAXPES STUDY OF A TERNARY PALLADIUM ALLOY METAL-ELECTROLYTE-INSULATOR-SEMICONDUCTOR SYSTEM

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To achieve optimal performance of gas sensors based on catalytically processes it is necessary to test new alloy compositions. Ternary alloy thin films studied are deposited as the catalytically active gate metal layer of a multi-layer sensor structure based on $LaF_3/Si_3N_4/SiO_2/Si$. The Metal-Electrolyte-Insulator-Semiconductor (MEIS) system works as a hydrogen sensor at room temperature for a wide range of hydrogen concentration [1].

Ternary Pd alloy thin films have been studied at the HIKE facility at the KMC-1 beamline at BESSY II, Berlin [2]. The films were deposited by magnetron dc-co-sputtering with a mosaic target consisting of palladium, nickel and cobalt. The experiments are focused on non-destructive determination of in depth gradients of elements constituting ternary alloys and the ways they might be altered due gas-surface interactions.

Two patches of different alloy composition were measured after preparation, after exposition to hydrogen and after exposition to hydrogen sulfide. The excitation energies of 2010, 4000 and 6000 eV selected by a Si (111) crystal have been chosen to measure Pd 3d, Ni 2p, Co 2p, S 2p and S1s core levels of each sample.

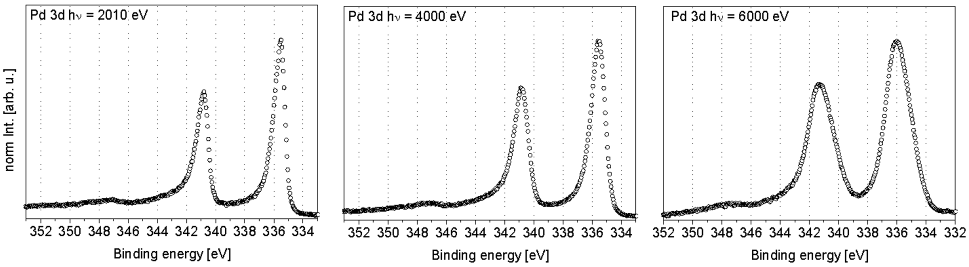

Fig.1: Pd 3d core photoelectron spectra recorded with a ternary Pd-Ni-Co alloy film at 2010, 4000 and 6000 eV using a Si (111) crystal of the KMC-1.

Hard X-ray photoelectron spectroscopy (HAXPES) has been used to study the effect of hydrogen and hydrogen sulfide on segregation phenomena in the outermost layers of a ternary Pd-Ni-Co alloy system. Other points are the acquisition of S 1s core level spectra at a binding energy of ~2470 eV and the analysis of the buried Alloy/LaF_3 interface which has been detected at an excitation energy of 6000 eV.

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P10

BURIED INTERFACE CHARACTERIZATION FOR A CLICK CHEMISTRY-DERIVATIZED SELF ASSEMBLED MONOLAYER ON GOLD

E. Darlatt (1)*, J. Kühn (1), J. Poppenberg (2), S. Richter (2), C. H.-H. Traulsen (2),
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An azide-terminated self assembled monolayer on a gold substrate was functionalized by an alkyne exploiting click chemistry (Figure 1). [1-2] The interface and surface analysis was carried out using X-ray photoelectron spectroscopy with excitation energies between 4000 eV and 260 eV. Additionally the results were cross checked with near-edge X-ray absorption fine structure spectroscopy (NEXAFS spectroscopy). Despite the relatively large space requirement of the terpyridyl groups the spectroscopy data show the complete absence of azide moieties after click reaction und thus the nearly quantitative course of that reaction. Due to the resulting dense organic layer stack the characterization of the gold sulfur interface was worse estimable with the S 2p low energy photoelectron emission but very good accessible with the S 1s photoelectron emission line at ~2470 eV.
Furthermore the coordination behavior with palladium(II) ions of these densely packed donor head group layer was investigated with the same analysis method.

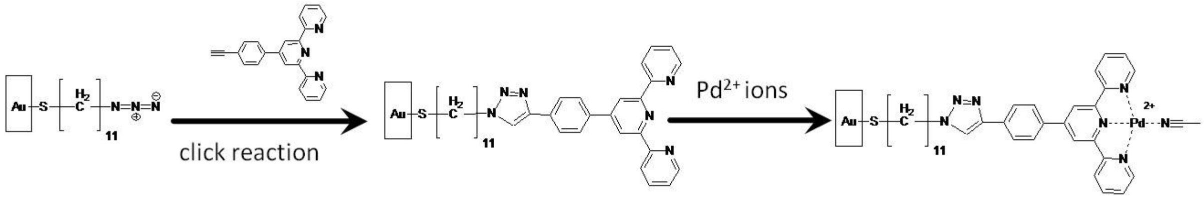

Figure 1: Reaction path of the click reaction and the subsequent complex formation

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the DFG (SCHA 893/9-1, UN 80/8-1), the Freie Universität Berlin, and the FCI for financial support. S. Richter thanks the FCI for a Ph.D. fellowship.

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HIGH-*K* / $In_{0.53}Ga_{0.47}As$ INTERFACE OXIDATION CONTROL CHARACTERIZED BY HAXPES

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During the past decade the semiconductor industry has introduced new elements in the form of novel materials systems at an unprecedented rate. This materials revolution, driven by the need to maintain the rapid rate of device scaling according to Moore's Law, has given rise to several fundamental modifications including; high permittivity (***k***) gate insulator films as replacements for SiO_2, ***p***- and ***n***-type workfunction metals as alternatives for B^+ and As^+ doped poly-Si electrodes, and the emergence of engineered substrates as a means of enhancing device mobility. The latter initiative includes strained Si, $Si_{0.7}Ge_{0.3}$, and intensive evaluations of III-V channel materials. Any effort focused on successful integration of high-***k*** gate dielectric layers on $In_{0.53}Ga_{0.47}As$ substrates must ultimately lead to controlled oxidation of the III-V constituents and control oxygen redistribution as a function of processing.

The HAXPES data presented in this work were acquired at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL) on National Institute of Standards and Technology (NIST) beamline X24A. An advantage of the HAXPES greater penetration depth to characterize buried layers and interfaces is that blanket films prepared for such experiments may be processed as more precise replications of capacitor and transistor film systems, enabling direct correlation with performance data.

3nm thick ZrO_2 and Al_2O_3 high-***k*** films deposited on $In_{0.53}Ga_{0.47}As$ have been processed with O_3 and H_2O exposure as well as with AlN substrate pretreatments for comparison.[1-3] HAXPES evidence for oxidation control and AlN passivation of As-As bond formation associated with aggressive reduction of As-O_x is presented in detail and correlated with performance (***C-V***) data. In addition, gettering of oxidized III-V elements (through the dielectric layers) by TiN electrodes is presented as a function of processing and a clear dielectric dependence is revealed. Figure 1 illustrates the advantage of AlN passivation and the impact of TiN gettering for ZrO_2 vs. Al_2O_3.

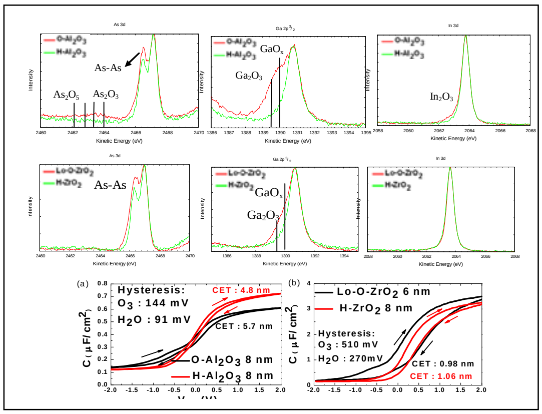

Fig1. Top panels : HAXPES of TiN/O-Al_2O_3 and TiN/H-Al_2O_3 shows TiN reduction of AsO_x, Mid panels: of TiN/O-ZrO_2 and TiN/H-ZrO_2, Bottom panels CV hysterysis shows lower bulk traps with H(H2O) than O (O3) process.

In summary, new findings include in-situ TMA clean, low O_3 precursor dose, replacement of O_3 with H_2O as the oxidizer, gettering of interfacial oxides by TiN metal gate all lead to changes at the high-k/ III-V interfaces. Specifically, significant reduction of CV hysteresis (37% in Al_2O_3 and 47% in ZrO_2), fast transient traps (15% in Al_2O_3 and 19% in ZrO_2), and mean interface traps (91% in Al_2O_3 and 29% in ZrO_2). H_2O-based high-k and a gettering TiN thereby reducing O content at high-k/III-V interface are process keys. These results positively impact the industry's progress toward III-V CMOS at the 11nm technology node.

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P12

CHARACTERIZATION OF InAs-BASED METAL-OXIDE-SEMICONDUCTOR STACKS USING HAXPES

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The development of Metal-Oxide-Semiconductor (MOS) devices is at a state where miniaturizing is not enough to keep up with the demands for higher speeds and less power consumption. One promising strategy for improving MOS field-effect-transistors is to use narrow band gap III-V semiconductors with high electron mobility, like InAs [1,2]. A high-k dielectric material is used as substitute for the native oxide to further increase the performance. Thereby the stoichiometry of the interface between the III-V semiconductor and the high-k dielectric plays a crucial role for the device performance.

This interface has widely been studied using X-ray photoelectron spectroscopy (XPS) [3,4]. However, such investigations are limited to structures with very thin high-k layers and without any gate metal on top due to the small probing depth of conventional XPS, thus neglecting the influence of a thicker dielectric layer and the impact of the top metal on the MOS structure behavior. Only the use of Hard X-ray PhotoEmission Spectroscopy (HAXPES) allows the investigation of realistic MOS stacks.

We have investigated InAs-HfO_2-W and InAs-HfO_2-Pd structures with HAXPES at BM25 at the ESRF, using photon energies varied between 11 and 20 keV. HfO_2 layers of either 8 or 15 nm thickness were formed by atomic layer deposition, while the 5 nm thick metal films were evaporated. InAs-HfO_2 samples without any metal on top served as reference.

The In *2p* [Fig. 1 (a)] and As *2p* [Fig. 1 (b)] core-level spectra demonstrate the ability of HAXPES to investigate an interface buried up to 20 nm below the surface. The peak shapes show no dependence on the imaging depth except of the varying instrumental broadening, indicating an abrupt interface between the InAs and the HfO_2, in agreement with conventional XPS studies [3,4]. From the comparatively narrow As *2p* peaks any significant amount of interfacial As-oxide can be excluded [Fig. 1 (b)]. The energy-dependent Hf *2p* spectra [Fig. 1(c)] reveal a homogeneous depth profile of both the 8 nm and 15 nm thick HfO_2 layers.

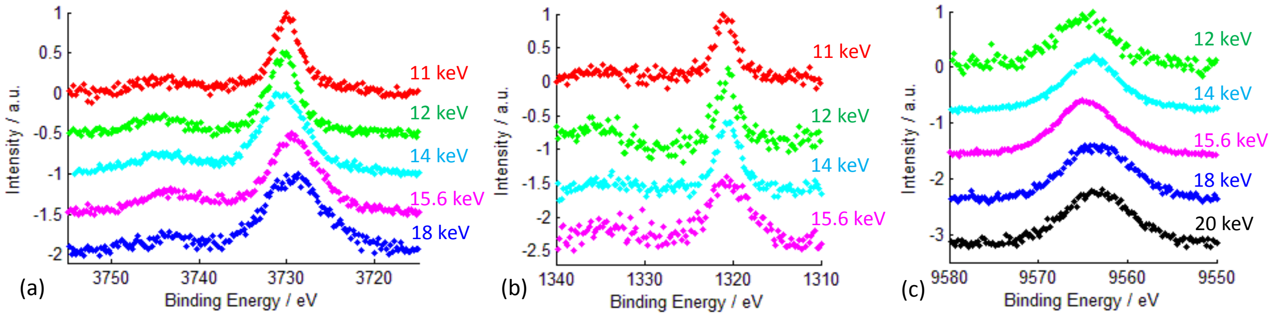

Fig. 1: (a) In *2p* spectra of a sample with 8 nm HfO_2 and 5 nm W. (b) As *2p* spectra of the same sample. (c) Hf *2p* spectra of a sample with 15 nm HfO_2 and 5 nm W. All spectra are normalized and shifted vertically for better visibility. Note that the instrumental peak broadening increases with increasing beam energy.

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CHARGE CARRIERS IN METAL OXIDES AND THEIR HETEROSTRUCTURES

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In recent years the quasi 2-dimensional electron gas (2DEG) observed at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface has become a model case demonstrating the exciting new properties that may exist at the interfaces of insulating complex oxide layers [1]. However, the origin of this conducting layer is still heavily debated. So far several explanations have been proposed, including intrinsic doping with electrons, formation of oxygen vacancies, interdiffusion or intermixing at the interface, formation of a conducting intermediate phase, and strain induced lattice distortions. The presence of such a 2DEG should be accompanied by filling of the valance states in the STO band gap up to the Fermi edge, which have been observed very recently on the surfaces of UHV cleaved, weakly doped STO [2, 3]. Similar signatures have not yet been reported for the buried LAO/STO interface, which can only be probed by HAXPES using a third generation synchrotron. In the light of the current ongoing discussion about the nature of the 2DEG at oxide interfaces, a more detailed study of the interfaces in direct comparison with the doped substrate materials is extremely important.

In this contribution we will report an x-ray standing wave (XSW) study of site-specific valence states of Nb-doped STO, oxygen deficient STO (after annealing at 1000°C for 4h), and a 6 unit cell LAO film grown on STO.

XSW modulated valence spectra were measured at three different photon energies around the STO(111) Bragg reflection to determine the partial yields associated with the Ti site and SrO plane. We observed clear XSW effects on the density of states near the Fermi edge of the Nb doped STO, which associated the shallow charge carriers with the Ti-Lattice site. For the oxygen deficient STO an additional in-gap state was found 1.3 eV below the Fermi edge [4] and associated also with the Ti site, as indicated by the strong standing wave modulation. We will show that the valence spectra measured from the conducting LAO/STO sample follow the characteristic line shape of the oxygen deficient STO.

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P14

NON-DESTRUCTIVE *IN-SITU* HAXPES STUDY OF RESISTIVE SWITCHING IN Ti/HfO$_2$/TiN RRAM CELLS

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A variety of different metal-insulator-metal (MIM) multilayered structures reveal reversible changes in resistance upon applying bias voltages across the layers. We utilize this phenomenon, which has not yet been fully understood, in Resistive Random Access Memory (RRAM) technology developed at our institute.

In order to identify whether the resistance variation is related to local changes in chemistry or in charge distribution we performed a hard x-ray photoelectron spectroscopy (HAXPES) study on the Ti/HfO$_2$/TiN system. Macroscopic 0.5 x 0.5 mm^2 large specimens of RRAM device cells structured as shown as in Fig.1, which are typically 1x1 μm^2 in size in functional devices prepared in the clean room facility of our institute, were specially prepared for this *in situ* biasing experiment.

The multilayered sample was set *in situ* at specific points of the I-V curve shown in Fig. 2 by means of a commercial semiconductor analyzer. Using the homemade setup shown in Fig. 3, high-resolution core level XPS spectra were recorded at 7 keV photon energy with a total energy resolution of better than 300 meV. Fig.4 shows spectra taken for the Ti 2*p* level. We will present a detailed discussion of the experimental results.

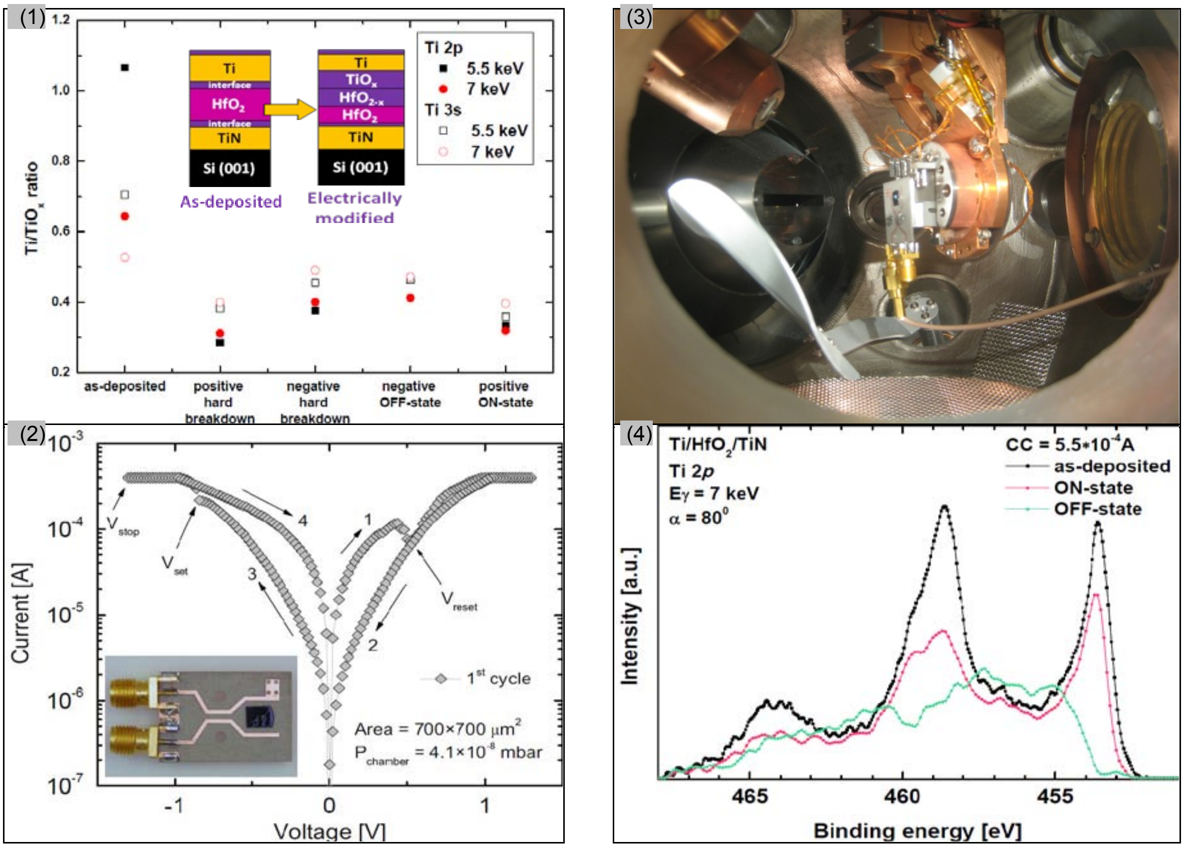

Fig.1 Ti/TiO$_x$ XPS intensity ratio for the MIM structure at specific points of the I-V-curve, (2) I-V curve of Ti/HfO$_2$/TiN cell obtained during the *in-situ* HAXPES measurements. Inset presents top view of the sample holder, (3) *In-situ* HAXPES setup, (4) Ti 2*p* HAXPES spectra taken for different resistance states of the Ti/HfO$_2$/TiN, while current compliance was set at 55 mA.

HAXPES CHARACTERISATION OF HIGH-K DIELECTRIC METAL OXIDE SEMICONDUCTOR STRUCTURES ON InGaAs SUBSTRATES

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The aim of this study was to use synchrotron radiation based hard x-ray photoelectron spectroscopy (HAXPES) measurements to study the intrinsic electronic properties of high-k dielectric metal oxide semiconductor (MOS) structures on InGaAs substrates. Lattice matched 0.2 µm thick $In_{0.53}Ga_{0.47}As$ layers, with both n and p doping (~$4x10^{17}$ cm^{-3}), were grown by MOCVD on InP n^+ and p^+ substrates, respectively. Hafnium oxide dielectric layers 5nm thick were then deposited ex-situ by atomic layer deposition (ALD) on the native oxide and ammonium sulphide treated InGaAs surfaces. MOS structures were prepared with both high (Pt) and low (Al) workfunction metal layers 5nm thick on these differently prepared surfaces. CV and IV measurements were also preformed on an identical sample set where the top metal contact was 115nm thick to facilitate electrical measurements. HAXPES measurements using a photon energy of 3578 eV were used to probe the MOS structures in order to investigate the differences in InGaAs core level binding energies caused by changes in doping type, surface preparation and metal workfunction. The sampling depth for these high energy photons was sufficient to detect core level peaks originating from the InGaAs substrate.

The binding energy of core levels in photoemission are referenced with respect to the Fermi level, therefore changes in the binding energy of a particular core level reflect differences in the position of the Fermi level in the semiconductor band gap. Binding energy measurements for the core levels of native oxide covered n-type doped InGaAs substrates with no metal cap were found to be consistently (~0.3eV) higher than p-type samples reflecting the fact that the Fermi level is in a different position in the band gap. These differences were lower (~0.15eV) for sulphur passivated samples than for the native oxide covered InGaAs surfaces. Variations in the binding energy and full width half maximum (FWHM) of the InGaAs core levels consistent with the differences in the workfunction of the Al and Pt caps and band bending in the InGaAs were detected. The FWHM of the Hf 3d core level for the Pt capped sample was ~0.2 eV greater than for the Al capped sample, consistent with a larger potential drop across the dielectric layer for the higher workfunction metal (1). As the escape depth of the photoemitted electrons is greater than the thickness of the dielectric stack, it is possible to detect valence band emission from all three layers, as shown in figure 1 where the Al/HfO_2/InGaAs spectrum is compared with that from HfO_2/InGaAs. Analysis of these spectra will be undertaken to extract the valence band offsets for the differently prepared surfaces. RMW acknowledges the support for this work under NSF award No. ECCS-0925844.

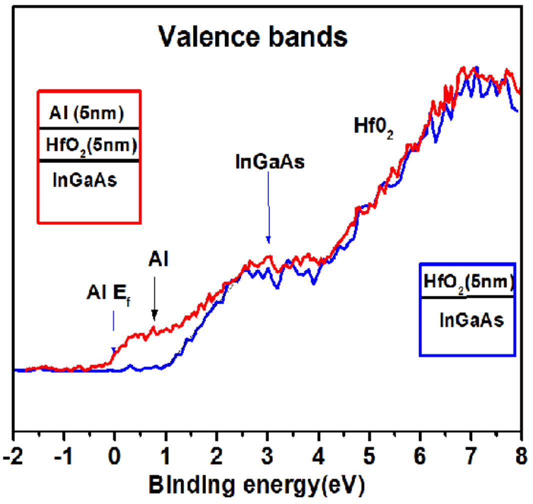

Figure 1 Valence band spectra acquired at 3578 eV photon energy showing valence band offsets in the HfO_2/InGaAs and Al/HfO_2/InGaAs structures

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HIGH TEMPERATURE ELECTRONIC AND SPIN STATES OF $LaCoO_3$: A HAXPES STUDY

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Strongly correlated transition metal oxides exhibit a wealth of interesting phenomena. Understanding the fundamental mechanisms in these materials is essential for a future use of their special properties in applications. Until recently, photo electron spectroscopy measurements were only performed at and/or below room temperature because these compounds suffer from surface oxygen loss at high temperatures which leads to distorted spectra. The increased probing depth of HAXPES allows us to look at the high temperature phases without significant contributions of oxygen deficient surface regions. By going to high temperatures it is possible to investigate disordered phases and to switch off different correlations.

$LaCoO_3$ has attracted considerable interest because of its unconventional magnetic properties which are interpreted in terms of a thermally induced spin state transition from a non-magnetic low-spin (LS) ground state to a paramagnetic finite spin state. The nature (intermediate- (IS) versus high- (HS) spin state scenario) of the thermally excited spin state of the Co^{3+} ions have been heavily debated for many years. Here we present valence band and Co 2*p* core level spectra for a wide range of temperatures giving direct experimental evidence for a LS-to-HS transition.

THE ELECTRONIC STRUCTURE OF MULTIFERROIC $BiFeO_3$ FROM HIGH ENERGY X-RAY PHOTO-ELECTRON SPECTROSCOPY AND FIRST PRINCIPLES THEORY

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BiFeO3 (BFO) is a multi-functional material with promise for a variety of applications enabled by the high ferroelectric and magnetic ordering temperature of BFO. For applications, fundamental understanding of the BFO electronic properties is a prerequisite. In this work we have investigated the electronic structure of (001) oriented 100nm rhombohedral BFO thin film [1] using high energy X-ray photoelectron spectroscopy (XPS). Additionally we performed ab inito calculations within the framework of QSGW method [2]. By making use of the variation of the relative cross sections for different valence states as a function of excitation energy in the range of 2-6 keV, we were able to selectively probe the elemental contributions to the valence band, i.e., Bi and Fe and O contributions. At high energies, states with high main quantum number will have a higher relative cross section for photo-ionization. This means that the Bi 6s and 6p contributions in the valence region are enhanced relative to the Fe 3d and O 2p contributions at higher excitation energy. Our data suggests that the Bi 6p states hybridize strongly with the valence band dominated by the Fe 3d and O 2p states. The hybridization results in a splitting of the 3d states due to bonding and anti-bonding combinations with the Bi 6p states. It is anticipated that this interaction will have decisive impact on the physical properties of the material, and that this hybridization is also a route to tune the properties of Bi-transition metal oxides by selective doping. Our results thus suggest that an previously relatively ignored electronic interaction needs to be considered when describing the BFO and related TM oxides with Bi like BiMnO3. Our results are corroborated with first principle calculations and we can conclude that including electron correlation beyond the local density approximation accounts for the experimental findings, indicating the importance of screened Coulomb correlations to describe Bi and Fe electronic states.

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P18

HARD X-RAY PHOTOELECTRON SPECTROSCOPY OF $LaVO_3/SrTiO_3$-HETEROSTRUCTURES

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At the interfaces of epitaxial grown heterostructures consisting of insulating oxides novel phases with unexpected properties may be generated. E.g., for $LaAlO_3/SrTiO_3$ (LAO/STO) a conducting interface is found if more than four monolayers (ML) of LAO are grown on STO. As possible explanations electronic reconstruction, but also extrinsic causes like oxygen vacancies are discussed.

Very similar to this extensively studied hybrid system, a thickness induced phase transition from conducting to insulating is triggered, if more than 10 ML $LaVO_3$ (LVO) are grown on STO. Here the overlayer is a Mott, instead of a band insulator as in LAO/STO. As also instrinsic cause, electronic reconstruction has been discussed as driving mechanism.

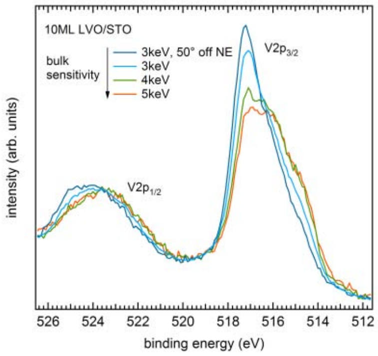

Fig. 1: Angle dependent V2p core level spectra of a 10ML LVO/STO sample

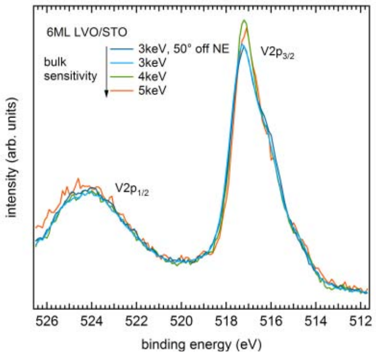

Fig. 2: Angle dependent V2p core level spectra of a 6ML LVO/STO sample

We performed depth profiling on LVO/STO by varying the photon energy and the detection angle. The V 2p core level is displayed for a 10ML (conducting) and 6ML (non-conducting) sample in Fig. 1 and Fig. 2, respectively.

The spin-orbit-split V2p core level shows a clear angle dependence for the 10ML sample. In contrast, the 6ML sample shows no angle dependence at all. Analyzing the V 2p3/2 core level of the 10ML sample in more detail, a transfer of spectral weight to the lower binding energy side was observed for more interface-sensitive measurements. This could be a hint for extra mobile electrons hosted by the V3d shell at sites near the interface as this behavior was only found for the conducting samples.

At variance with the LAO/STO system , however, no Ti3+ signature can be seen indicating that no extra electrons seem to reside at Ti sites. Instead the line shape seems to be asymmetric compared to LAO/STO and pure STO. Angle dependent measurements show that the asymmetry increases for more surface-sensitive measurements. As Ti 2p is a substrate core-level the asymmetry is biggest close to the interface. This could be interpreted as a band bending effect.

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ELECTRONIC STRUCTURE OF NEWLY DISCOVERED Yb-COMPOUNDS YbNi$_3$X$_9$ (X= Al, Ga) STUDIED BY HARD X-RAY PHOTOEMISSION SPECTROSCOPY

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Rare-earth compounds which have strongly correlated 4f electrons show various physical properties such as heavy-fermion behavior, non-Fermi liquid states, unconventional superconductivity and valence fluctuations. Recently, Ohara *et al.* have succeeded in synthesizing brand-new Yb-compounds, YbNi$_3X_9$ (X= Al, Ga) with trigonal ErNi$_3$Al$_9$-type structure.[1,2,3] YbNi$_3$Al$_9$ is a heavy-fermion antiferromagnet with a Néel temperature of T_N=3.4 K. On the other hand, YbNi$_3$Ga$_9$ is a mixed-valence compound in spite of its similar structure to YbNi$_3$Al$_9$ and substitution of Al by iso-valent Ga.[2] To reveal the difference of physical properties between these two compounds in terms of electronic structure, we have carried out hard x-ray photoemission spectroscopy (HAXPES).

HAXPES experiments with hν= 5.95 keV were carried out at the undulator beamline BL15XU of SPring-8. The total energy resolution was set to 150 meV. Single crystals of YbNi$_3X_9$ (X= Al, Ga) were synthesized by the flux-method. Clean surfaces of the samples were obtained by fracturing in situ.

The Yb 3d HAXPES spectra of YbNi$_3X_9$ measured at 300 and 20 K are shown in Fig.1. In the spectra of YbNi$_3$Ga$_9$, both Yb^{2+}- and Yb^{3+}- derived structures are observed, indicating its strong valence fluctuation in this compound. With lowering temperature, the intensity of Yb^{2+}- (Yb^{3+}-) structure gradually increases (decreases). The estimated Yb valence (z) is z~2.6 at 20 K. In the spectra of YbNi$_3$Al$_9$, on the other hand, the intensity of Yb^{2+}- structure is significantly weak, and, in comparison with the case of YbNi$_3$Ga$_9$, the spectrum shows almost no temperature dependence with z~3.0. We also observed that the Ni 2p core level shifts toward the lower binding-energy side on going from X= Al to Ga. Furthermore, similar behavior is observed in the Ni 3d structure in the valence-band spectra. These results indicate that not only conduction electrons from Al/Ga which is the nearest neighbor of Yb, but also those from Ni contribute to the c-f hybridization and the difference of physical properties between YbNi$_3$Al$_9$ and YbNi$_3$Ga$_9$.

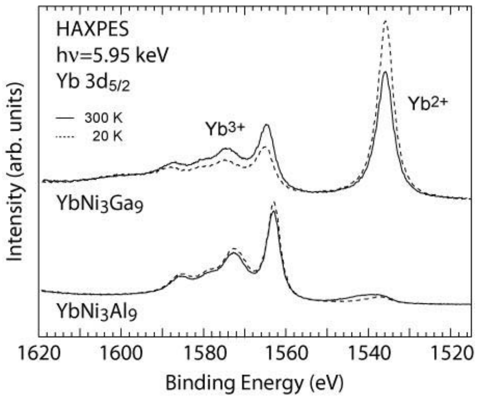

Fig1. Yb 3d$_{5/2}$ HAXPES spectra of YbNi$_3X_9$ (X= Al, Ga) at 300 (solid lines) and 20 K (dashed lines).

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LOCAL CORRELATIONS, NON-LOCAL SCREENING, MULTIPLETS, BAND FORMATION, AND NEAREST NEIGHBOR SPIN-SPIN CORRELATIONS IN NiO

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NiO is an antiferromagnetic insulator with T_N=523K and is considered a benchmark system in solid state physics. Its photoemission spectrum has been employed to critically test the accuracy of the different theoretical approaches used to describe the electronic properties of the system. Both Ni 2*p* core level and valence band have a characteristic double peak structure which cannot be explained with a local picture. Even recent (single-site) DMFT calculations cannot reproduce the line shape of valence band spectra. Here we report a clear change in the peak splitting in both Ni 2*p* core level and valence band spectra across T_N indicating that the origin of the double peak is related to the antiferromagnetic order and thus indeed a non-local screening effect.

Furthermore we have studied NiO impurities in MgO films and we have been able to determine reliably the parameters which describe the local correlations, thereby establishing the compensated-spin character of the first ionization state or the state created by hole doping. Using these parameters in a multisite cluster model we are able to reproduce nicely the double peak structure of the bulk NiO spectrum.

P21

ELECTRONIC STRUCTURE ANALYSIS OF $Pr_{1-x}A_xCo_{3-\delta}$ (A = Sr and Ca)

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Rare-earth cobaltates $RCoO_3$ (R = rare-earth ions) have been extensively studied, because they have unique electronic and magnetic properties such as colossal magnetoresistance and metal-insulator transition, when alkaline-earth ions were substituted at rare-earth site, i.e, $R_{1-x}A_xCoO_{3-\delta}$ (A = alkali-earth ions) [1-3]. It is essential to know the electronic structures of vallence and conduction bands of these materials to understand such properties. When the alkaline-earth ion is incorporated into $PrCoO_3$, one or both of the followings should occur to keep the system electrically neutral, i) Co and/or Pr ions controls charge balance of the system, i.e., $Co^{3+} \rightarrow Co^{4+}$ or $Pr^{3+} \rightarrow Pr^{4+}$, ii) oxygen vacancy is created. However, these mechanisms of charge compensation have not yet been fully investigated for these materials. Then the electronic structure analysis of valence and conduction bands of $Pr_{1-x}Sr_xCoO_{3-\delta}$ and $Pr_{1-x}Ca_xCoO_{3-\delta}$ are systematically carried out here by the X-ray photoemission spectrum (XPS) and the X-ray absorption near-edge structure (XANES) measurements.

All the samples were synthesized by the conventional solid-state reaction method. Co-K and Pr-$L_{2,3}$ XANES spectra were collected at BL01B1 in SPring-8 by the conventional transmission method and Co-$L_{2,3}$ XANES spectra were collected at BL4B in UVSOR by the total electron yield method. The XPS spectra of O-1s and valence band were collected by JPS-90SX (JEOL) using Mg-Kα X-rays. All the samples were confirmed to be single-phased orthorhombic perovskite structures (Pbnm) by the X-ray diffraction (XRD) measurements.

Observed Co-L_3 XANES spectra of $Pr_{1-x}Sr_xCoO_{3-\delta}$ are shown in Fig. 1, which were deconvoluted into four peaks using the Gaussian function. The fine structure of Co-L_3 XANES spectra of $Pr_{1-x}Sr_xCoO_{3-\delta}$ changes depending upon the concentration of doped Sr^{2+} ions, i.e., intensity of peak A increases as increment of doped Sr^{2+} concentration. The O-1s and valence band XPS and Co-K XANES spectra also chanegs in accordance with the doped Sr^{2+} concentrations. On the other hand, Pr-$L_{2,3}$ XANES spectra are almost identical when doped Sr^{2+} concentration changes. These experimental results suggest that charge state of Co ions in $Pr_{1-x}Sr_xCoO_{3-\delta}$ changes continuously as increment of Sr concentration, while that of Pr ions do not change. Other experimental results will be shown on site.

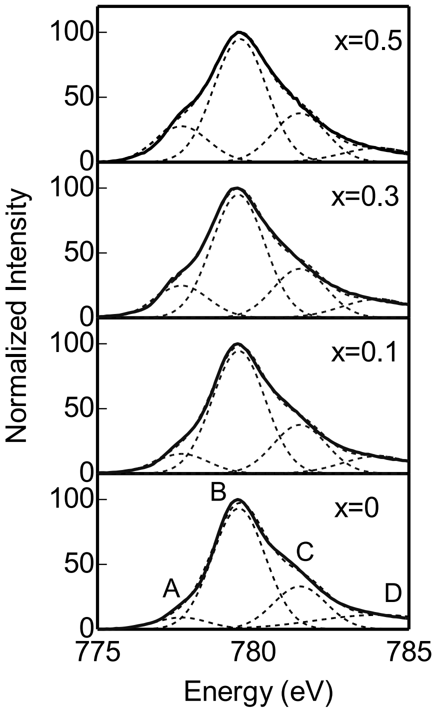

Fig1. Observed Co-L_3 XANES spectra of $Pr_{1-x}Sr_xCoO_{3-\delta}$.

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P22

INTERFACE CHARACTERIZATION OF ALL-HEUSLER GMR MULTILAYER STRUCTURES

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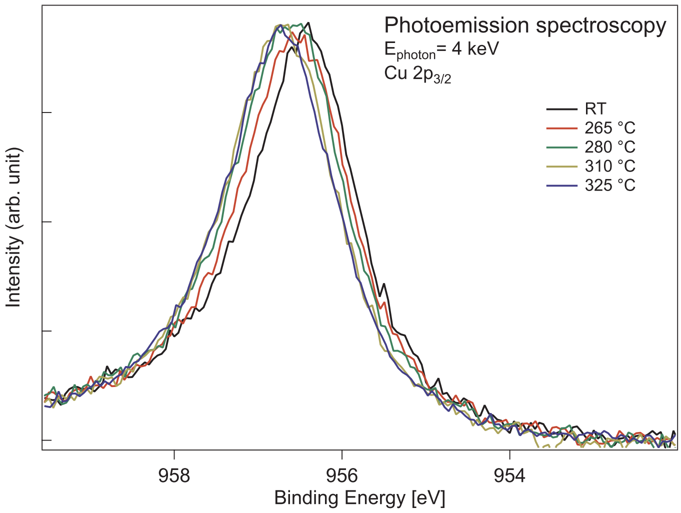

Fig 1. *Cu 2p shifts to higher binding energies as the intermixing of multilayers increases due to annealing.*

Current-perpendicular-to-plane (CPP) giant magneto-resistance (GMR) heads based on specially designed ternary Heusler alloys have been found to be a potential alternative to current tunnel magneto-resistance (TMR) based technology, which has complications arising from overall resistance when downsizing the TMR sensor. Read heads based on alternating layers of magnetic (Co2MnGe) and non-magnetic (Rh2CuSn) Heusler alloys have been shown to be promising for magnetic recording reader applications with an MR of 7 % and RA of 4 mΩμm2 [1]. This combination of ferromagnetic and non-magnetic Heusler alloys were proposed by Ambrose and Mryasov [2] to maximize interface spin asymmetry by the right band matching at the interfaces. A determining factor for the performance of a CPP-GMR device is the ability to achieve high spin polarization which is in reality limited by defects and specific details of the interface structure regarding roughness and intermixing. It is therefore essential to understand the nature of the interfaces between the ferromagnetic and non-magnetic layers. We have used high kinetic energy photoemission to investigate the chemical roughness and the degree of intermixing [3] depending on preparation conditions and post-annealing conditions for a set of all-Heusler GMR-type structures. We find that the sensitivity of the GMR structure to post-annealing is strongly dependent on the thickness of the magnetic layer. At the important annealing temperature used for establishing the pinning layer in spin-valve structures, XMCD does not only show a change but also different behaviors of the magnetic constituents as the layer thicknesses are varied. These results are further corroborated with resonant magnetic scattering and neutron reflectivity data obtained for similar post annealing conditions, which allows us to specifically address magnetic interface properties. We also have performed broad-band ferromagnetic resonance experiments to investigate the correlation between interface properties and the damping parameter of the spin resonance dynamics. We employ the WKB model and first-principles calculations [1] to investigate the role of the observed disorder on the spin dependent interface scattering.

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MAGNETIC DICHROISM IN ANGLE-RESOLVED HARD X-RAY PHOTOEMISSION FROM BURIED LAYERS

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This work reports the measurement of magnetic dichroism in angular-resolved photoemission from in-plane magnetized buried thin films. The high bulk sensitivity of hard X-ray photoelectron spectroscopy (HAXPES)[1,2] in combination with excitation by circularly polarized X-rays makes this method to be a unique tool for investigation of the electronic and magnetic structure of deeply buried layers and interfaces [3].

HAXPES experiments with excitation energy of 8 keV were performed on two different types of exchange-biased structures with epitaxially grown CoFe and Co_2FeAl ferromagnetic layers. In the on-top sample arrangement the topmost pinned magnetic layer was CoFe on top of $Ir_{78}Mn_{22}$ pinning layer. The on-bottom configuration was realized with Co_2FeAl underneath $Ir_{78}Mn_{22}$. Both structures were protected with thin oxide capping layer.

It was shown that IrMn exchange-biasing layers keep thin films of CoFe or Co_2FeAl remanently magnetized in a well-defined direction. A pronounced magnetic dichroism is found in the Co and Fe 2*p* core levels of CoFe and deeply buried Co_2FeAl and the asymmetries up to 58% detected. The localization of the magnetic moments at the Fe site conditioning the peculiar characteristics of the Co_2FeAl Heusler compound, predicted to be a half-metallic ferromagnet, is revealed from the magnetic dichroism detected in the Fe 2*p* states.

Financial support by Deutsche Forschungsgemeinschaft and the Strategic International Cooperative Program of JST (DFG-JST: FE633/6-1) is gratefully acknowledged. We are thankful to the Japan Synchrotron Radiation Research Institute (JASRI) for the support of experiments within approved 2009B0017 proposal. The team of Hokkaido University acknowledges the support of MEXT, Japan (Grants-in-Aid 20246054, 21360140 and 19048001). X.K. acknowledges the support of the graduate school of excellence MAINZ.

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P24

VALENCE STATES OF OFF-STOICHIOMETRIC THIN FILMS BASED ON THE HEUSLER COMPOUND Co_2MnSi

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This work reports on high resolution high energy photoelectron spectroscopy of the valence states of buried off-stoichiometric $Co_2Mn_\alpha Si$ thin films. Being a half-metallic ferromagnet, $Co_2Mn_\alpha Si$ exhibits distinctive transport properties and provides a perfect spin-polarized electrical current that is of a great importance when being used in high-performance spintronic devices. This behaviour of such Heusler compounds is determined by their intrinsic electronic structure in the vecinity of the Fermi energy [1,2]. Hard X-ray photoemission spectroscopy with excitation energies of about 3.24 keV and 7.94 keV was applied as a non-destructive bulk probing technique for investigation of the electronic structure of the thin films [3,4]. The changes of the density of states upon variation of the Mn content in $Co_2Mn_\alpha Si$ thin films investigated experimentally were compared to ab-initio calculations. Both present experimental and theoretical results agree well with the previous studies and the proposed composition formula. Sputter deposition of $Co_2Mn_\alpha Si$ together with co-sputtering of Mn is shown to be an appropriate method to tune the composition of such ferromagnetic layers and thus their electronic structure. This technique provides the possibility to vary the features of the electronic band structure within the valence band and, as a direct consequence, the magnetoresistive characteristics of Co_2MnSi based tunnel junction.

The financial support by Deutsche Forschungs Gemeinschaft (DFG) and the Japan Science and Technology Agency (JST) (grant no.: FE633/6-1) is acknowledged. The Mainz group greatfully acknowledges the support by DFG (TP 1.2-A and TP 1.3-A of the Research Unit 1464 *ASPIMATT*), the Hokkaido University group acknowledges the support by a Grantin-Aid for Scientific Research (A) (Grant No. 20246054) from the MEXT, Japan, and by the Strategic International Cooperative Program of JST. The synchrotron radiation HAXPES measurements were performed at BL47XU with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (Long-term Proposal 2008B0017, 2009A0017) and at BL15XU with the approval of NIMS (Nanonet Support Proposal 2008B4903). The HAXPES experiment at BL15XU was partially supported by the Nanotechnology Network Project MEXT (Japan). X. K. acknowledges the support by the graduate school of excellence MAINZ.

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P25

SYMMETRY OF VALENCE STATES OF HEUSLER COMPOUNDS EXPLORED BY LINEAR DICHROISM IN HARD X-RAY PHOTOELECTRON SPECTROSCOPY

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The linear dichroism in the angular distribution (LDAD) of photoelectrons has attracted considerable interest as a powerful probe to study the symmetry, orientation, and alignment phenomena in photoionization. Thus far, most studies dealing with LDAD have been based on soft radiation in the range from the vacuum ultraviolet region (ultraviolet photoelectron spectroscopy, UPS) to the soft X-ray region (X-ray photoelectron spectroscopy, XPS), resulting in a very limited probing depth that is suitable only for the examination of surface effects. Therefore, LDAD from real 3D bulk states has not yet been observed.

This study reports on the linear dichroism in angular-resolved photoemission from the valence band of a Gold single crystal as well as the Heusler compounds NiTi0.9Sc0.1Sn and NiMnSb. High-resolution photoelectron spectroscopy was performed with an excitation energy of hv = 7.938 keV. The linear polarization of the photons was changed using an in-vacuum diamond phase retarder. The use of hard X-rays for excitation together with the high kinetic energies of the emitted electrons affords the advantage of making all surface effects negligible. The valence band spectra exhibit the typical structure expected from first-principles calculations of the electronic structure of these compounds [Fig.1]. Noticeable linear dichroism is found in the valence band of both materials and this allows for a symmetry analysis of the contributing states. The differences in the spectra are found to be caused by symmetry dependent angular asymmetry parameters, and these occur even in polycrystalline samples without preferential crystallographic orientation [1].

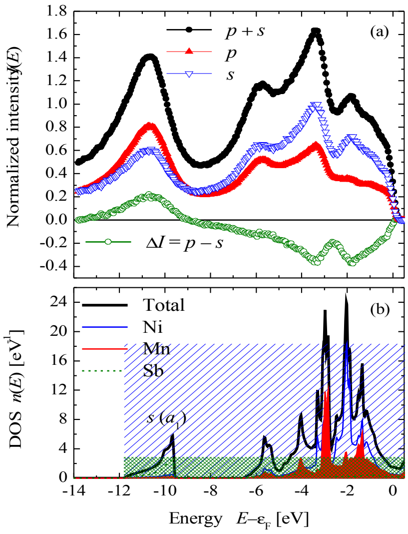

Fig1. Electronic structure and polarization dependent photoelectron spectra of NiMnSb. (a) Valence band spectra obtained with ***s*** and ***p*** polarized light together with the sum and difference and (b) total and partial density of states (DOS).

The authors gratefully acknowledge the financial support by the DFG (P 1.3-A in FOR 1464 ASPIMATT). The synchrotron radiation measurements were performed at BL-47XU with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (Proposal No. 2009B0017).

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SPIN POLARIMETRY IN HARD X-RAY PHOTOELECTRON SPECTROSCOPY ON BURIED MAGNETIC LAYERS

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Exploration of the electronic structure of buried ferromagnetic electrodes of tunneling magnetoresistive (TMR) junctions is of a great importance for the selection of optimal materials for TMR based devices. HArd X-ray Photoelectron Emission Spectroscopy (HAXPES) was proven to be a bulk sensitive probe of the electronic band structure [1,2] and provides the possibility to study the electronic structure of buried layers. Growing interest in search and development of spintronic materials requires spin resolved studies of their electronic structure. Thus, extension of HAXPES technique with a spin polarimeter enables the investigation of the spin-resolved electronic structure of buried layers and interfaces involved in spintronic devices. The spin-resolved HAXPES technique facilitates complete studies of electronic band structure resolving electron energy, momentum and spin degrees of freedom with rather high bulk sensitivity. Presently available spin-detection techniques are based on spin-dependence in electron scattering and diffraction originating from i) spin-orbit interaction and ii) exchange scattering. The reported spin-resolved ptotoelectron emission studies were performed up to now for the photoelectrons with kinetic energies of only UPS-XPS range implying a strong surface sensitivity. We report on the implementation of the first spin-resolved HAXPES experiment at BL47XU beamline (SPring-8) using SPLEED-type spin detector.

The spin-resolved HAXPES experiment has been performed on an exchange-biased $Co_2FeAl_{0.5}Si_{0.5}$ (CFAS) buried magnetic layer shown to be a half-metallic Heusler alloy with a high spin-polarization. The measurements prove that a spin polarization of about 50% is retained during the transmission of the photoelectrons through a 3 mm thick oxide capping layer. The reported spin-resolved spectra agree well with the features of magnetic circular and linear dichroism in photoelectron emission. One can elucidate the magnetic states from the magnetic dichroism measurements providing much higher detecting efficiency [3] than achieved in spin-resolved measurements with a spin detector. However, this does not exclude the necessity in direct spin-resolved measurements with spin detectors. The information content of the spin polarization and magnetic dichroism signals are different and their combination provides a detailed insight into the dynamics of photoemission from a ferromagnetic material. The reported Spin-HAXPES experiment paves the way to spin-resolved spectroscopy of buried layers and buried interfaces, issues being inaccessible by the classical low-energy approach.

Financial support by DFG-JST (FE633/6-1) is gratefully acknowledged. The experiments at BL-47XU (Spring-8) were performed within the proposal (2009B0017) approved by JASRI. X.K. acknowledges the support of the graduate school of excellence MAINZ.

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P27

SPIN DEPENDENT CORE HOLE SCREENING OF 2p AND 3s PHOTOEMISSION IN FERROMAGNETIC TRANSITION METALS

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We discuss the 2p and 3s core level x-ray photo emission spectroscopy (XPS) in ferromagnetic transition metals Fe, Co, and Ni. We calculate the spectra using a band structure calculation based on the local density functional approximation. The method is an extension to the ab initio level of that Feldkamp and Davis adopted for analyzing the 6eV satellite in the Ni 2p XPS [1].

It is well known that the 3s spectra in the majority spin channel exhibit the specific strong satellite intensity. On the other hand, in the minority spin channel the 3s spectra show almost single peak structures in these metals. In contrast to the 3s excitation, the Fe 2p spectra do not show remarkable satellite intensity while the Ni 2p spectra show the notable 6eV satellite. These behaviors depending on spin channels, excited cores, and elements relate with the spin dependent core hole screening by the conduction electrons.

In the calculation we assume that the initial and the final states are described by the single Slater determinant wave functions which consist of the Kohn-Sham one electron wave functions. The one electron wave functions for the final states are calculated with keeping a core hole at a photo excited site. In order to simulate the photo excited states, we adopt super cell approximation where one core hole exists in each cell. The obtained self-consistent state may be considered as the fully screened (relaxed) state with a core hole. The one electron wave function for the initial state is also calculated using the super cell with no core holes. The spectral intensity is calculated exploiting Fermi's golden rule. The overlap integrals are evaluated using the one electron wave function.

We show the calculated Fe 2p, Fe 3s, Ni 2p, and Ni 3s spectra in the majority spin channel in figure 1. We do not include the spin-orbit interaction. The calculation well reproduces the spin channel, excited core, and element dependences of the spectra. Although the satellite appears around 6eV higher energy region from the threshold in the experiments, the calculation gives that around 4eV. This might result from the longer screening time constant in Ni than in Fe [2]. The fully screened state might not be proper for the final state of the Ni core level XPS. We discuss the behaviors of the line shapes in terms of the difference in the one-electron states screening the core-hole potential.

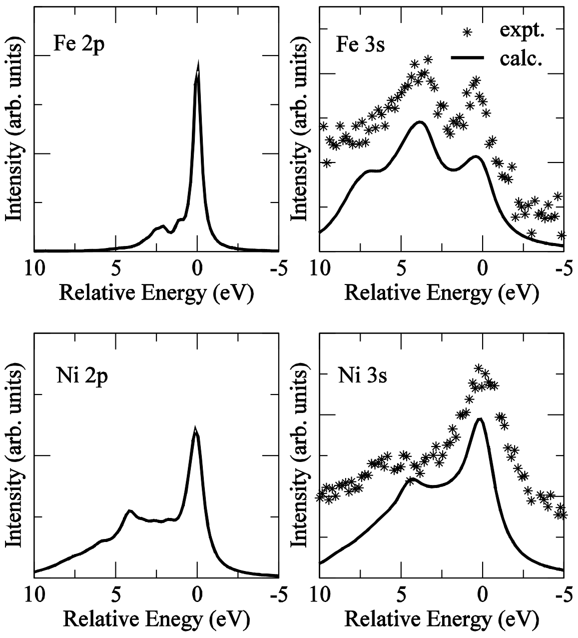

Figure 1: Calculated spectra corresponding to the 2p and 3s core level XPS in Fe and Ni for majority spin channel. Spin orbit interaction is not included.

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P28

EXPLORATION OF "IN GAP" STATES OF THERMOELECTRIC HEUSLER COMPOUNDS BY MEANS OF HARD X-RAY PHOTOELECTRON SPECTROSCOPY

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Hard x-ray photoelectron spectroscopy HAXPES became a powerful tool to investigate the bulk electronic structure of materials in a variety of applied fields such chemistry, physics, materials science, and industrial applications [1]. Several studies using high-resolution HAXPES have been realized, at solids (e.g. to study valence transitions in bulk systems) as well as multilayer systems and the valence band of buried thin films.

The XYZ Heusler compounds (X, Y transition metals, Z main group element) crystallize in the cubic MgAgAs-type structure (F-43m, $C1_b$). Most of those with 18 valence electrons in the primitive cell exhibit a closed shell type behavior with filled bands and therefore are found to be semimetals or semiconductors. They are considered to be promising thermoelectric materials. The conductivity and Seebeck coefficients, as key quantities of the thermoelectric properties, are controlled by the electronic states close to the Fermi energy ε_F.

This study reports on high resolution photoelectron spectroscopy of the valence states of substituted Heusler Compounds $NiTi_{1-x}M_xSn$ and $CoTi_{1-x}M_xSb$ (M= Zr, Hf, Sc, V) to examine the influence of electron- and hole-doping on the transport properties of the compounds. The HAXPES measurements were performed at BL15XU and BL47XU of Spring8.

Figure 1(a) shows the valence band spectra of compounds with selected composition. Already for the pure parent compound massive "*in gap*" states are observed (Fig. 1(b)). The present study proves that the electronic states close to ε_F play the key role on the behavior of the transport properties [2]. Especially, they are responsible for the high power factor, conductivity, and Seebeck coefficient of the compound.

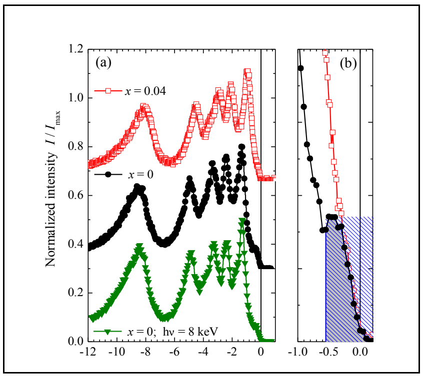

Fig1 : Valence band spectra of $NiTi_{0.3-x}Sc_xZr_{0.35}Hf_{0.35}Sn$ (x=0, 0.04). The *in gap* states are marked by the shaded area in (b).

The authors gratefully acknowledge the financial support by Federal Ministry of Economics and Technology (Grant No.0327876D thermoHEUSLER) and Stiftung Rheinland Pfalz für Innovation (Project No. 863). The synchrotron radiation measurements were performed at BL15XU with the approval of NIMS (Nanonet Support Proposal No. 2010A4903) and at BL47XU with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (Proposal No. 2009B0017).

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P29

HAXPES CHARACTERISATION OF THE nm-THICK PROTECTING OXIDE LAYER ON NEW Al-Cr-Fe COMPLEX METALLIC ALLOYS

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Al-Cr-Fe Complex Metallic Alloys (CMA) are Al- based crystalline intermetallic phases characterised by large unit cells and very complex structures (hundreds atoms/unit cell) that show high corrosion resistance for pH's ranging from 0 to 14[1,2]. This remarkable corrosion behaviour can be combined with their additional low adhesion, low friction coefficient and low reflectivity and exploited in resistant "multifunctional" coatings. However, the influence of ageing of the nm-thick surface oxide (referred as passive film) in relation with the surface properties of Al-Cr-Fe CMA still needs to be fundamentally understood. Recently, single phase large grain single- or poly-crystals of the orthorhombic $Al_{80}Cr_{15}Fe_5$ (unit cell dimensions a = 12.5006 Å, b = 12.6172 Å and c = 30.6518 Å and 306 atoms) were prepared and their electrochemical behaviour characterised. The HAXPES technique has been found particularly suited for the study of the in depth composition gradients of the protecting passive oxide layer (approximately 5-8 nm thick) and of its buried metal/oxide interface. In order to probe different penetration depths, two excitation energies, 3 keV and 6 keV and different electron escape angles (30°, 45°, 58°) were used, exploiting the highest spectral resolution possible at ID32 beamline of ESRF[3]. HAXPES characterisation allowed proposing a model for the protecting oxide that is described by a stacking of Al and Cr oxy-hydroxide layers.

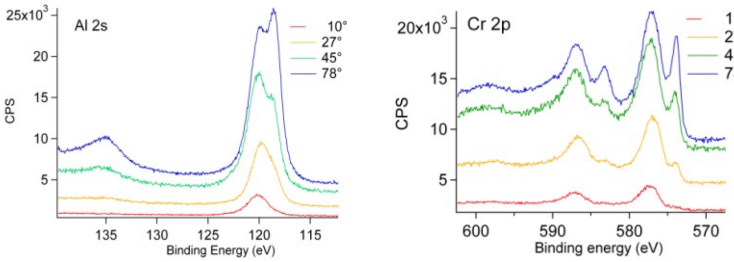

Figure *Al 2s and Cr 2p region of the alloy electrochemically treated and studied at 6 keV.* The structure/composition of the oxide layer after electrochemical treatment in very aggressive solutions (H_2SO_4 pH 0 and 2) and the behaviour of isostructural alloys having different composition will be discussed in detail, paying particular attention to the role of Cr content in the stability of the alloy .

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P30

SOFT X-RAY ANGLE-RESOLVED PHOTOEMISSION STUDY ON IRON PNICTIDE

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Since the discovery of superconducting state in an Iron-based layered material LaOFeP [1], Iron-based superconductors have attracted much attention because of the unexpected high transition temperatures [2]. The mechanism of superconducting state in Iron pnictides is considered to be different from high-T_c cuprates. In contrast to the two-dimensionality of Co-O plane in cuprates, optimally hole-doped $Ba_{1-x}K_xFe_2As_2$ (BKFA) has been reported to show the superconducting gap depending on k_z momentum [3]. Investigation of bulk three-dimensional electronic structure will provide therefore further understanding of physical properties of BKFA.

Soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) is one of the most promising methods to measure bulk band structure of materials due to the increase of probing depth and high k_z-momentum resolution. In this study, we have investigated the shape and k_z-dependence of the Fermi surfaces (FSs) in BKFA. The measurements were performed at SX-ARPES end station of ADRESS beamline in Swiss Light Source [4].

Figure 1 shows an experimental FS map of BKFA taken at $h\nu$ = 900 eV. The experimental FSs show in-plane shapes alternating between a circle-like and flower-like appearance when going from the Γ_0 point to higher Brillouin zones. Additionally, we observed modulations of FSs along k_z direction corresponding to periodicity of the Brillouin zones. All these effects show clear linear-polarization dependence reflecting orbital character of the bands forming the FS. These results provide with experimental information on the dimensionality and orbital character of FSs.

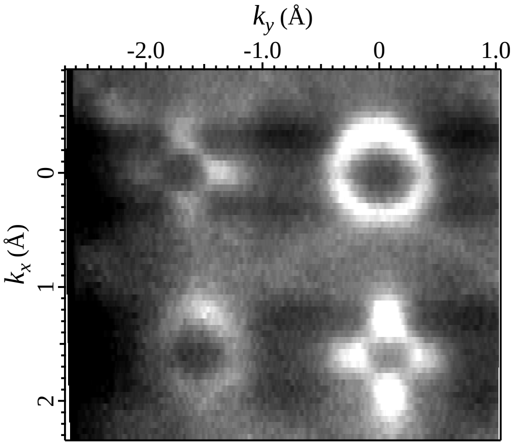

FIG.1 Fermi surface map of BKFA at 900 eV.

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P31

CORE DISORDER BROADENING IN PdAg (100) SURFACE ALLOYS

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One important issue in condensed matter physics is the role played by disorder on electronic and magnetic properties of solids. Materials are never perfectly ordered and some amount of disorder is always present which influences the local environment around atomic sites. Since core level photoemission is very sensitive to variations in the local electrostatic potential (initial state) and also relaxational contributions (final state), disorder effects may result in a significant broadening of core level lines[1]. This was first observed for the binary random Cu_xPd_{1-x} alloy system by Cole et al[2] and later also reported for several other random alloys[3]. The experimentally observed core disorder broadening (CDB) in various random alloys has been accounted for satisfactorily using model and *ab initio* calculations, whereas the anomalous core disorder broadening observed in PdAg(100) alloys[4] could not be satisfactorily explained[5].

PdAg(100) ordered surface alloys with compositions Pd_5Ag_{95}, $Pd_{15}Ag_{85}$, $Pd_{20}Ag_{80}$, $Pd_{25}Ag_{75}$ and $Pd_{30}Ag_{70}$ have been prepared *in situ* using the THE-XPS instrument at DORIS III wiggler beamline BW2 (DESY) by e-beam evaporation of Pd onto a clean Ag(100) single crystal kept at 250^{0}C. The surface alloy was investigated using hard X-ray photoelectron spectroscopy (HAXPES) and normal incidence X-ray standing wave (NIXSW) techniques. The Ag(200) reflection at 3034.8 eV was used for the NIXSW measurements; HAXPES data were obtained at the same photon energy. The total energy resolution was set to 0.45 eV. The Ag $3d_{5/2}$ spectra of pure Ag, $Pd_{15}Ag_{85}$ and $Pd_{25}Ag_{75}$ alloys are shown in Fig. 1. The lines exhibit a shift to lower B.E. with increasing Pd concentration. The inset shows the aligned spectra (relative to the $3d_{5/2}$ B.E. in Ag(100), i.e. 368.4 eV). Clearly, the width of the Ag $3d_{5/2}$ line increases with Pd concentration in the alloy. The Ag $3d_{5/2}$ line shape was modeled using Doniach–Sunjic (DS) functions broadened by a Gaussian to account for both instrumental and disorder broadening. Surprisingly, the CDB (0.66 eV) obtained for the 30% Pd ordered surface alloy is much larger than the CDB in the random bulk AgPd alloy. Single crystalline alloys are supposed to exhibit sharper core levels as compared to random bulk alloys. A change in composition with depth is ruled out as electron emission angle dependent spectra for Ag and Pd do not show any changes in relative intensity. Possibly, the extra CDB is contributed by strain in the surface alloys.

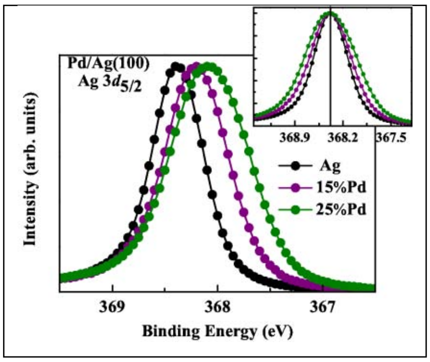

Fig 1. Core level shifts and CDB (inset) in PdAg alloys

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P32

CORROSION RESISTANCE OF Fe-Al ALLOYS: THE ROLE OF Cr

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The good corrosion resistance of Fe–Al alloys in oxidizing environments at high temperatures is due to the formation of highly stable protective Al oxide scale on the surface of the alloys. However, a high concentration of Al makes the alloys brittle. Therefore, the Al concentration in the bulk material needs to be reduced without weakening the high surface Al content. Chromium addition to Fe–Al is known to boost the Al driving force from bulk to the surface.

We have previously investigated the oxidation of Fe–Al and Fe–Cr–Al alloys in ambient conditions: by successive sputtering and Auger electron spectroscopy (AES) measurements of the oxidized surfaces, combined with theoretical considerations, it was possible to construct a model for possible oxidation related atomic processes in the metal-oxide interface region[1,2]. In addition, the boosting effect of Cr and the initial oxidation of Fe–Cr–Al at low oxygen pressure atmosphere were studied by X-ray photoelectron spectroscopy (XPS)[3]. By adding 10 at.% Cr to Fe–Al, the Al concentration in bulk can be reduced from 15 to 3 at.% without weakening the protective surface layer, and at the same time, the Al surface concentration was increased by 30 %[1-3]. It was found that the increased Al driving force is mainly due to bulk properties and thus insensitive to the type of the surface, e.g. whether it is metal or oxide[1,2]. In the present study we focused on the Al diffusion through the Fe|Fe–Al and Fe|Fe–Cr–Al interfaces. The theory predicts enhancement of Al diffusion when Cr is added to the alloy[2]. The use of high kinetic electron photoelectron spectroscopy (HIKE or HAXPES) provides a non-destructive way to study the interfaces and perform depth profiling.

The measurements were performed at the KMC-1 beamline in HZB-BESSY II, Berlin. Photon energies of 2500, 4000, and 7500 eV were used. The alloys examined were Fe10Al, Fe5Cr10Al, and Fe10Cr10Al (the bulk concentrations given as at. % in alloy formulas) with a thin layer of Fe on top of them.

The addition of Cr to the Fe-Al alloy increased the Al diffusion through the Fe|Fe-Cr-Al interface after heating the samples at 450 °C, as expected from the theory[2]. Figure 1 shows the concentration ratio of Al and Fe (estimated from the Al 1s and Fe 2p photoemission components) in the Fe-alloy interface region as a function of heating time.

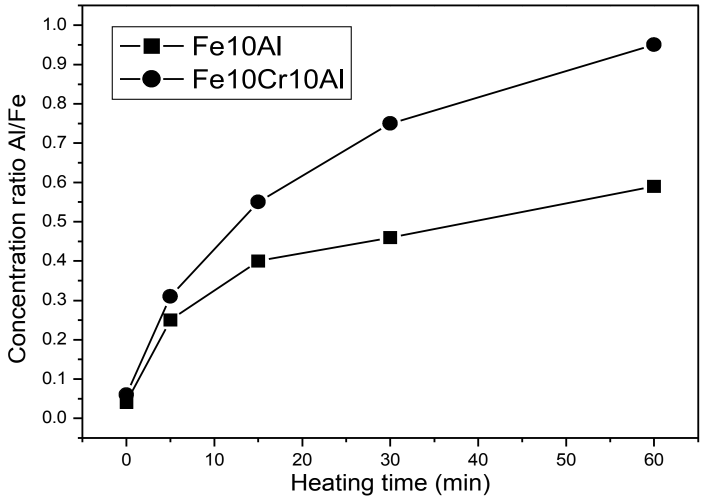

Fig1. Concentration ratios of Al and Fe as a funtion of heating time at 450°C at the interfaces Fe|Fe-Al and Fe|Fe-Cr-Al as taken from Al1s and Fe 2p photoemission components.

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HAXPES OF STRAINED $SrRuO_3$ THIN FILMS

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Transition metal oxides show a plethora of intriguing physical properties such as high-temperature superconductivity, colossal magnetoresistance, ferroelectricity, or multiferroicity [1]. Ferromagnetic metallic $SrRuO_3$ (SRO) films are of particular interest, since their perovskite crystal structure in combination with adequate electrical conductivity favor, e.g., an application as electrode material in novel oxide devices [2]. However, it was shown that the geometric, electronic, and magnetic properties of SRO films are very sensitive to the growth parameters [3]. For example, enhanced magnetization in strained SRO films has been reported [4]. This finding, in particular, make SRO films ideal candidates for studying magnetostriction effects, which play a key role in novel oxide–based magnetoelectric composites. These composites are studied in the SFB 855 with the specific long–term objective to build a magnetic field sensor with ultra–high sensitivity for medical applications.

For our investigations we prepared SRO thin films (5 nm) in different in-plane strain states. Static strain was induced to pulsed laser deposited (PLD) films by choosing single crystal substrates with a lattice mismatch between +2.2% ($SrTiO_3$) and -1.2% ($NdGaO_3$).

Performing Angle Resolved Photoelectron Spectroscopy (ARPES) as well as Hard X-ray Photoelectron Spectroscopy (HAXPES) we could clearly resolve changes in the electronic structure near the Fermi energy as well as corresponding variations in the binding energy of the Ru 3***d*** core levels (see Fig. 1). The measurements strongly indicate a boost of electronic correlation effects towards compressively strained films and will help to model the magnetic properties of strained SRO thin films. In future studies using piezoelectric $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTi0_3$ (PMN- PT) substrates strain can be tuned continously by applying an external voltage. This will allow a more detailed investigation of the interplay between strain and the electronic structure in SRO thin films.

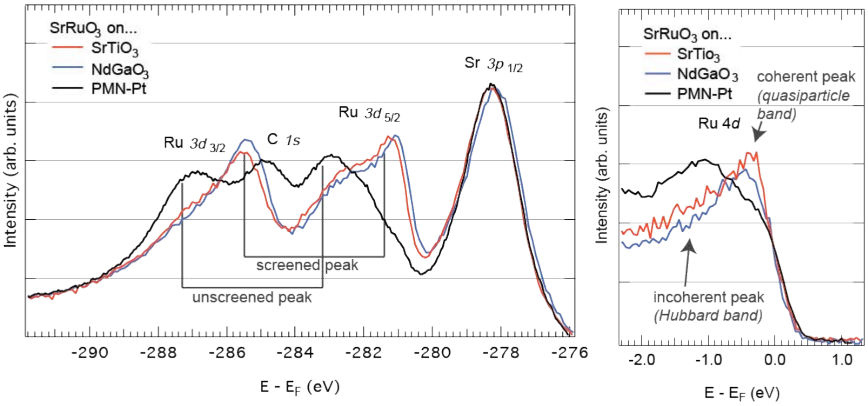

Fig1. Comparison of different in-plane strain states of SRO thin films. Compressive strain changes the spectral weight from the coherent screened to the incoherent, unscreened peak. [5]

The experiments were performed at beamline BW2 of HASYLAB (Hamburg). This work is funded by the DFG through SFB 855.

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COMPOSITION OF CuAu ALLOYS AND CHANGES UPON CORROSION INVESTIGATED BY HAXPES

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Metals and their alloys are of fundamental importance in industry and our daily life, but unfortunately highly susceptible to corrosion in wet or humid environment. Dealloying is a particular type of corrosion, attacking practically all metals in industrial use, which are usually alloys i.e., composed of metals of different “nobility”. When a metal alloy is coming into contact with an electrolytic solution, the less noble metal tends to dissolve, typically causing crack formation and subsequent material failure upon stress [1].

We used bulk sensitive HAXPES with an excitation energy of 6.0 keV as powerful tool to investigate the chemical composition of alloys and changes upon dealloying, studying Cu_xAu (with x = 4.1) alloy films of 9 to 50 nm thickness. HAXPES measurements were done at the ID32 beamline of the ESRF, Grenoble, France using monochromatic (energy resolution (ΔE/E) ~ 1.3 x 10^{-4}) and focused x-radiation from two undulators. A clean gold sample served as reference for the measured binding energies.

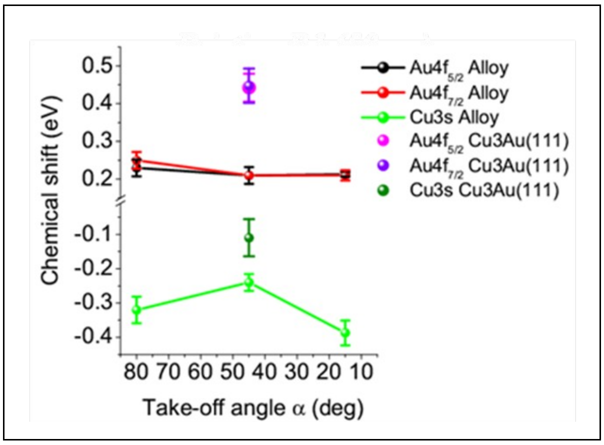

Fig1. Chemical shift of CuAu alloy as a function of Take-off angle.

The HAXPES analysis revealed that characteristic chemical shifts of metal core-levels, i.e. Au4f and Cu3s, can be used as a benchmark for the alloy composition. Figure 1 shows the determined binding energy shifts for a 50 nm thick alloy film before dealloying and in comparison the chemical shifts for a Cu3Au(111) single crystal sample. HAXPES data, recorded as a function of electron emission angle, which allowed depth sensitive determination of the chemical composition before and after dealloying in sulphuric acid, will be discussed in detail.

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P35

SPECTROSCOPIC FINGERPRINT OF ELECTRON LOCALIZATION IN THE ANOMALOUS METALLIC REGIME OF κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br

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Sulphur 2s core-level photoemission in the hard X-ray range (hν = 6keV, beamline P09 at PETRA III (DESY, Hamburg)) was employed as local spectroscopic probe in the ET-layer of the title compound. The large inelastic electron mean free path at such high photoelectron energies provides an information depth of >10nm, i.e. true bulk sensitivity. In this compound the BEDT-TTF (in short: ET) molecules arrange in layers with strong dimerisation. Each ET-dimer donates one electron to the counterion layer, leading to a half-filled band so that metallic behaviour is expected. The rich phase diagram allows to cross three different regimes (correlated good metal, anomalous metal and “ethylene liquid” range) just by varying the temperature (the superconducting state is below T_{min} of our setup).

The single-line S 2s spectrum at temperatures between 14 and 40K confirms the metallic behaviour found in conductivity measurements (regime of coherent transport). At the T* crossover at 45K the spectrum suddenly changes: The main line intensity drops and two additional signals occur that are indicative of electron localization. The “localization pressure” is caused by band-narrowing due to thermal lattice expansion. Electrons leaving the itinerant band state give rise to the “anomalous-metal regime” between 45 and 70K (see Fig1.).

At 75K the spectrum changes dramatically: the main-line intensity drops to about 50% of its initial value and a new, strongly shifted signal appears. This is the temperature of the thermal glass-like transition T_g where configurational switching of the ethylene groups in the ET molecules is activated. HAXPES results are compared with transport and thermal expansion data [1], fluctuation spectroscopy [2] and muon-spin relaxation measurements [3].

We will also discuss new results for a related family of compounds (TMTTF)$_2$X that undergo a charge-ordering transition. In this state we find charge residing at the surface for macroscopic times.

Funded by DFG, Transregio SFB TR 49.

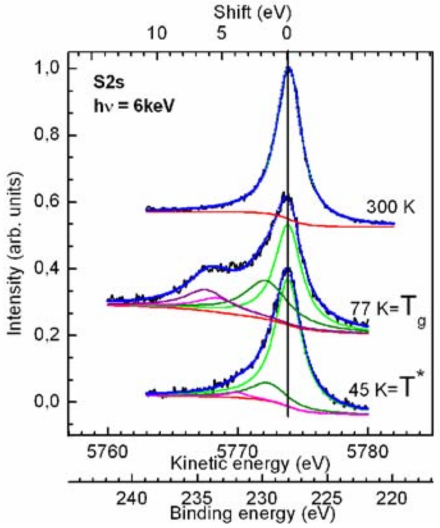

Fig1. Temperature series of sulphur 2s HAXPES core level spectra for the CT complex *κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br.*

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INVESTIGATIONS OF THE VALENCE BAND OF THERMOELECTRIC HEUSLER COMPOUNDS BY HIGH ENERGY PHOTOELECTRON SPECTROSCOPY

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Hard x-ray photoelectron spectroscopy HAXPES has emerged as a powerful tool to investigate the bulk electronic structure of materials in a variety of applied fields such chemistry, physics, materials science, and industrial applications. Several studies using high-resolution HAXPES have been realized on the valence band of bulk systems as well as multilayers and buried thin films.

Heusler compounds with a 1:1:1 composition crystallizes in the cubic MgAgAs-type structure (F-43m, $C1_b$). Most of those with 18 valence electrons in the primitive cell exhibit a closed shell type behavior with filled bands and therefore are found to be semimetals or semiconductors. They are considered to be promising thermoelectric materials. A key to control the electronic transport and thermoelectric properties of Heusler compounds is the electronic structure close to the Fermi energy ε_F. In particular, high conductivities and Seebeck coefficients, that both depend strongly on the states at ε_F, are needed to reach high power factors for power generator applications.

This study reports high energy valence band photoelectron spectroscopy on Heusler compounds. It was performed on the substituted compounds $Ti_{0.5}Zr_{0.25}Hf_{0.25}$ $NiSn_{1-x}Sb_x$ to examine the influence of anti-site disorder and doping on the transport properties. The high resolution HAXPES experiments were performed at the new undulator beamline P09 of PETRA III.

The measured valence states (see Figure 1) agree well with theoretical predictions. In addition, pronounced "*in gap"* states, those are states in the semiconducting gap, are observed already for the pure, parent compound. These states emerge from anti-site disorder and increase the conductivity by self-doping. They are influenced under substitution. This observation proves that the electronic states close to ε_F play a key role on the behavior of the transport properties. Especially, they are responsible for the high conductivity and Seebeck coefficient of the compounds.

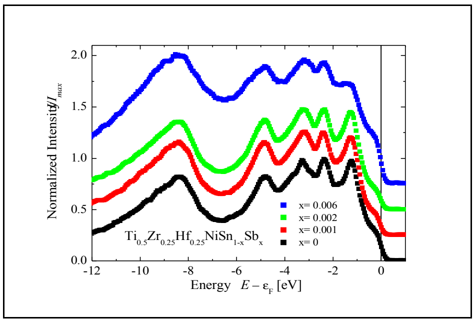

Fig1 : Valence band spectra of $Ti_{0.5}Zr_{0.25}Hf_{0.25}$ $NiSn_{1-x}Sb_x$ (x=0, 0.001, 0.002, 0.006).

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BULK-SENSITIVE PHOTOEMISSION STUDY OF FeSe AND RELATED COMPOUNDS

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Fe-based high-T_c superconductors have attracted enormous attention for their possibly new-type superconducting mechanism and the potential of breaking the deadlock in the high-T_c superconductor research field. A simple Fe-Se binary compound FeSe has been discovered to show superconductivity below 27 K under 1.5 GPa, which consists of the two dimensional Fe plane in the Fe_2Se_2 layer [1]. The appearance of superconductivity in the FeSe system indicates Fe_2X_2 (X=P, As, and Se) layer is essential for the superconductivity in Fe-based superconductors. The density functional study has pointed out that FeSe is not a conventional electron-phonon superconductor, being similar to $LaFeAsO_{1-x}F_x$ system [2].

We have performed the soft-x-ray and hard-x-ray photoemission spectroscopy (SXPES and HAXPES) of the FeSe superconductor and related compounds in order to quantitatively evaluate the electron correlation effect in the bulk. The SXPES and HAXPES have been widely recognized as the powerful techniques which can reveal bulk electronic structures due to the long inelastic mean-free path of photoelectrons excited by high-energy x-ray. It is found in the angle-integrated PES spectrum of FeSe that a large Fe 3d spectral weight is located in the vicinity of the Fermi level (E_F) and it decreases steeply toward E_F, being a similar feature to those in the other Fe-based superconductors non-doped LaFePO and $LaFePnO_{0.94}F_{0.06}$ (Pn=P, As). Considering the self-energy correction to the results of band structure calculations, the experimentally observed band narrowing and the energy shift of the band toward E_F are fully explained. The correction also provides the renormalization factor Z of C 0.28 and enables us to separate the incoherent part of the quasi-particle spectrum [3].

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IMMOBILIZED PALLADIUM CATALYSTS ON SULFUR-TERMINATED SUBSTRATE STUDIED BY HARD X-RAY PHOTOEMISSON

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The immobilization technology of highly efficient catalysts on a substrate is a key aspect of green chemistry to enable easy recycling of catalysts and small leaching of catalysts into product materials. We have recently found promising organopalladium catalysts immobilized on sulfur-terminated GaAs(001) [1,2] or Au [3]. Although sulfur often seems to be catalytic poison, sulfur contributes to the high performance of the catalysts in this work. We speculated that sulfur works as a binder at the junction of Pd and GaAs substrate (Pd-S-GaAs structure). We have carried out hard X-ray photoemission spectroscopy (HX-PES) measurements of this catalyst before and after catalytic reaction to reveal the mechanism of its high efficiency. HX-PES enables us to detect palladium and sulfur beneath surface residual products after catalytic reaction.

HX-PES measurements were performed with 5945 eV X-rays at the NIMS beamline BL15XU of SPring-8. Figure 1 shows the Pd 3d spectra of Pd-S-GaAs before and after being subjected to the Heck reaction of iodobenzene and methyl acrylate. The chemical state of Pd for the catalysts was close to metallic, and was different from an original divalent state of organopalladium $Pd(OCOCH_3)_2$. It suggests that $Pd(OCOCH_3)_2$ was reduced in the initial fixing of $Pd(OCOCH_3)_2$ on a sulfur terminated GaAs. The evidence of metallic Pd is consistent with the well-known knowledge that the existence of zero-valent Pd is essential for the Heck reaction, and the retention of metallic state after catalytic reaction should be the cause of high recycling capability. The S 1s spectra originating from sulfur terminated GaAs were clearly observed and remained after cycles of reactions. We can conclude that sulfur on GaAs is stable and works as a reaction site of the formation and fixing of metallic Pd on GaAs substrate.

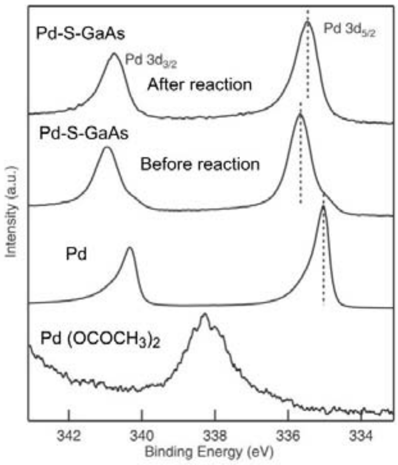

Fig.1 Pd 3d spectra of Pd-S-GaAs catalysts before/after Heck reaction. Reference spectra of Pd and $Pd(OCOCH_3)_2$ are also shown.

Acknowledgements

We are grateful to Mr. K.Tateishi and Mr. T.Toujyou of Anan National College of Technology and Dr. N.Nishiwaki of Kochi University of Technology and Dr. N.Hoshiya of Hokkaido University and Mr. N.Isomura, Mr. H.Yokota , Mr. Y.Furukawa, and Prof. K.Iizuka of Nippon Institute of Technology and Dr. T.Ogiwara of NIMS for their contribution of experiments and discussions. We also thank HiSOR, Hiroshima University, and JAEA/SPring-8 for their contributions to the construction of HX-PES station at BL15XU of SPring-8.

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THE ONE-STEP MODEL APPROACH TO HAXPES

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A brief introduction to the theory of angle-resolved photoelectron spectroscopy (ARPES) of solid materials is given with an emphasis on the so-called *one-step-model of photo emission t*hat describes excitation, transport to the surface and the escape into the vacuum in a coherent way. The main features of the theory and its implementation within the Munich SPR-KKR program package [1] will be discussed. Attention will be put on the possibility to account for correlation effects and chemical disorder using the LSDA+U or DMFT (dynamical mean field theory) schemes in combination with the Coherent Potential Approximation (CPA) alloy theory, respectively. Furthermore, the rule of the photon momentum, the description of the final state for high excitation energies and aspects of temperature will be discussed. To illustrate the applicability of the new formalism several examples of soft- and hard X-ray ARPES calculations from simple metals as well as from complex disordered alloys will be presented [2,3,4].

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MULTIPOLE CONTRIBUTIONS TO THE PHOTOELECTRIC ABSORPTION DETERMINED BY XSW/ HAXPES

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Hard X-ray photoelectron spectroscopy when combined with the X-ray standing wave technique (XSW) offers, among other advantages, access to a wider section of the reciprocal space. Unfortunately, with the increasing kinetic energy of photoelectrons the basic assumption of dipole approximation to the matrix element describing the photoionization process becomes invalid and higher order multipole terms must be taken into account [1]. We present study of the non-dipolar effects on two model systems, chlorine adsorbate on Cu(001) and graphene on SiC(0001).

Generally, the multipole contributions manifest themselves in the photoelectron angular emission profile by a forward/backward asymmetry with respect to the photon polarization direction, in contrast to the symmetric dipole emission [2]. The influence of this asymmetry is enhanced when using XPS in conjunction with the XSW technique because of the presence of two X-ray waves travelling in different directions. The precise knowledge of multipole differential cross sections is thus required, besides of fundamental reasons, for an accurate interpretation of result of XSW XPS experiments.

The influence of multipole contributions on XSW XPS data is the strongest in the backscattering geometry, i.e. when the incident photon energy is tuned such that the Bragg angle is almost 90° and the two X-ray waves are travelling in opposite direction. Our back-scattering XSW experiment was performed in two geometries: with the electron analyzer pointing at 45° from the incident photon beam (and thus at 45° with respect to its polarization direction) and at 90° off the beam (i.e. pointing toward the polarization vector). The former geometry is the most sensitive to the multipole contributions to the photoelectron cross section while the latter configuration is insensitive to quadrupolar terms when the electrons are excited from states with angular momentum $l=1$ [3].

Two model systems were chosen to clarify the role of solid state effects in the non-dipolar contributions to the photoelectron cross section. Cl on Cu(001) represents an adsorbate system with negligible elastic scattering of photoelectrons and with a choice of substrate that ensures that the in parallel detected Cl fluorescence cannot be excited (significantly) by scattering from the substrate. The fluorescence yield, free from non-dipolar effects, has been recorded as a reference for “multipole free” coherent fraction/coherent position values.The graphene on SiC(0001) represents a combination of adsorbate (graphene), bulk (carbon of the SiC substrate) and an intermediate layer (“zerolayer graphene”), all of which can be identified in the XPS spectrum by their distinct chemical shift.

Data at several Bragg reflections recording yield from different photoemission lines (i.e. different angular momentum states) and Auger lines will be shown and discussed in the presentation.

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IMPROVED TOUGAARD BACKGROUND CALCULATION USING PREDETERMINED INELASTIC ELECTRON SCATTERING CROSS SECTION FUNCTIONS λ(E)·K(E,T) USING THE SOFTWARE *UNIFIT 2011*

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The shape of the background in x-ray photoemission spectra may be affected by secondary electrons and inelastic energy loss processes. A polynomial of low order has very often turned out to model the secondary electron background. The Tougaard background model [1] has been successfully used to characterise the inelastic loss processes. However, the correct usage of the Tougaard background needs a well defined λ(E)·K(E,T) function (T = energy loss). The introduction of a four parameter loss function

$$\lambda(E)\cdot K(E,T)=\frac{BT}{(C+C' T^2)^2+DT^2}$$

with the fitting parameters B, C, C' and D implemented in the fittable background function [2] allows the improved estimation of the λ(E)·K(E,T) function. The results will be compared with the recommended parameters by Tougaard. The calculation of Inelastic Electron Scattering Cross Sections of clean surfaces from different materials using UNIFIT will be demonstrated [3].

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COMPARATIVE STUDY OF IMPROVED TOUGAARD BACKGROUND AND SHIRLEY BACKGROUND CALCULATION USING TEST FUNCTIONS AND REAL PHOTOEMISSION SPECTRA

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The shape of the background in x-ray photoemission spectra may be affected by secondary electrons and inelastic energy loss processes. A polynomial of low order has very often turned out to model the secondary electron background. The Tougaard background model [1] has been successfully used to characterise the inelastic loss processes. However, the correct usage of the Tougaard background needs a well defined $\lambda(E)\cdot K(E,T)$ function (T = energy loss). The introduction of a four parameter loss function

$$\lambda(E)\cdot K(E,T)=B\cdot T/((C+C'\cdot T^2)^2+D\cdot T^2)$$

with the fitting parameters ***B,C,C'*** and ***D*** implemented in the fittable background function [2,3] permits the generation of an improved Tougaard background. The fitting results of test spectra and real photoemission measurements using the improved Tougaard background and the traditional Shirley background will be compared.

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INTERFACE QUALITY FROM THEORETICAL CORE-LEVEL SHIFTS

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We perform *first principles* calculations of core-level binding energy shifts (CLS) for metallic systems using density functional theory (DFT). The high sensitivity of core-level binding energies to the chemical environment of an atom makes CLS a very valuable tool for structural characterization. Recently, theoretical layer resolved shifts and measurements from nondestructive high-kinetic-energy photoelectron spectroscopy were used to study the interface quality in Cu/Ni multilayered systems [1]. Here, we demonstrate the use of layer resolved CLSs as a probe of the interface quality in thin Cu films embedded into Fe, Co and Ni metal matrices, comparing the results with disordered alloys. We find a sensitive dependence of shifts to the interface quality [2].

An efficient computation is accomplished with the use of a Green's function method within DFT and by representing interfaces with alloy intermixing profiles – controlled by a single parameter. All the CLS calculations are performed within the complete screening picture, including both initial and final state effects in the same computation scheme. Recent applications include the study of embedded thin films and the disorder broadening of spectral core-lines, a summary of the studies are found in [3].

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FREE-ELECTRON FINAL-STATE CALCULATIONS FOR THE INTERPRETATION OF HARD X-RAY ANGLE-RESOLVED PHOTOEMISSION

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A simple two-step numerical procedure has been developed in order to interpret the electron band dispersions measured by angle-resolved photoemission at energies where free-electron final states are a good approximation. The useful photon energy range is from above approx. 50 eV up until several keV, while for much higher energies the modulations due to band dispersions are smeared out by the photon effects in experimental data.

In the first step the ***k***-point position in the Brillouin zone is calculated taking into account the vector momentums of the emitted electron and incoming photon. A macro written in Matlab allows full 3D geometry by means of matrix rotations and can automatized for predicting the trajectory in the Brillouin zone or the Fermi or constant energy surfaces.

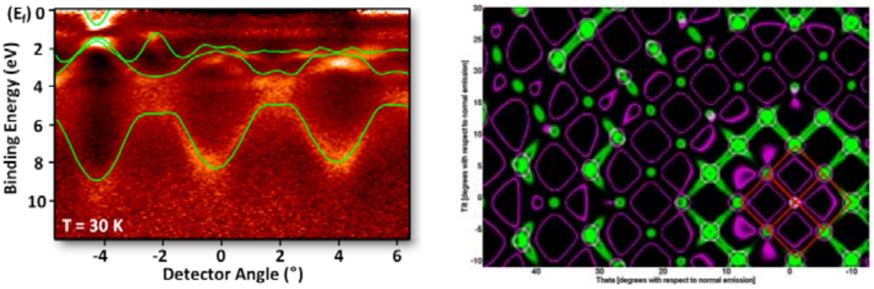

Fig1. ***Left***: comparison between the experimental and free-electron band dispersions for tungsten (110) crystal at approx. 6 keV [1]. ***Right***: The cut through a Fermi surface of LaSrMnO as predicted for ARPES at 833.2 eV photon energy, different colors refer to majority and minority electron spin.

In the second step the set of ***k***-points calculated by macro is plugged into the DFT code which calculates the electron eigenvalues at these points. It can be done by virtually any code, but we found the WIEN2k in particular useful due to its convenient interface, no need to use pseudopotentials, and excellent online support.

The left panel in Fig. 1 presents excellent agreement between the theory and experiment at several keV photon energy [1] where purely bulk states are probed, while the right panel presents the abilities of our procedure in calculating Fermi and constant energy surfaces.

We will present results of the free-electron final state calculations for various materials at various photon energies from VUV up to hard x-rays, and compare them to the experimental results and one-step model photoemission calculations.

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BOND STRENGTH INFLUENCE ON THE RECOIL EFFECT IN CARBON BASED MATERIALS: A HAXPES STUDY

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In the past couple of years hard x-ray high kinetic energy photoelectron spectroscopy (HAXPES) has lead to a break-through in the field of photoemission due to its non destructive way of investigating the bulk electronic properties of materials and in particular buried interfaces. In the present contribution we will report recent experiments performed at the hard x-ray HIgh Kinetic Energy (HIKE) photoelectron spectroscopy facility [1] at the Berliner synchrotron light source BESSY II of the HZB. The facility successfully combines the bending magnet source of the KMC-1 beamline [2] with a new generation electron spectrometer optimized for high kinetic energy electrons up to 10keV. In the present contribution we will discuss the recoil effect of high energy photoelectrons from carbon based materials.

In soft x-ray photoemission the photoelectron momentum transfer is small and thus any recoil effects can be neglected. However in HAXPES recoil effects result in rather large core level energy shifts and can not be disregarded any further. Moreover different bonding strength seems to define the recoil energies. Here we will show recoil effects given by 2 to 9 keV photons in diamond and HOPG with emphasis on the carbon bond strength differences.

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NEW OPPORTUNITIES FOR A SPIN RESOLVED SOFT AND HARD X-RAY PHOTOEMISSION EXPERIMENT AT BESSY II

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Nanolayered systems are the keystones of current and future spintronics devices. The electronic, magnetic and magneto-transport properties of these structures are determined not only by the characteristics of each layer, but also by their interfaces. Magnetic coupling phenomena and spin-dependent transport are largely affected by the interface electronic states, which consecutively are determined by the structure, the bonding situation and the magnetic nanostructure of the individual constituents.

The present project concentrates on the development of a unique experimental combination of spin resolved soft and hard x-ray photoelectron spectroscopy to study both surface and bulk electronic structures additionally providing the spin information. Employing a new undulator source which will be soon installed in the BESSY II ring, the beamline will be optimized for high throughput and high resolution within the energy range of 60 eV to 6 keV. The special design of the beamline allows both soft and hard x-ray beams to have the same focal point thus making use of only one experimental end-station. The experimental chamber will be equipped with a high resolution electron analyzer and highly efficient spin detector.

XSW AND HAXPES AT THE ID32 BEAMLINE

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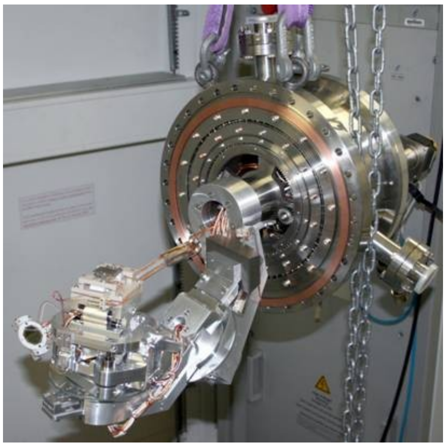
The ID32 beamline is dedicated to surface and interface science with two experimental hutches for diffraction and hard X-ray photoemission spectroscopy (HAXPES) studies, respectively [1].The beam is monochromatized by a double crystal Si(111) monochromator. Higher energy resolution can be achieved using two secondary monochromator, each equipped with Si(111), Si(220), Si(311) channel-cut crystals. Employing different crystal combinations allows tuning the bandpass of the x-rays from $\Delta E/E \approx 10^{-4}$ to 10^{-6}. Focusing is achieved with the help of a Be lens exchanger (transfocator) equipped with 34 parabolic beryllium lenses with 1500 μm and 500 μm radii. Eight pneumatic pistons allow computer controlled focusing in both experimental hutches on a wide energy range from 2.15keV (1500 μm radius lens) to 21.3 keV (all lenses) [2]. The transfocator is located right behind the monochromator thus demagnifying the source by a about a factor of two at the sample positions(s). The combination of the lenses with the two different radii allows obtaining a minimal focal spot size for 127 discrete energies in the range 2.15 to 21.3 keV.

For HAXPES measurements, a state-of-the art Phoibos 225 HV (SPECS) analyzer is installed in the main chamber associated with a delay-line detector. It is able to detect electrons with kinetic energy up to 15 keV and an energy resolution < 50 meV at 10 keV has been demonstrated [3].

The HAXPES UHV system is equipped with a chamber for sample preparation and characterization. LEED, ion sputtering, sample cooling (80 K) or heating (1500 K) can be performed and various ports are available for user equipment (evaporators etc.).

A three-circle, x,y,z UHV manipulator (ID32/ESRF design) using the Kappa geometry is equipped with an in-vacuum photodiode detector arm (see picture) on a fourth circle. Encoder feedback allows high accuracy and excellent reproducibility of all motions. This unique set-up opens the way for XSW measurements in all possible geometries. The manipulator also features a cryostat for controlling the sample temperature from about 30K to 450K.



For the XSW acquisition (which needs to acquire several XPS spectra when changing the excitation and thus the electron kinetic energy) a set of macros is available for enabling the communication between the beamline control software and the PHOIBOS analyzer. It now allows a convenient and user-friendly interface for batch acquisition.

*Now at DIAMOND Light Source. Didcot, UK

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HIGHLY EFFICIENT MULTICHANNEL SPIN POLARIMETER

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Since the original work by Mott, the low efficiency of electron spin polarimeters has prohibited many fundamental experiments, suffering from low intensity. Here we report a solution to this problem using a novel concept of multichannel spin-polarization analysis that provides a stunning increase in efficiency by four orders of magnitude in comparison to the performance of single-channel state-of-the-art electron spin detectors. The novel approach paves the way to spin-resolved HAXPES in the valence region and to single-shot experiments at low-repetitive FEL sources. The novel principle was demonstrated in spin-resolved UPS for Heusler compounds [1] and for Fe and O p(1x1)/Fe. An imaging set-up proved the principal capability for parallel acquisition of 3800 spin-polarization data points [2].

The relevant quantity for the statistical performance of a polarimeter is its figure of merit FoM = S^2I/I_0 with S being the asymmetry function and I/I_0 the ratio of scattered versus incoming intensity [3]. Up to now, spin-polarization detectors were based on single-channel electron scattering, which is characterized by an FoM of $\approx 10^{-4}$. In spin-integral electron spectroscopy, the situation developed differently. With the advent of multichannel detection, the efficiency of spectrometers increased strongly. Today, state-of-the-art hemispherical analyzers feature efficient multichannel detection with $>10^4$ data points being acquired simultaneously. When comparing spin-resolved with spin-integral electron spectroscopy, we are thus faced with a difference in counting efficiency of eight orders of magnitude.

The novel multichannel concept is based on the idea of preserving a two-dimensional electron distribution in the spin-polarized low energy electron diffraction process as sketched in Fig.1a,b. In our first instrument, the analyzer crystal is mounted in specular geometry, under an impact angle of 45°. The conservation of $k_{||}$, guarantees a transfer of the two-dimensional lateral image information that is encoded in the scattering angle. The Ewald-construction (Fig.1c) reveals how energy and angular variations act on the kinematic diffraction conditions.

The basics of the method are discussed, first results are presented and the potential and expected improvement for spin analysis in a HAXPES spectrometer is outlined.

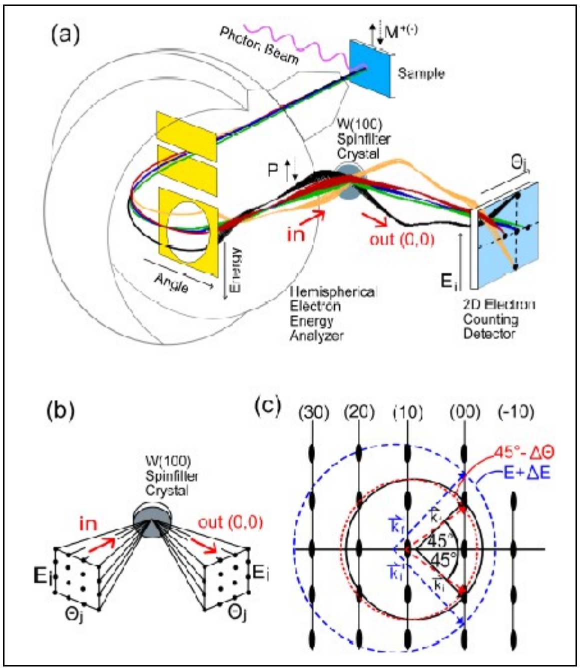

Fig.1: Geometry and scheme in *k*-space

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A NEW OPPORTUNITY FOR HAXPES AT DIAMOND LIGHT SOURCE

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A new beamline for studying surfaces and interfaces is under construction at Sector 9 at Diamond Light Source. It is scheduled to receive its first light in January 2012 and to host its first user experiment in October 2012. The beamline will be a dedicated facility for high-resolution investigations of atomic structures and electronic properties of a wide range of surfaces and interfaces using photoelectron spectroscopy (PES), x-ray standing waves, near edge x-ray absorption fine structure, photoelectron diffraction and x-ray reflectivity. To apply the different techniques to the same sample, and to access more absorption edges, which can be highly beneficial in solving complex surface/interface problems, two canted undulators installed in a modified long straight section will be used to provide both soft (150 eV – 2.1 keV) and hard (2.1 – 18 keV) x-ray beams, which will be directed to the same spot on the sample in one of the end-stations equipped with an high energy electron analyzer capable of detecting electrons emitted over an angle of 60º. Such a wide photon energy range, which can be translated into an electron mean free path of 0.5 to larger than 5 nm, offers a unique opportunity for probing the electronic structures of buried layers and interfaces in either an angle-integrated or angle-resolved mode. To facilitate HAXPES experiments, the beamline optics have been designed to achieve an energy resolution of 50 – 100 meV with strong horizontal focusing to allow a grazing incident sample geometry.

P50

HARD X-RAY PHOTOELECTRON SPECTROSCOPY AT PETRA III – BEAMLINE P09

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Photoelectron spectroscopy probably is the most important tool for studying the electronic structure of surfaces. Utilizing hard X-ray excitation and taking advantage of the increased photoelectron inelastic mean free path expands the applicability of this tool to investigating buried interfaces and the bulk of solids. Hard X-ray photoelectron spectroscopy (HAXPES) at third generation synchrotron sources uses tunable X-rays ranging from about 2 to 15 keV in energy and yields bulk representative electronic information from depths of typically 10-20 nm below sample surfaces.

The new high resolution HAXPES instrument at undulator beamline P09 of the 6 GeV storage ring PETRA III (DESY) has been in user operation since summer 2010. The high heatload primary monochromator provides two pairs of remotely interchangeable crystals, Si(111) and Si(311), yielding high flexibility for the experiments. Using the Si(311) crystal pair, a total energy resolution below 200 meV can already be achieved up to 6 keV with an appreciable photon flux of $2x10^{12}$ Ph/s. When needed, even better resolution is obtained by moving in an additional Si channel-cut post-monochromator. Circular and variable linear polarization can be generated by a diamond phase retarder remotely placed in the beam path. A beam spot of currently 200(v) x 400(h) μm is produced at the sample position located 95 m from the source by a primary set of focusing mirrors. A Kirkpatrick-Baez mirror system close to the endstation will be implemented in 2012 to reduce the spot size down to about 2×2 μm. The beamline is optimized for HAXPES experiments up to 12 keV allowing also two different geometries of the SPECS Phoibos 225 HV analyser, which is equipped with a delayline detector. Electron spin detection at several keV photoelectron energy has recently proved feasible using a four-channel micro-Mott detector [1]. The UHV analysis chamber is equipped with a custom made OMICRON 5-axes manipulator with LHe cooling. Selected experimental results obtained at the P09 HAXPES station will be presented.

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P51

HIGH ENERGY PHOTOEMISSION SPECTROSCOPY ENDSTATION AT THE SXRMB BEAMLINE OF CLS

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A High Energy X-ray Photoemission Spectroscopy (HXPES) system is being developed at the Soft X-ray Micro-characterization Beamline (SXRMB) of the Canadian Light Source. SXRMB is a bending maganet based, medium energy range beamline with the main features summarized in Table 1.

Table 1. The feature of SXRMB beamline at CLS

Source	Bending Magnet	
Monochromator	Double InSb (111) crystal	Double Si(111) crystal
Energy range	1.7 – 3.7 KeV	2.1 – 10.0 KeV
Resolution	2.63×10^{-4} eV	1.0×10^{-4} eV
Flux	$> 1 \times 10^{11}$	
Beam spot size	< 1 mm × 1mm (focused by toroidal mirror)	

The HXPES system consists of six components. (1) The main chamber made of stainless steel with single Mu – metal Liner with a residual magnetic field lower than 0.5 micro Tesla. (2) A 5-axis manipulator (x, y, z, primary rotation and azimuthal rotation) with an open cycle cryostat and both resistive and EB heaters. (3) A VG Scienta R4000 analyzer with < 35 meV energy resolution installed at 90 degree from the incident beam, minimizing the inelastic photoemission background while optimizing the photoelectron yield. This high resolution electron energy analyser is designed to measure electrons with kinetic energies up to 10 keV. (4) The load-lock system with a sample storage that can accommodate up to 5 samples. (5) The vacuum system designed to reach a base pressure of $< 1\times 10^{-10}$ Torr at the main chamber. (6) The four movements (x, z, roll and pitch) motorized support base designed to allow for the remote control and transport of the HXPES system. Furthermore, a four cells electron beam evaporator, ion sputtering gun and RHEED are equiped onto the main chamber for MBE thin film growth and in-situ investigation of surface and interface. The system is under commissioning, ready for users in 2012.

Fig1. The HXPES end station at SXRMB beamline of Canadian Light Source.

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HAXPES 2011

4th International Workshop on Hard X-ray Photoelectron Spectroscopy

September 14 – 16, 2011
DESY, Hamburg, Germany

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HAXPES 2011

4th International Workshop on Hard X-ray Photoelectron Spectroscopy

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PRACTICAL INFORMATION

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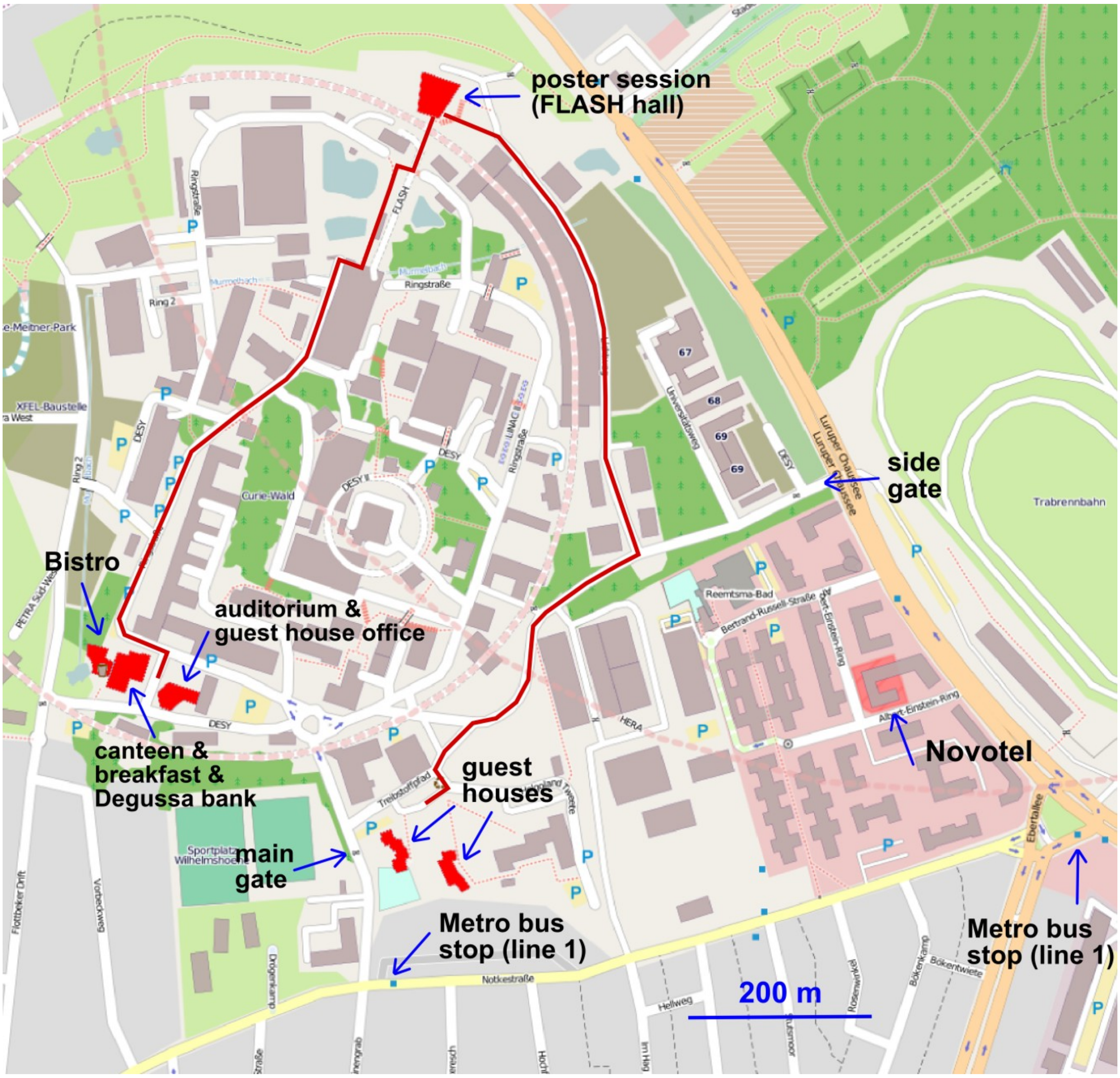

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  Sat/Sun : closed

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- Rooms in the guest have wireless access and a DESY campus phone (4-digit numbers)

- Drop off room keys at the guest house office (opening hours see above) or main gate

- A Taxi can be ordered at the main gate (phone 3333).

- Public transportation:
  the nearest bus stop to the main gate is "Zum Hünengrab / DESY" (Metro bus line 1)

Internet access

Wireless Web access is provided during the workshop:
network name: **HAXPES2011**
WPA/WPA2-PSK: **Ar3ah45h58u**
Two computers are available for public access in the lobby of the auditorium.

Oral sessions

Speakers are requested to copy their presentations onto the workshop PC in the auditorium well before the session starts (a USB stick is available if needed).

Poster session

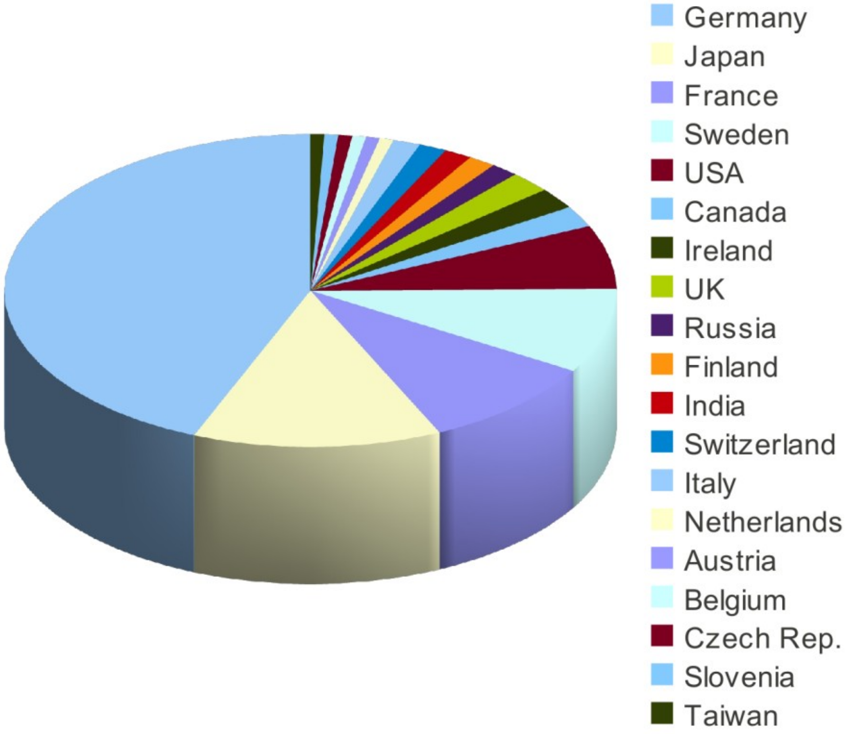
Posters can be set up in the FLASH hall (see map) starting from Wed. 13:00 and should be removed by 21:00.

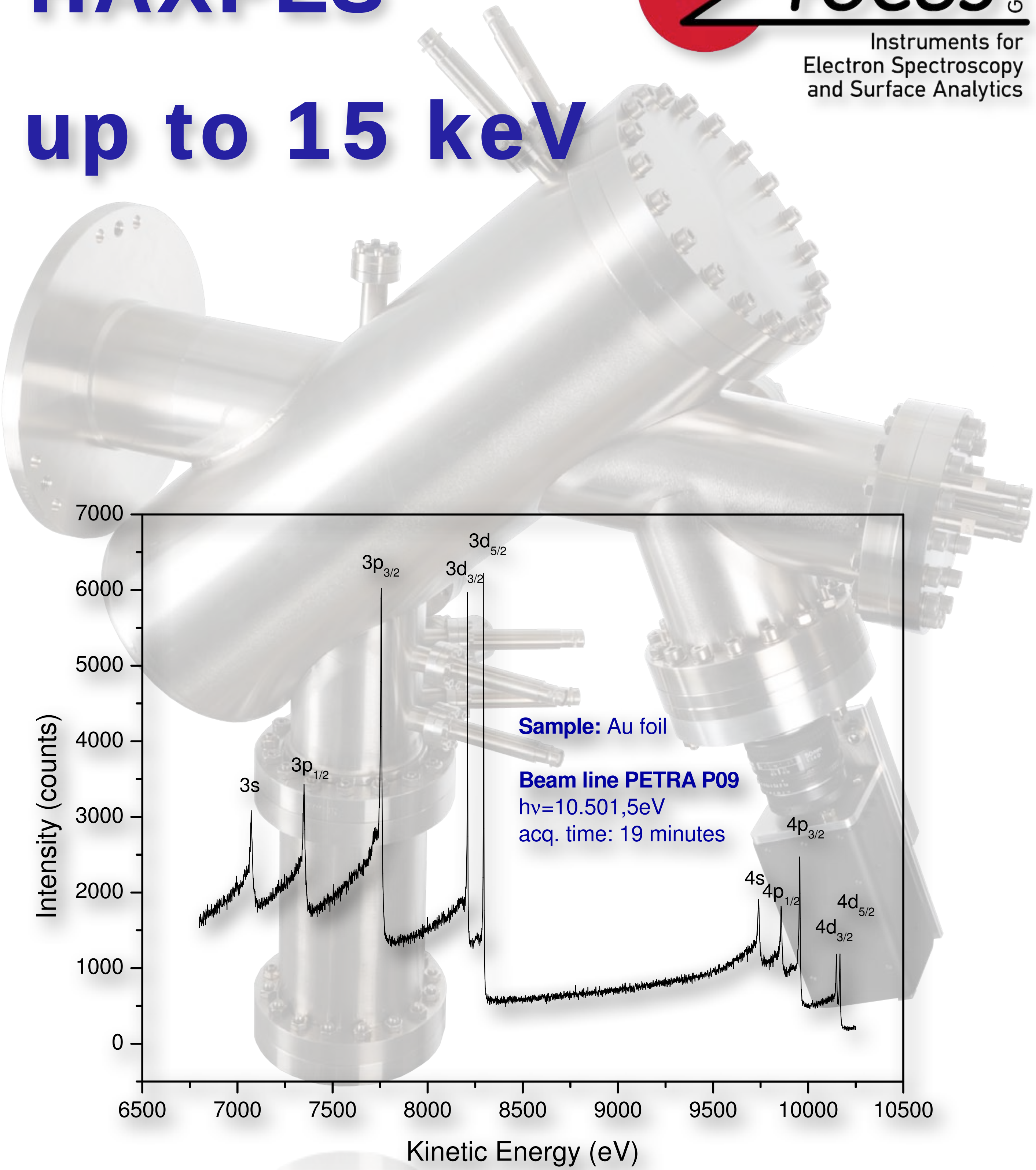
Contacts:

Workshop secretary: Mrs. Susanne Weigert, office phone 1803 (if not at the registration desk)

Participant Statistics

Germany	60
Japan	18
France	13
Sweden	12
USA	9
Canada	3
Ireland	3
UK	3
Russia	2
Finland	2
India	2
Switzerland	2
Italy	2
Netherlands	1
Austria	1
Belgium	1
Czech Rep.	1
Slovenia	1
Taiwan	1
	137





Intensity (counts)
Kinetic Energy (eV)
0
1000
2000
3000
4000
5000
6000
7000
6500
7000
7500
8000
8500
9000
9500
10000
10500
3s
3p1/2
3p3/2
3d3/2
3d5/2
4s
4p1/2
4p3/2
4d3/2
4d5/2
Sample: Au foil
Beam line PETRA P09
hν=10.501,5eV
acq. time: 19 minutes

VG Scienta Highlights
HARD X-RAY PHOTOELECTRON SPECTROSCOPY

R4000 HE Angular Resolved Mode for Band Mapping

The emerging field of hard x-ray photoelectron spectroscopy (HAXPES, HXPS) sets new demands on instrumentation. The first challenge is to be able to handle high retardation voltages in order to achieve spectra with high resolution and high transmission in a stable manner. Early models of VG Scienta analyzers were capable of measuring up to 6 keV, but in 2003 VG Scienta took a further step and developed a high energy version of the R4000 L1 analyzer, capable of recording spectra up to 10 keV. In addition, the novel angle-resolved mode possible in the R4000 L1 analyzer can for example be used for bulk band structure mapping via hard x-ray ARPES (HARPES). Figure 1 shows the first such HARPES spectra from GaAs (001) and W(110) recorded at 30 K and with excitation energies of 3242 eV and 5956 eV respectively. This opens the possibility of truly bulk sensitive electronic structure studies in the future. Data from SPring8, BL15XU, courtesy of Dr. K. Kobayashi, SpPring8, and Prof. Charles S. Fadley, UC Davis.

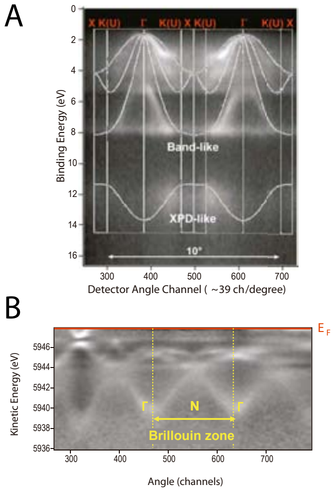


Figure 1: Angle-resolved valence-band spectra of (A) GaAs(001) and (B) W(110) recorded at 30K with an excitation energy of 3242 eV and 5956 eV respectively. Data courtesy of K. Kobayashi and C. S. Fadley.

VG Scienta High Pressure and High Energy

VG Scienta have in collaboration with the Advanced Light Source (ALS) developed a high pressure photoemission (HiPP) version of the R4000 (M. E. Grass et al, RSI 81 (2010) 053106). This analyzer houses a 2D detector and is capable of measuring both in spatial and angular mode under HiPP conditions. Figure 2 shows the band structure of graphite recorded at 0.2 Torr CO pressure using the VG Scienta R4000 HiPP analyzer. The band dispersion of the graphite is clearly seen together with the CO valence. Data courtesy of Dr. Zhi Liu, ALS.

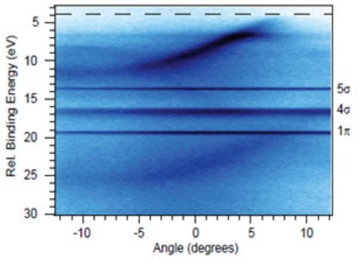


Figure 2: Band structure of graphite recorded at 0.2 Torr CO pressure. Data courtesy of Dr. Zhi Liu.

VG Scienta future plans for instrumental development includes combining the field of HAXPES with HiPP. The goal is to produce a HiPP-HAXPES analyzer with an angle resolved mode for the hard x-ray regime.

info@vgscienta.com - www.vgscienta.com

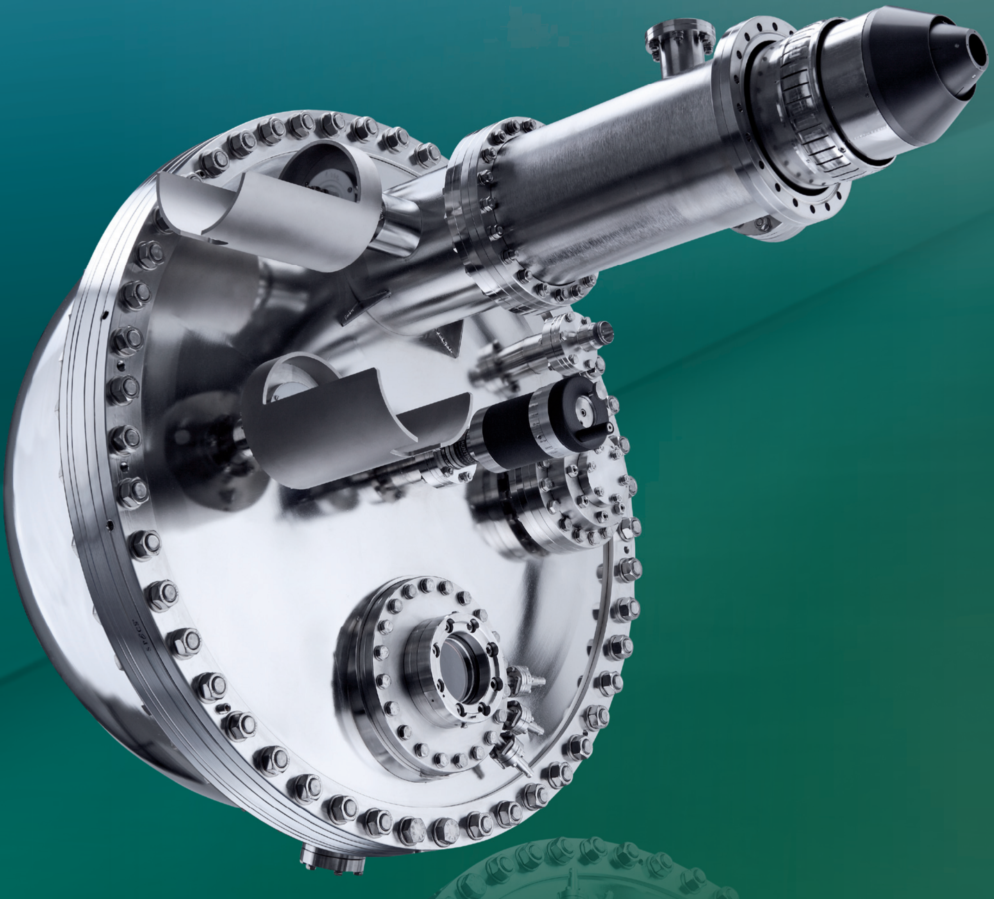
VG SCIENTA
a gammadata company

PHOIBOS 225 HV

THERE IS NO BETTER CHOICE FOR HARD X-RAY PHOTOEMISSION SPECTROSCOPY

KEY FEATURES

- For Electron Energies up to 15 keV
- Different Modes of Operation (UPS, XPS and HAXPES)
- Ultra High Energy Resolution
- Angular Mapping (Δθ < 0.1°)
- CCD, DLD and DLD/SPIN Detection Available



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