DS 6: Thin Film Characterization: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS,...)

Time: Monday 15:00–20:00 Location: CHE 89

DS 6.1 Mon 15:00 CHE 89

Lattice Dynamics and Hyperfine Interactions in fcc Europium Islands — •Olga Bauder[1,2], Przemyslaw Piekarz[3], Anja Seiler[1,2], Shyjumon Ibrahimkutty[1,2], Daniel G. Merkel[4], Marcin Zajac[4], Rudolf Rüffer[4], Tilo Baumbach[1,2], Krzysztof Parlinski[3], and Svetoslav Stankov[1,2] — [1]Laboratory for Applications of Synchrotron Radiation, Karlsruhe Institute of Technology, Germany — [2]Institute for Photon Science and Synchrotron Radiation, Karlsruhe Institute of Technology, Germany — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Poland — [4]European Synchrotron Radiation Facility, France

Employing in-situ nuclear inelastic scattering on 151Eu we investigated the phonon DOS of fcc europium islands with a nominal coverage of 2, 3, 5, 10, and 24 monolayers (ML) grown on the Nb(110)/Al2O3 and compared the results with that of the bulk bcc Eu. The experimental results reveal a systematic shift of the phonon spectrum to high energies and significant suppression of the low-energy phonon modes as the nominal Eu coverage is reduced. The observed phenomenon is attributed to the notable lattice compression of about 9 % in the fcc Eu islands, as well as to the naturally formed monolayer of EuO on the oxygen-induced (6x2) reconstructed Nb(110) surface. These findings are supported by the in-situ nuclear forward scattering spectra that reveal the presence of quantum beats attributed to the difference between the isomer shift of the EuO interface layer and the metallic Eu.

DS 6.2 Mon 15:15 CHE 89

In situ PLD synchrotron characterization for the detection of domain formation during Ba0.5Sr0.5TiO3 growth on MgO — Sondes Bauer[1], •Alan Molinari[2], Sergey Lazarev[1], Andreas Breitenstein[1], Philipp Leufke[2], Robert Kruk[2], Horst Hahn[2], and Tilo Baumbach[1] — [1]Karlsruhe Institute of Technology (KIT), Synchrotron Facility ANKA, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

A highly sophisticated pulsed laser deposition (PLD) chamber has recently been installed at the Nano beamline of the synchrotron facility ANKA (Karlsruhe, Germany), which allows for comprehensive studies on the PLD growth process of thin films by combining in situ reflection high energy electron diffraction (RHEED) with the in situ synchrotron high resolution X-ray diffraction and surface diffraction methods.

Ba0.5Sr0.5TiO3(BST) grown on MgO is the first system studied in this in situ PLD chamber being analyzed by in situ X-ray reflectivity, in situ two-dimensional reciprocal space maps (2D-RSMs) and acquisition of time resolved diffraction profiles during the ablation process. The stability of morphology during the PLD growth is demonstrated to be seriously affected by the film thickness: after a critical thickness of hc = 107 nm, BST on MgO reveals a splitting of the diffraction peak into two distinguishable peaks proving the formation of a new kind of domain.

DS 6.3 Mon 15:30 CHE 89

RF-sputtering deposition of Ag: in-situ time-resolved GISAXS investigation — •Gonzalo Santoro[1], Shun Yu[1], Sarathlal K. Vayalil[1], Ralph Döhrmann[1], Daniel Moseguí-González[2], Peter Müller-Buschbaum[2], Margarita Hernández[3], Concepción Domingo[3], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, D-22607, Hamburg, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, D-85748, Garching, Germany — [3]Institute of Structure of Matter, IEM-CSIC, Serrano 121-123, E-28006, Madrid, Spain

Ag nanocoatings have shown to exhibit excellent properties that can be exploited for applications such as antibacterial coatings, plasmonic devices or sensors [1-3]. However, in order to fully control the desired final properties of the nanocoatings, that are very sensitive to the morphology developed during the deposition, it is mandatory to achieve a profound understanding of the growth kinetics of Ag.

This work presents in-situ time-resolved Grazing Incidence Small Angle X-ray Scattering (GISAXS) results concerning the time evolution of the nanostructures developed during the RF-sputtering of Ag . The Surface Enhanced Raman Spectroscopy (SERS) activity of the prepared Ag coatings for different film thicknesses is also presented and correlated to their nanostructure.

[1] F. Faupel, et al., Adv.Eng. Mat. 12, 1177 (2010); [2] M. Rycenga, et al., Chemical Reviews 111, 3669 (2011); [3] J. Chen, et al., Biosens. Bioelectron. 44, 191 (2013).

DS 6.4 Mon 15:45 CHE 89

metal layer growth on Alq3: towards OLEDs — •Shun Yu[1], Yuan Yao[2], Gonzalo Santoro[1], Peng Zhang[1], Sarathlal Koyiloth Vayalil[1], Matthisas Schwartzkopf[1], Ezzeldin Metwalli[2], Peter Müller-Buschbaum[2], and Stephan V. Roth[1] — [1]Photon Science, DESY, Notkestraße 85, 22607, Hamburg — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic light emitting diodes have entered the market as the next generation digital displays and solid-state lighting devices. Its typical multilayer device structure emphasizes the significance of understanding the interfacial structure and properties. Comparing to evaporate the metal contact, Here we used sputter deposition to prepare Al, Ag and Au electrical contact onto Tris(8-hydroxyquinolinato)aluminium (Alq3), the activating layer. The interaction between metals and Alq3 has been studied by different spectroscopic techniques and theoretical methods at atomic level. The growth of metallic thin film demands deep understanding concerning the dynamic process. In this work, we have exploited in situ grazing incidence small angle X-ray scattering technique to monitor the growth of metallic thin film on top of Alq3 layer during the sputtering process in real time. We elucidate interesting results that the highly reactive Al manifest completely different growth mode compared to the Ag and Au, showing three-stage growth mode, nano-pillar structure and great roughness correlation to the substrate. Whereas, Ag and Au grow in a continuous way involving clustering and coarsening.

DS 6.5 Mon 16:00 CHE 89

Epitaxial MgO/GaAs(001) studied by in-situ X-ray diffraction — •Thomas Hentschel, Michael Hanke, Oliver Bierwagen, Andre Proessdorf, and Jens Herfort — Paul-Drude-Institut Berlin, Hausvogteiplatz 5-7, 10117 Berlin, Germany

The integration of Magnesiumoxide MgO into magnetic tunnel junctions or ferromagnet/semiconductur-hybrid structures acting as a potential tunnel and diffusion barrier has drawn much attention in the last years. Although the growth of MgO by different procedures is well established and used in various applications, its structural properties and growth mechanisms apparently have not been of much interest yet.

This contribution presents *in-situ* X-ray diffraction measurements carried out during molecular beam epitaxy of 5 to 30 nm thick MgO films on GaAs(001). All samples were grown at a substrate temperature of $T_S = 350$ °C by evaporating metallic Mg from an effusion cell with a sapphire crucible and providing additional molecular oxygen at a partial pressure of 10^{-6} mbar. It is observed that the in-plane orientation of MgO depends on the growth rate, while the ouf-of-plane orientation remains unchanged with $MgO_{[001]} \| GaAs_{[001]}$. For a growth rate of 1 Å/min the cubic rocksalt structure-like MgO with a misfit of about 25% to GaAs grows directly cube-on-cube on top of the substrate with an in-plane orientation of $MgO_{[110]} \| GaAs_{[110]}$. If the growth rate is increased by a factor of 4 the in-plane orientation rotates by 45°. The resulting orientation is $MgO_{[100]} \| GaAs_{[110]}$. We attribute this in-plane rotation to unoxidized Mg clusters formed at the GaAs interface.

DS 6.6 Mon 16:15 CHE 89

Optimization of crystal and morphological Parameters wetchemical synthesized $LiNbO_3$-Films — •Doreen Eger, Diana Karsch, Erik Mehner, Hartmut Stöcker, and Dirk Meyer — TU Freiberg - Institut für experimentelle Physik

Lithium niobate is a versatile applicable material. Some applications require thin films on substrates, which can be produced only with high effort until now. The wet-chemical synthesis is an environment friendly alternative for coating. In this contribution the influence of

processing parameters of annealing on substrates made of silicium are investigated.

Samples dip-coated with three different sols or solutions are annealed at different high temperatures. For morphology analysis of the films mainly confocal and scanning electron microscopy are used. The portions of crystalline lithium niobate and other phases are investigated by grazing incidence X-ray diffraction.

The coating based on $NbCl_5$ shows the best results. The annealing at about 800 °C for 4 h yields the maximum amount of crystalline Lithium niobate with in parallel minimal impurity phases.

Coffee break (15 min)

DS 6.7 Mon 16:45 CHE 89

Spray pyrolysis of Mo-based nanostructures and thin films — •Marlis Ortel and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The high potential of Transition Metal Dichalgonides (TMD) in 2D electrical thin film devices was shown recently. A major bottle neck of the material system is the lack of suitable deposition methods for large-area applications. Up to now mainly electrical devices applying mechanical exfoliation have been reported.

In this work we report on spray pyrolysis of Mo-based nanostructures. Therefore concentration dependent ageing tests of the precursor solution (e.g. H2O, DMSO) were conducted in order to find an optimized starting solution. The layers were grown on silicon dioxide and mica substrates. The solvents utilized were altered with respect to Leidenfrost temperature, surface energy and solubility of the precursor material. Finally the material parameters were correlated with measurements conducted by AFM (atomic force microscopy) and SEM (scanning electron microscope) in order to investigate the physical mechanisms causing the growth of different types of nanostructures, i.e. layers or rods. A fluid mechanics based growth model was developed assuming colloidal growth of the nanostructures in the precursor.

DS 6.8 Mon 17:00 CHE 89

Chemical composition of Mo-based layers deposited by spray pyrolysis — Marlis Ortel, •Torsten Balster, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Mechanical and liquid exfoliation are well known techniques to produce nano flakes for high performance transition metal dichalcogenide (TMD) thin film transistors (TFTs). However, up to now there is a lack of deposition processes for large area processing.

In this work, the focus is on spray pyrolysis which is a suitable deposition technology for large area thin film growth. Understanding of decomposition processes during growth is essential to deposite high quality thin films. The chemical composition in the deposited layer results from those decomposition processes and can be monitored by X-ray photoelectron spectroscopy (XPS). The investigated MoS_2 thin films were deposited from non-toxic precursor solutions, e. g. ammonium tetrathiomolybdate (ATTM) dissolved in dimethyl sulfoxide (DMSO). The chemical composition of the thin films was analyzed with respect to the decomposition temperature of the precursor and whether Mo and S can be provided from a single source. Generally, it was found that Mo-based thin films deposited far above the decomposition temperature (e.g. at 360°C) require an additional sulfur source to successfully grow MoS_2.

DS 6.9 Mon 17:15 CHE 89

Combinatorial epitaxial strained film growth: a new tool to adjust functional properties — •Sandra Kauffmann-Weiss[1,2,3], Sven Hamann[4], Ludwig Reichel[1,2], Alexander Siegel[4], Vasilis Alexandrakis[4], Rene Heller[5], Alfred Ludwig[4], Ludwig Schultz[1,2], and Sebastian Fähler[1,3] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Institute for Materials Science, 01062 Dresden, Germany — [3]Technische Universität Chemnitz, Faculty of Natural Science, Institute of Physics, 09107 Chemnitz, Germany — [4]Ruhr-University Bochum, Faculty of Mechanical Engineering, Institute of Materials, 44801 Bochum, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

Whereas in bulk lattice parameters can only be changed by composition or temperature, coherent epitaxial growth of thin films allows adjusting the lattice parameters independently. Up to now only discrete values were accessible by using different buffer layers or substrate materials. As a new tool for an efficient search for optimum parameter we present a continuous variation of lattice parameters of an alloy buffer layer by combinatorial film deposition of a Cu-Au layer on wafer level. These libraries are versatile as they allow tuning functional properties of various types of materials, ranging from (magnetic) shape memory alloys over multiferroics to permanent magnets.

Work was funded by DFG through SPP 1239 and EU through REFREEPERMAG.

DS 6.10 Mon 17:30 CHE 89

Investigating the oxidation process of the $Pt_3Ti(111)$ alloy surface on the atomic scale — •Marco Moors[1,2], Maria Buchholz[2,3], Séverine Le Moal[2,4], Klaus Wandelt[2,5], and Rainer Waser[1] — [1]Forschungszentrum Jülich — [2]Universität Bonn — [3]Karlsruher Institut für Technologie — [4]Université Paris Sud — [5]University of Wroclaw

The oxidation of reactive bimetallic alloys like the $Pt_3Ti(111)$ surface is a promising approach to grow atomically thin titanium oxide films with a high degree of surface order on a metallic conducting substrate. Depending on the used preparation conditions several ordered oxide phases with both rectangular and hexagonal symmetry have been observed. The morphology of these phases is dominated by the surface strain caused by the interplay of the hexagonal substrate symmetry and the favoured rectangular oxide symmetry.

In this presentation the focus is set on the investigation of the first steps of the complex oxidation process on the atomic scale. At low oxygen pressures a titanium oxide phase with a characteristic zigzag structure is formed by a temperature induced segregation process of titanium atoms from the bulk to the outermost surface layer. By variation of the oxygen dosage and temperature the oxide coverage can be controlled ranging from small single islands up to the complete coverage of the entire surface. Due to the surface strain in all cases a regular arrangement of surface defects along the trenches between the zigzag lines can be observed, which may be important for the catalytic activity as well as for self assembly processes.

DS 6.11 Mon 17:45 CHE 89

Isolating free-standing diamond-like carbon membranes from coated biodegradable plastic materials — •Christian B. Fischer, Bastian Pause, Lukas Hoffmann, Alberto Catena, and Stefan Wehner — Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany

Diamond-like carbon (DLC) as an isolated single free-standing thin film is a very exciting material since it exhibits outstanding properties like high hardness, chemical inertness, selective barrier characteristics etc. The preparation of a 100 nm thick single free-standing DLC-film follows the route of depositing carbonaceous precursors on selected supporting materials first. The isolation of single DLC-pieces is very challenging and comprises several single steps in general. In the present work we report an easy access for stable isolated amorphous carbon (a-C:H) films via delamination from a coated biodegradable polymer. DLC contains a mixture of sp3- and sp2-centers determining its intrinsic hardness. By enhancing the proportion of sp2-carbons a more flexible carbon layer on the pure bioplastic polyhydroxybutyrat (PHB) foil as support is realized by PECVD. Delamination is performed using several organic solvents. The surface structures of uncovered materials and isolated thin films have been analyzed by SEM and AFM spectroscopy. Significant differences of the contact side depending on the used solvent are found. This provides further insights into the interaction of hard DLC coating and soft plastic material.

DS 6.12 Mon 18:00 CHE 89

Strontium segregation in LaAlO3/SrTiO3 and NdGaO3/SrTiO3 oxide heterostructures investigated by XPS — •Uwe Treske[1], Nadine Heming[1], Martin Knupfer[1], Bernd Büchner[1], Emiliano Di Gennaro[2], Umberto Scotti di Uccio[2], Fabio Miletto Granozio[2], and Andreas Koitzsch[1] — [1]Institute for Solid State Research, IFW-Dresden, P.O. Box 270116, DE-01171 Dresden, Germany — [2]CNR-SPIN and Dipartimento di Fisica, Complesso Universitario di Monte S.Angelo, Via Cintia, 80126 Naples, Italy

Pulsed laser deposition grown $LaAlO_3$ and $NdGaO_3$ on TiO_2-terminated $SrTiO_3$ with different film thicknesses were investigated by soft X-ray photoemission spectroscopy. The surface sensitivity of the measurements has been tuned by varying photon energy $h\nu$ and emission angle Θ. In contrast to the core levels of the other elements, the

Sr 3*d* line shows an unexpected splitting for higher surface sensitivity, signaling the presence of a second unexpected strontium component. From our quantitative analysis we conclude that during the growth process Sr atoms diffuse away from the substrate and segregate at the surface of the heterostructure, possibly forming strontium oxide.

Coffee break (15 min)

DS 6.13 Mon 18:30 CHE 89

Structural characterization of CeO2 thin films grown on Yttria-Stabilized Zirconia — •Björn Arndt[1,2], Patrick Müller[1,2], Heshmat Noei[1], Thomas Keller[1], Vedran Vonk[1], Andreas Nenning[3], Jürgen Fleig[3], and Andreas Stierle[1,2] — [1]Deutsches Elektron-Synchrotron (Desy), D-22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]Institute of Chemical Technologies and Analytics, Vienna University of Technology, 1060 Vienna, Austria

Apart from its use in catalytic converters, CeO2 offers a variety of possible applications: for hydrogen production via photon induced water-splitting, as a support for metal nanoparticles, or as an electrolyte or anode material for Solid-Oxide Fuel Cells. The reason for this lies in the ability of CeO2 to form oxygen vacancies in the bulk and at the surface, thus being able to store, conduct and release oxygen. Doping with a trivalent oxide (in this case Gadolinia) induces oxygen vacancies, making them available under non-reducing conditions. For a better understanding of the above mentioned properties of Ceria, it is important to study its structure under oxygen-deficient conditions. Therefore, 10% Gd-doped CeO2 thin films were grown on Yttria-Stabilized Zirconia (110) and (111) by pulsed laser deposition, inducing a nominally 5% oxygen vacancy concentration in the films. The films were studied by grazing incidence x-ray diffraction, x-ray reflectivity and atomic force microscopy. XRD-Measurements were performed at the ID03-Beamline at the ESRF as well as using a conventional lab source. The films are shown to be atomically smooth and epitaxial to the YSZ substrates.

DS 6.14 Mon 18:45 CHE 89

Partial Crystallinity in Alkylsilanes Monolayers — •Hans-Georg Steinrück[1], Moshe Deutsch[2], Ben Ocko[3], and Andreas Magerl[1] — [1]1Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg, Germany — [2]Bar-Ilan University, Ramat- Gan, Israel — [3]Brookhaven National Laboratory, Upton NY, USA

Alkylsilane (denoted as Cn, n = 12, 14, 18, 22, 30) self-assembled monolayers (SAMs) on the amorphous oxide of silicon are vertically aligned and densely packed as shown by X-ray reflectivity. A new 3-slab model simulating the electron density profile was developed yielding only four free fit parameters (roughnesses of each interface and the density of one slab). All other parameters for the alkyl chain were fixed to the values in the rotator phase [1] and to the chemical bond length in the linker group region. For all Cn, expect C12, a hexagonal ordering with a lattice constant of a = 4.82 $\AA$ is revealed by X-ray grazing incidence diffraction. Interestingly, the analysis of the intensity distribution along q_z (Bragg rod) reveals that crystalline phase is less than the length of the molecule. We argue that this reflects gauche defects at the chain ends [2] as well as steric hindrance in the linker group region [3]. The percentage of the surface normal crystalline part of the alkyl chain increases up to 60% for C18 and linearly drops down to 40% for C30.

[1] Ocko, B.M. et al., PRE 1997, 55, 3164-3182.
[2] Allara, D.L. et al., Langmuir 1995, 2357-2360.
[3] Prasad, S. et al., A. PRL 2008, 101, 065505-065505.

DS 6.15 Mon 19:00 CHE 89

Non-destructive and non-preparative chemical nanometrology of interfaces at tunable high information depths — •Beatrix Pollakowski[1], Peter Hoffmann[2], Marina Kosinova[3], Olaf Baake[2], Valentina Trunova[3], Rainer Unterumsberger[1], Wolfgang Ensinger[2], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]Technische Universität Darmstadt, Materials Sciences, Darmstadt, Germany — [3]Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

The development of improved characteristics of functional nanoscaled devices involves novel materials, more complex structures and advanced technological processes, requiring analytical methods to be well adapted to the nanoscale. Thus, non-destructive and non-preparative techniques for chemical nanometrology providing sufficient sensitivity, reliable quantification and high information depths to reveal interfacial properties. Appropriate measurement strategies adapted to a nanoscaled stratified sample enables the combined technique NEXAFS and GIXRF to provide interfacial species information. The validation of this method for interface speciation has been performed at nanolayered model structures consisting of a Si substrate, a physically vapor deposited Ni metal layer and, on top, a chemically vapor deposited $B_xC_yN_z$ light element layer. The chemical bonds in the interfaces were to be determined by the GIXRF-NEXAFS technique. B. Pollakowski et al., Anal. Chem. 85,193 (2013)

DS 6.16 Mon 19:15 CHE 89

Quantitative grazing incidence X-ray fluorescence analysis for reference-free elemental depth profiling of thin films — •Cornelia Streeck[1], Beatrix Pollakowski[1], Christian Herzog[2], Janin Lubeck[1], Martin Gerlach[1], Philipp Hönicke[1], Rainer Unterumsberger[1], Stephan Brunken[3], Christian Kaufmann[3], Burkhard Beckhoff[1], Birgit Kanngiesser[2], and Roland Mainz[3] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 12109 Berlin

Synchrotron-radiation based X-ray fluorescence analysis under grazing incidence (GIXRF) conditions provides a non-destructive access to the compositional depth profile of thin films in the nano and micro meter range. Using reference-free GIXRF measurements and a fundamental parameter based quantification no well-characterized standards for calibration purposes are required. As an example, thin films of Cu(In,Ga)Se2 (CIGSe) have been were investigated, which are used as absorber layer of thin film solar cells. In the case of CIGSe, a graded band gap is created by a depth-dependent variation of the absorber matrix elements. To correlate the device functionality with the respective material properties, both the absolute composition and the in-depth gradient in CIGSe thin films require reliable determination. Due to the lack of appropriate reference materials, non-destructive GIXRF is used to address this analytical challenge.

DS 6.17 Mon 19:30 CHE 89

Resonant Soft X-Ray Reflectometry on strained $LaSrMnO_4$ thin films — •Martin Zwiebler[1], Jorge-Enrique Hamann-Borrero[1], Mehran Vafaee[2], Ronny Sutarto[3], Feizhou He[3], Lambert Alff[2], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW Dresden, Helmholtzstraße 20, 01097 Dresden, Germany — [2]Institute of Material Sciences, Technische Universität Darmstadt, 64287 Darmstadt, Germany — [3]Canadian Light Source Inc., 44 Innovation Boulevard, Saskatoon SK S7N 2V3, Canada

The strong electron-lattice coupling in the perovskite manganites provides a unique opportunity to tune the electronic properties of these materials via lattice strain. $LaSrMnO_4$ is a good model material with well-known orbital occupation in the bulk material. We present a study of the depth-resolved electronic properties in a tensile strained $LaSrMnO_4$ film by the means of resonant X-ray reflectometry (RXR) and XAS. We find evidence for Mn^{2+} on the surface and we extract the depth profile of the Mn valence throughout the film.

DS 6.18 Mon 19:45 CHE 89

Resonant X-ray reflectometry study of $YBa_2Cu_3O_{7-\delta}$ thin films: An atomic approach to reflectivity — •Jorge E. Hamann-Borrero[1], Sven Partzsch[1], Benjamin Gray[2], Sebastian Macke[3], Enrico Schierle[4], Martin Zwiebler[1], John W. Freeland[5], Jak Chakhalian[2], Bernd Buechner[1], and Jochen Geck[1] — [1]IFW-Dresden — [2]Department of Physics University of Arkansas, USA — [3]Max Planck-UBC Centre for Quantum Materials, Vancouver, Canada — [4]Helmholtz-Zentrum Berlin für Materialien und Energie — [5]Advanced Photon Source, Argonne National Laboratory, Illinois, USA

We present a Cu $L_{2,3}$ Resonant X-ray Reflectometry study of a (001)-YBCO thin film grown on $SrTiO_3$. The reflectivities measured using σ and π polarized light show a strong dichroism due to the local anisotropy of the different copper sites at the plane and chain layers of this compound. Within the scanned **q**-range also the (001) Bragg reflection appears highlighting the importance of the interference between the different scattering centers in the sample.

In order to describe the observed intensities, traditional models such

as the Parrat's formalism fail, since they neglect the interference between the atomic scatterers. Therefore, we employed a new atomistic approach to model reflectivity where the most important structural, finite size, surface and interface effects, are considered by explicitly defining the atom positions together with their anisotropic scattering form factors. First calculations will be presented and discussed.