MI 4: 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, DF, GP, MA, MI, MM; related to SYXD)

Time: Tuesday 9:30–12:45 Location: EMH 225

Invited Talk MI 4.1 Tue 9:30 EMH 225

The discovery of X-ray interferences, the role of characteristic radiation therein and potential applications of the Laue method in modern engineering. — •Hans-Jürgen Ullrich[1], Siegfried Däbritz[2], Enrico Langer[2], Jürgen Bauch[1], Andreas Danilewsky[3], and Peter Paufler[4] — [1]Institute of Materials Science at the TU Dresden — [2]Institute for Solid State Physics at the TU Dresden — [3]Institute of Crystallography at the University of Freiberg — [4]Institute of Structural Physics at the TU Dresden

It was during a noteworthy conversation between Paul Peter Ewald and Max von Laue in the English Garden in Munich in early 1912 that the foundation for the discovery of X-ray interferences was laid. They were debating which effects can be expected when short-wave electromagnetic radiation is allowed to impinge on crystals, and in a eureka moment Max von Laue theorized that interference phenomena are caused.

The first diffraction experiments were founded on the notion that the interferences in question might be characteristic radiation. The effect subsequently searched for was eventually discovered by Walther Kossel and his colleagues in 1934 (interferences from lattice sources, Kossel interferences). It is with this fact in mind that our lecture will look at the significance of Laue and Kossel diffraction patterns during the initial research into X-ray physics and their influence on all further academic work in this area. In the past, Laue's discovery was mainly applied within the natural sciences, but more recently the Laue method has also been employed successfully in engineering, for example:

- for quality assessment procedures used within the framework of semiconductor chip production
- as diagnostic techniques for gas turbine blades.

MI 4.2 Tue 10:00 EMH 225

Thermal diffuse scattering as a complementary tool in the study of lattice dynamics — Björn Wehinger, Alexeï Bosak, and •Michael Krisch — ESRF, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble, France

Thermal diffuse scattering (TDS) in combination with inelastic x-ray scattering (IXS) and lattice dynamics calculations allows the reconstruction of the lattice dynamics in the entire Brillouin zone. X-ray scattering by thermally populated phonons in crystals reduces the intensity of Bragg spots and substantially increases the intensity of the diffuse scattering which has a rich structure in reciprocal space [1,2]. In combination the two techniques can serve as a rigorous benchmark for parameter free lattice dynamics calculations [3]. The proposed method can be used for the precise detection of mode softening, for the study of lattice dynamics under extreme conditions and for time resolved measurements. In metallic systems it is possible to map the Fermi surface in tree dimensions by directional tracing of Kohn anomalies [4]. The presented results on β-tin illustrate the functionality of the proposed combined approach with new insights into the dynamical properties on this system.

[1] Wooster, Diffuse X-ray reflections from crystals, Clarendon Press, Oxford (1962)

[2] Xu RQ, Chiang TC, Z. Kristallogr. 220, 1009 (2005)

[3] A. Bosak, et al., Z. Kristallogr. preprint: doi: 10.1524/zkri.2012.1432

[4] A. Bosak, et al., PRL, 103, 076403 (2009)

MI 4.3 Tue 10:15 EMH 225

Brillouin scattering of ultrashort optical and x-ray pulses from quasi-monochromatic phonon wavepackets — •Marc Herzog[1], André Bojahr[1], Jevgenij Goldshteyn[2], Steffen Mitscherling[1], Wolfram Leitenberger[1], Dmitry Khakhulin[3], Michael Wulff[3], Ionela Vrejoiu[4], Roman Shayduk[2], Peter Gaal[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France

We excite a $SrRuO_3$ thin film transducer epitaxially grown on a $SrTiO_3$ substrate with pulse trains of ultrashort laser pulses. Each laser pulse launches single bipolar strain pulses of broad bandwidth into the substrate [1] which coherently add up to form a quasi-monochromatic sub-THz phonon wavepacket. The generation and dynamics of these phonon pulses is investigated by Brillouin scattering using visible and hard x-ray photons. The combination of both methods reveals the excited narrow phonon spectrum as well as the phonon lifetime which is on the order of a few 100 ps in the considered frequency range. This lifetime is explained by anharmonic phonon interactions.

[1] Thomsen *et al.*, Phys. Rev. B 34, 4129 (1986).

MI 4.4 Tue 10:30 EMH 225

Following Strain-Induced Mosaicity Changes of $PbZr_{0.2}Ti_{0.8}O_3$ Thin Films by Ultrafast Reciprocal Space Mapping — •Daniel Schick, André Bojahr, Marc Herzog, Peter Gaal, and Matias Bargheer — Institut für Physik & Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam/Golm

We studied the propagation of coherent sound waves in a $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) - $SrRuO_3$ (SRO) bilayer sample after optical excitation of the metallic SRO layer. We observed changes of the out-of-plane lattice constant and structure factor of the ferroelectric PZT layer that can be exclusively attributed to the transient strain wave launched from within the SRO layer. In addition to this we are also able to follow in-plane structural dynamics simultaneously utilizing a new ultrafast reciprocal space mapping technique. Thereby we observed a transient change of the mosaicity of the PZT layer on a ps timescale which is again directly coupled to the coherent sound wave travelling through the layer.

MI 4.5 Tue 10:45 EMH 225

Analysis of the size and shape of colloidally prepared nanocrystals by Rietveld refinement — •Holger Borchert, Xiaodong Wang, Marta Kruszynska, Joanna Kolny-Olesiak, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

Many properties of colloidal nanocrystals can be tuned by controlling the crystal size and shape. Examples are the quantum size effect in the case of semiconductors or size-dependent catalytic properties in the case of metals. Establishing correlations between the structure and other properties relevant for applications requires suitable methods to characterize the size and shape of nanocrystals. Most evident are imaging techniques like transmission electron microscopy (TEM). However, as a disadvantage only a limited number of particles can be evaluated. Powder X-ray diffraction (XRD), in contrast, probes a large ensemble of nanocrystals, but it remains a challenge to reliably extract information on the crystallite size and shape from XRD data. In this work, colloidal chemistry was used to prepare mono- and bimetallic Pt and Pt/Sn nanocrystals as well as semiconductor nanocrystals of ZnO, CuInS2 and composite particles consisting of CuInS2 and Cu2S. The samples were analyzed by TEM and XRD. Rietveld refinement of XRD data was done with a program enabling to simulate also anisotropic crystallite shapes. This approach turned out to be suitable for the determination of the average size and shape, in particular also in the case of nanorods and composite nanomaterials.

MI 4.6 Tue 11:00 EMH 225

Strain measurement in semiconductor nanostructures by convergent electron nanoprobe diffraction — •Knut Müller[1], Andreas Rosenauer[1], Marco Schowalter[1], Josef Zweck[2], Rafael Fritz[3], and Kerstin Volz[3] — [1]Universität Bremen, Germany — [2]Universität Regensburg, Germany — [3]Universität Marburg, Germany

The fundamental but simple Bragg law is exploited to measure lattice strain with a precision of $7\cdot 10^{-4}$ and a spatial resolution of $0.5-0.7$ nm directly from convergent beam electron diffraction (CBED) patterns. In particular, we present 3 different algorithms for pattern recognition to measure CBED reflection positions accurately: The first detects edges in a patch around each CBED disc and iteratively finds all edge points which lie on the disc boundary by circle fitting. The second takes a rotational average in the patch and maximises the gradient in radial direction by optimising the centre of the rotational average. The third and fastest method exploits cross-correlations between each reflection patch and different types of masks. Besides results for a 350 nm wide $In_xGa_{1-x}N_yAs_{1-y}/GaAs$ highly strained quantum layer stack with alternating compressive/tensile strain, we present prospects for the operation and acquisition hardware of a TEM, directly deduced from the three algorithms above to allow for a fast strain map acquisition directly at the microscope in future. For the present study we operated an FEI Titan (S)TEM microscope in STEM mode to record a series of energy filtered CBED patterns on CCD.

15 min. break

MI 4.7 Tue 11:30 EMH 225

Theory of Electron Magnetic Circular Dichroism — •Jan Rusz — Dept. of Physics and Astronomy, Uppsala University, Sweden

Electron magnetic circular dichroism (EMCD) is an electron microscopy analogue of the established x-ray magnetic circular dichroism, that can provide atom-specific spin and orbital moments. EMCD, compared to its x-ray counterpart, offers a potential of significantly better spatial resolution, potentially in the Angstrom range. Presently, the technique is limited by difficulties of reaching sufficient signal to noise ratio and complexity of the accompanying dynamical diffraction effects, both of which make quantitative analysis demanding and prone to systematic errors.

We present recent theoretical developments in the field of EMCD, namely, 1) influence of plural scattering and associated spectral post-processing corrections; 2) convergence of the dynamical diffraction calculations in electron energy loss spectroscopy (ELNES), and 3) decomposition of the signal in diffraction plane to maps of various irreducible operators, such as orbital and spin magnetic moments, number of holes, orbital and spin-orbital anisotropy tensors.

These developments improve our understanding of deviations of recent quantitative EMCD experiments from expected values, allow more accurate predictions of the signal distribution, and uncover the wealth of information contained in electron energy loss spectra and thus aid in improving the methods of extraction of the magnetic signal from experimental datasets.

MI 4.8 Tue 11:45 EMH 225

Magnetic structure of magnetoelectric $NdFe_3(BO_3)_4$ under applied magnetic fields — •Jorge E. Hamann-Borrero[1], Sven Partzsch[1], Sergio Valencia[2], Claudio Mazzoli[3], Christian Hess[1], A. Vasiliev[4], L. Bezmaternikh[5], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW-Dresden — [2]Helmholtz-Zentrum-Berlin — [3]ESRF, Grenoble, France — [4]Moscow State University, Russia — [5]L. V. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia

The magnetic structure of the magneto-electric $NdFe_3(BO_3)_4$ is studied by means of Resonant X-ray Magnetic Scattering (RXS) at the Nd $L_{2,3}$ and Fe K edges. The temperature dependent experiments show below $T_N = 30$ K the appearance of commensurate (CM) magnetic superlattice reflections with Miller indices $(0, 0, l \pm 3/2)$ (where $l = 3n$ and $n =$ integer). By further cooling, at $T_{ICM} \sim 16$ K, a transition into an incommensurate (ICM) spin helix structure is observed in agreement with recent neutron experiments[1, 2]. Detailed mean field based analysis of the x-ray diffracted intensities show, that the Nd and Fe magnetic sublattices behave differently. In fact the magnetization of the Nd sublattice is induced by the Fe moments. At $T<T_{ICM}$, by applying an external magnetic field **B** parallel to the *ab*-plane, the magnetic structure suffers a reorientation transition from a spin helix configuration to a collinear structure where all the moments align perpendicular to **B** in the basal plane.

[1] M. Janoschek et al. Phys. Rev. B, 2010, 81, 094429
[2] P. Fischer et al. Jour. Phys. Cond. Matt., 2006, 18, 7975-7989(15)

MI 4.9 Tue 12:00 EMH 225

Monoclinic Symmetry in Barium Titanate — Christian Eisenschmidt, •Hans Theo Langhammer, and Günther Schmidt — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik

The tetragonal-orthorhombic phase transition of barium titanate crystals has been investigated by XRD measurements during slow cooling. Additional diffuse scattering intensity between the (002) and (200) reflexes as well as a shift of the (200) reflex towards higher 2Θ values develop with decreasing temperature and time. The tetragonal-orthorhombic phase transition takes place obviously via a monoclinic intermediate stage. This can be understood by assuming this order-disorder phase transition is initiated by increasing short-range order (SRO) of Ti ions followed by rearranging of Ba ions similar to the 'tetragonal' SRO below the Burns temperature above the transition cubic-tetragonal. This results, finally, in nucleation and transition to the long-range ordered orthorhombic phase. Conclusions of the proposed mechanism in compositionally disordered systems like Ba(Ti,Sn)O3, PMN-PT et al. are discussed.

MI 4.10 Tue 12:15 EMH 225

Multilayer Optics for Modern X-ray Analytical Equipment — •Andreas Kleine, Jörg Wiesmann, Bernd Hasse, Jürgen Graf, Uwe Heidorn, Steffen Kroth, Frank Hertlein, and Carsten Michaelsen — Incoatec GmbH, Max-Planck-Str. 2, 21502 Geesthacht, Germany

Even 100 years after the first publication of the Bragg equation, there are current developments which are still mainly based on this fundamental law. One of these developments are multilayer optics which are used for beam shaping of X-rays e.g. for focusing the X-rays onto the sample. The multilayer optics simulate an artificial crystal with the typical distance d of the Bragg equation. It is advantageous that this distance can be changed and thus adapted to the specific application and setup. The development of multilayer optics allowed a performance increase of modern diffractometers by more than one order of magnitude.

In this contribution, we will give an overview of current developments of multilayer optics. We will explain the design and the manufacturing process of the optics and give some examples of typical applications which benefit from the new possibilities, especially in combination with modern microfocus X-ray sources. Applications like GISAXS, high-pressure XRD or micro-diffraction known from synchrotrons, can be realized now in the home-lab.

MI 4.11 Tue 12:30 EMH 225

Reconstruction phenomena at the interfaces of $LaCoO_3$ single films: A resonant x-ray reflectivity study — •Jorge E. Hamann-Borrero[1,2], Abdullah Radi[2], Woo Seok Choi[3], Sebastian Macke[4], Ronny Sutarto[5], Feizhou He[5], George A. Sawatzky[2], Ho Nyung Lee[3], and Vladimir Hinkov[4] — [1]IFW-Dresden — [2]University of British Columbia, Vancouver, Canada — [3]Oak Ridge National Laboratory, Materials Science and Technology Division, USA. — [4]Max Planck-UBC Centre for Quantum Materials, Vancouver, Canada — [5]Canadian Light Source, Saskatoon, Canada

A series of $LaCoO_3$ (LCO) single films grown on polar $NdGaO_3$ (NGO) and non polar $SrTiO_3$ (STO) substrates were studied by means of Resonant Soft X-ray Reflectivity (RXRR) and X-ray Absorption Spectroscopy (XAS). The RXRR measurements were performed at photon energies close to the Co $L_{2,3}$ edges. The detailed analysis of the energy dependent measurements at fixed Q values corresponding to maxima and minima of the RXRR Kiessig fringes reveals a strong signal contribution to the line-shapes which can not be attributed to pure Co^{3+}. By considering the polar nature of the LCO structure we find that, at interfaces with polar discontinuity, e.g., at LCO/STO and LCO/Vaccum, reconstruction phenomena take place.

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