

KR 2: Poster Crystallography

Time: Monday 19:00–21:00

Location: Poster C

KR 2.1 Mon 19:00 Poster C

Magnetic properties of high quality single crystals of the electron underdoped cuprate superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ — ●ALMA DORANTES, CAI QI, MARK KARTSOVNIK, and ANDREAS ERB — Walther-Meißner Institut, Walther-Meißnerstraße 8 D-85748 Garching

We present investigations of the magnetic properties of the electron-doped cuprate superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO) with particular attention to the underdoped regime of the phase diagram. Special attention is given to the region between the antiferromagnetic (AF) and superconducting (SC) state of the electron-doped cuprate superconductors. We tried to investigate whether the AF and SC regions are separated by an intrinsic phase separation or if a microscopic coexistence exists between these two states. Experiments on high quality single crystals were performed to probe the relation between the transition temperature (T_c) and dopant concentration x , and to estimate the superconducting volume fraction. The results indicated that a SC transition can be observed after an appropriate annealing process, even for highly underdoped samples and that bulk superconductivity is present. In addition we find indications of a deviation in the monotonic doping dependence of the transition temperature T_c between samples with 12% and 13% Ce doping, which could signify a first evidence of the so-called 1/8 anomaly in the electron-doped cuprate superconductors.

KR 2.2 Mon 19:00 Poster C

Towards neutron scattering experiments with microsecond time resolution — ●FRANZ ALOIS ADLMANN¹, PHILIPP GUTFREUND², JOHN ANKNER³, JIM BROWNING³, ANDRE PARIZZI³, BOGDAN VACALIUC³, CANDICE HALBERT³, JASON RICH³, ANDREW DENNISON², and MAX WOLFF¹ — ¹Uppsala University, Box 516, 751 20, Uppsala, Sweden — ²Institut Laue Langevin, BP 156, 38042, Grenoble, France — ³Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Due to the interaction with the nucleus, neutrons offer unique opportunities for the study of condensed matter. However, the neutron flux on nowadays source is relatively low. To overcome this limitation we have developed a new technique for periodic excitations. Our approach takes full advantage of data storage in list mode combined with the time dependent information on the excitation as meta-data in the event-stream of the neutron data. Re-binning of the neutron data with respect to the periodic excitation is done in the post processing. This has the advantage that the time slices and resolution can be defined after the experiment is completed. We applied our approach in a combined neutron reflectivity and rheology study to probe the solid-liquid interface of a micellar system. LAOS (Large Amplitude Oscillatory Shear) was applied to highlight the complex rheological behavior. We extract the intensity of a Bragg reflection with a time resolution of less than one millisecond and show that it follows the oscillatory shear.

KR 2.3 Mon 19:00 Poster C

Application of polychromatic X-ray Laue diffraction for the analysis of dislocation structures using a PNCCD — ●ALI ABOUD¹, SEBASTIAN SEND¹, ULLRICH PIETSCH¹, CHRISTOPH KIRCHLECHNER², LOTHAR STRÜDER⁴, JEAN SEBASTIAN MICHA⁵, and JOZEF KECKES³ — ¹Department of Physics, University of Siegen, Siegen, 57072, Germany — ²Max Planck Institut für Eisenforschung GmbH, Max-Planck-Str.1, 40237 Düsseldorf, Germany — ³Montanuniversität Leoben, Leoben, 8700, Austria — ⁴PNSensor GmbH, Munich, 80803, Germany — ⁵CEA-Grenoble/DRFMC/SprAM, 17 rue des Martyrs, Grenoble Cedex 9, F-38054, France

uLaue diffraction with a polychromatic X-ray beam can be used to measure strain fields and crystal orientations of micro crystals. In the vicinity of a Bragg reflection the intensity distribution of the reciprocal space is sensitive to the distribution and type of dislocations. By using a pnCCD, the energy and the 2D intensity distribution of the Bragg reflections can be measure simultaneously. This allows to obtain the hydrostatic strain and the deviatoric strain tensors. We present an application of white beam uLaue X-ray diffraction on a bent Copper crystal to measure local strain along the bending beam by using a PNCCD detector.

KR 2.4 Mon 19:00 Poster C

Structural Information Beyond the Ensemble Average From Colloidal Crystals Using X-Ray Cross-Correlation Analysis — ●MATTHIAS KAMPMANN^{1,2}, MICHAEL SPRUNG¹, BILL PEDRINT³, TUSHAR SANT², FALCO ZIEGERT⁴, and CHRISTIAN GUTT² — ¹DESY, Hamburg, Germany — ²Universität Siegen, Germany — ³Paul Scherrer Institut, Villigen, Switzerland — ⁴Universität Rostock, Germany

Fluctuations in X-ray scattering intensity from particle ensembles carry structural information beyond the pure ensemble average, which can be mined using X-ray cross correlation analysis (XCCA). Kam was the first to propose applying higher order intensity correlation functions to solution scattering data of macromolecules for obtaining structural information [Kam1]. His ideas were far beyond the power of X-ray sources and detectors in the 1970s. But they gained new interest with the ultrafast snapshot capabilities of X-ray free-electron laser sources, not only for solving particle structures but also in a more statistical context for densely packed systems [Wochner].

Here we present an XCCA analysis of diluted suspensions of small micrometer sized colloidal crystals. In a coherent X-ray scattering experiment we have measured several thousand diffraction patterns of colloidal sample systems and calculated the corresponding higher order correlation functions. The data reveal strong angular modulations of the XCCA signal, which are a fingerprint of the single particle diffraction properties.

Kam1: Z. Kam, *Macromolecules* 10, 927-934 (1977)

Wochner: P. Wochner et al., *PNAS* 106, 11511-11514 (2009)

KR 2.5 Mon 19:00 Poster C

Kinetics of the hydrogen defect in lithium niobate and lithium tantalate — ●THOMAS KÖHLER, ERIK MEHNER, JULIANE HANZIG, GÜNTER GÄRTNER, HARTMUT STÖCKER, and DIRK C. MEYER — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, 09596 Freiberg, Germany

LiNbO_3 and LiTaO_3 crystals are used in many optical devices, therefore, understanding the structural defects is helpful to control optical and electrical properties. The incorporation of hydrogen in the two materials is investigated by FT-IR and UV/VIS spectroscopy using different crystallographic orientations and excitation polarisations. The aim of the study is the development of a structural model for the kinetic and the diffusion of the OH defect. The examined congruent crystals are cube shaped, cut and polished along the $[2\bar{1}\bar{1}0]$, $[01\bar{1}0]$ and $[0001]$ directions. The used stoichiometric crystals are plates, polished and cut in $[0001]$. Depending on the stoichiometry the hydrogen defect causes an OH band with several sub-bands, at different spectral positions. In congruent material two sub-bands are detectable, whereas near stoichiometric material exhibits four. The composition of the OH band with respect to formation or decline of sub-bands under oxidizing and reducing conditions shows the transport mechanisms within the crystals. The protonation in hot water shows a formation of new sub-bands at higher energies. We have found three and six sub-bands in congruent and near stoichiometric crystals, respectively. The results show that the hydrogen is disordered and can migrate to different binding sites within the crystal.

KR 2.6 Mon 19:00 Poster C

Impact of temperature and barometric pressure fluctuations on X-ray beam intensities — ●TINA WEIGEL¹, MATTHIAS ZSCHORNAK¹, MARCO HERRMANN², MANUEL ROTHENBERGER¹, TILMANN LEISEGANG², and DIRK C. MEYER¹ — ¹Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany — ²Saxray GmbH, Maria-Reiche-Str. 1, 01109 Dresden, Germany

Essential to X-ray analysis in crystallography, such as diffractometry and spectrometry, is a stable and reproducible X-ray beam intensity. Particularly, changes in environmental conditions, such as temperature, humidity and barometric pressure, and cooling water fluctuations can affect the beam intensity significantly. In this comprehensive qualitative as well as quantitative study, the impact of the environmental conditions and cooling water fluctuations on the primary beam intensity of a sealed tube with Cu anode are determined. This should be of wide interest for all who are dealing with X-ray analyzes, in particular in the field of crystallography, where accurate experimental data are

a prerequisite for deriving high-quality structure parameters. With a common set-up, the X-ray intensities are detected by a scintillation counter. Laboratory as well as external conditions are monitored simultaneously. Their individual influence on the X-ray intensity and

their correlations are evaluated by statistical analysis including time lag. The study shows significant correlations in respect to ambient conditions and in particular with daily and weekly cycles, which affect the intensity nearly instantaneous.