BP 4: Symposium SYXD: 100 years of X-ray diffraction: from the Laue experiment to new frontiers (with KR, CPP, DF, MA, MM, GP)

Time: Monday 15:00–17:30 Location: H 0105

Invited Talk BP 4.1 Mon 15:00 H 0105

Disputed discovery: The beginnings of X-ray diffraction in crystals — •Michael Eckert — Deutsches Museum, Forschungsinstitut, Museumsinsel 1, D-80538 München

The discovery of X-ray diffraction in crystals was based on misconceptions about the nature of X-rays. The background of "Laue's discovery" and its early repercussions are described from the perspective of contemporary views in 1912. The riddle concerned the origin of the monochromacy observed in the Laue spots.

Invited Talk BP 4.2 Mon 15:30 H 0105

Why are quasicrystals quasiperiodic? — •Walter Steurer — Laboratorium für Kristallographie, ETH Zürich, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Schweiz

It took more than two years until Dan Shechtman could publish his finding of a rapidly solidified Al-Mn phase with sharp Bragg reflections and icosahedral point group symmetry. His results were not accepted, initially, since they seemed to contradict fundamental laws of crystallography. A further twenty-seven years had to pass by until his discovery of quasicrystals was honoured by the Nobel Prize in 2011. This discovery was fundamental because quasiperiodic order represents a novel equilibrium state of solid matter fundamentally different from the common periodic one.

At present, stable quasicrystals have been found in more than fifty binary and ternary intermetallic systems. They show mostly decagonal or icosahedral diffraction symmetry contrary to soft quasicrystals. These are mainly qasiperiodic structures resulting from the self-assembly of either micelles in a liquid or of terpolymers with dodecagonal symmetry. The so far most promising applications of quasiperiodic structures seem to be in the field of photonic and phononic crystals.

The focus of the talk will be on the driving forces for the formation and stablization of quasiperiodic structures.

Invited Talk BP 4.3 Mon 16:00 H 0105

Coherent Diffraction Imaging with Free-Eletron Lasers — •Massimo Altarelli — European XFEL GmbH, 22607 Hamburg

One hundred years after the discovery of x-ray diffraction from crystals, spatially coherent, ultra-brilliant and ultra-short pulses of x-ray radiation from free electron lasers (FEL's) open the way to structure solution without the hurdle of crystallization. Biological objects such as cells, viruses, possibly down to individual macromolecules and to atomic resolution, and individual nanostructures in material sciences are eligible for these novel studies. An overview of the x-ray FEL sources and their basic physical principles and properties, of the strategies for sample handling and data collection and a glimpse of the necessary algorithms to phase the diffraction patterns are given. Example of results from the soft x-ray FLASH source in Hamburg and from the Linac Coherent Light Source in Stanford are illustrated. The perspectives and the challenges of the high repetition rate (up to 27 000 pulses/s) of the European XFEL, under construction in the Hamburg region, are also briefly discussed

Invited Talk BP 4.4 Mon 16:30 H 0105

X-ray free-electron lasers - emerging opportunities for structural biology — •Ilme Schlichting — Max Planck Institute for Medical Research, Heidelberg, Germany

X-ray crystallography is a mature yet still advancing method for structure determination of molecules with any molecular weight. Facilitated greatly by synchrotron X-ray sources, the method is limited only by the quality and size of the crystals and by radiation damage. Free-electron lasers (FELs) provide orders of magnitude brighter and shorter X-ray pulses than conventional synchrotron sources. It has been proposed that radiation damage, which limits the high resolution imaging of soft condensed matter, can be "outrun' by using ultrafast and extremely intense X-ray pulses that pass the sample before the onset of significant radiation damage [1]. Thus, one of the most promising scientific applications of XFELs is in sub-nanometer resolution imaging of biological objects, including viruses, macromolecular assemblies, and nanocrystals. The concept of "diffraction-before-destruction" has been demonstrated recently at the Linac Coherent Light Source (LCLS) [2], the first operational hard X-ray FEL, for protein micro- and nanocrystals [3] and single mimivirus particles [4]. These experiments and recent developments and progress will be presented.

[1]. Neutze et al., Nature 406, 752-757 (2000). [2]. Emma, Nature Photonics 4, 641-647 (2010). [3]. Chapman et al., Nature 470, 73-77 (2011). [4]. Seibert et al., Nature 470, 78-81 (2011).

Invited Talk BP 4.5 Mon 17:00 H 0105

Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling — •Tim Salditt — Georg-August-Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Classical x-ray diffraction has been based on three constraints: (i) averages over macroscopic accumulation time and sample sizes, which are many orders of magnitude larger than the structures to be resolved; (ii) homeogeneous "well ordered" samples which are - if not crystalline - characterized by well-defined correlation functions; (iii) data analysis by fitting to modeled diffraction data. However, many condensed matter problems, in particular in functional materials, soft matter and biomolecular samples, address non-equilibrium states with competing length scales, hierachical structures, and intrinsic dynamics. Progress in x-ray sources and optics has helped to meet these challenges. Conceptually often still close to the Laue experiment, far-field diffraction data can now be collected in controllable field of vies, with highly focused beams reaching the 10 nm range. Biomolecular diffraction signals can be recorded from hierachical structures such as a biological cells. Perhaps most importantly, fully coherent illumination enables data inversion without prohibitive model building. How these advances serve science, will be illustrated by examples in neuro-biophysics. We present experiments addressing different structural levels and bridging length scales, from proteins and lipid assemblies up to a complete organelle such as the synaptic vesicle, from an isolated axon up to an unsliced nerve, from tissue slice to the sensory organ.