Symposium Diffractive Imaging (SYDI)

jointly organized by
the Molecular Physics Division (MO) and
the Atomic Physics Division (A)

Jochen Küpper
Fritz-Haber-Institut der MPG
Faradayweg 4-6
14195 Berlin
jochen@fhi-berlin.mpg.de

Overview of Invited Talks and Sessions

(lecture room E 415)

Invited Talks

SYDI 1.1	Fr	10:30–11:00	E 415	**Flash diffraction imaging with X-ray lasers** — •Janos Hajdu
SYDI 1.2	Fr	11:00–11:30	E 415	**The hitchhikers guide to cryo-electron tomography - A voyage to the inner space of cells** — •Juergen Plitzko
SYDI 1.3	Fr	11:30–12:00	E 415	**Far-Field Optical Nanoscopy by Optical Switching** — •Andreas Schönle, Stefan Hell
SYDI 1.4	Fr	12:00–12:30	E 415	**Coherent Diffractive Imaging at LCLS** — •Henry Chapman
SYDI 2.1	Fr	14:00–14:30	E 415	**High Harmonic Generation from Molecules: Prospects for ultra-fast imaging of molecular structure and dynamics** — •Jonathan Marangos
SYDI 2.2	Fr	14:30–15:00	E 415	**Time-resolved diffraction from selectively aligned molecules** — •Ernst Fill, Martin Centurion, Peter Reckenthäler, Werner Fuss, Ferenc Krausz
SYDI 2.3	Fr	15:00–15:30	E 415	**Imaging Molecules from Within: Ultra-fast Structure Determination of Molecules via Photoelectron Holography with Free Electron Lasers.** — •Joachim Ullrich, Faton Krasniqi, Bennaeur Najjari, Alexander Voitkiv, Sascha Epp, Daniel Rolles, Artem Rudenko, Lothar Strüder
SYDI 2.4	Fr	15:30–16:00	E 415	**Ultrafast processes and imaging of clusters** — •Thomas Möller

Sessions

SYDI 1.1–1.4	Fr	10:30–12:30	E 415	**Imaging of biological systems**
SYDI 2.1–2.4	Fr	14:00–16:00	E 415	**Diffractive Imaging of complex molecules in the gas-phase**

SYDI 1: Imaging of biological systems

Time: Friday 10:30–12:30 Location: E 415

Invited Talk SYDI 1.1 Fr 10:30 E 415

Flash diffraction imaging with X-ray lasers — •Janos Hajdu — Laboratory of Molecular Biophysics, Uppsala University, Husargatan 3 (Box 596), SE-751 24 Uppsala, Sweden

Short, intense and coherent pulses from X-ray lasers provide exciting new capabilities in understanding the structure of biological cells, complex materials, and matter under extreme conditions. In previous work at FLASH (Hamburg), we have demonstrated that the imaging process can be faster than the damage process, which is a significant step towards our long-term goal of single-particle imaging at atomic resolutions. Biomolecular imaging has become one of the most exciting potential applications of X-ray lasers like the Linac Coherent Light Source (LCLS) at Stanford. However, the rate at which a large biomolecule explodes in the LCLS pulse while it is being imaged is one of the largest unknowns in this kind of experiment and will likely be one of the major factors in determining if such imaging will succeed. The dynamics of this explosion are complex, depending on an interplay of various aspects of energy deposition, evolution of ionization, and electron heating in the system. Therefore, it is a high priority to understand these dynamics. Experiments at the LCLS-AMO end station explore the underlying physics of how the LCLS pulse deposits energy in large clusters of atoms/molecules and the nature of the subsequent explosion. In parallel, new imaging experiments were also performed at LCLS and show interpretable diffraction data from single virus particles. The talk will survey recent experimental results.

Invited Talk SYDI 1.2 Fr 11:00 E 415

The hitchhikers guide to cryo-electron tomography - A voyage to the inner space of cells — •Juergen Plitzko — Max Planck Institute of Biochemistry, Department of Molecular Structural Biology, Martinsried, Germany

'One Picture is Worth Ten Thousand Words'; this slogan from former times depicts clearly the fact that human beings are, by and large, visually centred. A long hold dream, for example, of biologists is the ability to 'zoom' in on very fine details of living matter, literally in one go, from the complete organism to one single cell and beyond. However, today, we have to utilize different microscopes operating at different resolution levels to make this dream halfway come true. Therefore researchers use different probing signals to cover the different length scales and to visualize the gamut of organic and cellular functions. The cornucopia of available imaging methods and techniques is enormous, and we have already travelled a long way to reach our ultimate goal - the voyage to the inner space of cells. At the level of a single cell we might think that we already know a great deal, but at the supramolecular level the cell is still an uncharted territory. With this presentation we are trying to explain in detail the method of cryo-electron tomography and to teach the audience in the major concepts of tomographic imaging for structural biology. Moreover, we want to provide an outlook into future developments especially regarding hybrid approaches, where several methods are combined to work in unison for the one goal, which we have already stated - a voyage to the inner space of a cell.

Invited Talk SYDI 1.3 Fr 11:30 E 415

Far-Field Optical Nanoscopy by Optical Switching — •Andreas Schönle and Stefan Hell — Dept. for NanoBiophotonics, MPI f. biophysical Chemistry, Göttingen, Germany

In 1873 Ernst Abbe recognized that the resolution of every far-field microscope is fundamentally limited by diffraction and this barrier is indeed an unalterable fact for purely optical imaging. For more than a century it was thus naturally assumed that imaging systems operating with visible light will never be able to resolve features smaller than about 250nm. However, recent advances in optical microscopy have radically overcome this limit and resolutions of better than 10nm have been demonstrated. This groundbreaking development is based on the simple but powerful insight that the light-dye interaction rather than the propagation of waves have to be put at the core of the image formation process: The ability to transiently confine adjacent molecules to different states allows the time-sequential recording of spatial features thus eluding the limitations of diffraction. In 1994, the invention of stimulated emission depletion (STED) microscopy demonstrated the feasibility of this approach and several other more or less related diffraction-unlimited far-field optical approaches were successfully implemented since then. All these techniques switch molecules between states in order to record them sequentially in time, either by addressing molecule ensembles inside sub diffraction sized volumes or by stochastically turning on isolated single markers. The resulting resolution is then no longer fundamentally limited by diffraction and can be pushed to the macromolecular scale.

Invited Talk SYDI 1.4 Fr 12:00 E 415

Coherent Diffractive Imaging at LCLS — •Henry Chapman — CFEL, DESY, Hamburg, Germany

The ultrafast pulses from X-ray free-electron lasers may enable the determination of structures of proteins that cannot be crystallized. The specimen would be completely destroyed by the pulse, but that destruction will ideally only happen after the termination of the pulse. In order to address the many challenges that we face in attempting molecular diffraction, we have carried out experiments in coherent diffraction from protein nanocrystals at the Linac Coherent Light Source (LCLS) at SLAC. The periodicity of these objects gives us much higher scattering signals in order to determine the effects of pulse duration and fluence on the high-resolution structure of single objects. The crystals are filtered to sizes less than 2 micron, and delivered to the pulsed X-ray beam in a liquid jet. Diffraction patterns are recorded at the LCLS repetition rate with pnCCD detectors. Preliminary results will be presented on our first LCLS experiments.

This work was carried out as part of a collaboration, for which Henry Chapman is the spokesperson. The collaboration consists of CFEL DESY, Arizona State University, SLAC, Uppsala University, LLNL, The University of Melbourne, LBNL, the Max Planck Institute for Medical Research, and the Max Planck Advanced Study Group (ASG) at the CFEL. The experiments were carried out using the CAMP apparatus, which was designed and built by the Max Planck ASG at CFEL. The LCLS is operated by Stanford University on behalf of the U.S. Department of Energy, Office of Basic Energy Sciences.

SYDI 2: Diffractive Imaging of complex molecules in the gas-phase

Time: Friday 14:00–16:00 Location: E 415

Invited Talk SYDI 2.1 Fr 14:00 E 415

High Harmonic Generation from Molecules: Prospects for ultra-fast imaging of molecular structure and dynamics — •Jonathan Marangos — Imperial College London, UK

High harmonic generation (HHG) in a strong laser field is a coherent and highly non-linear process. It is initiated by laser ionisation and the key component of the process is the laser driven recombination of an energetic (10 - 100 eV) electron with the molecular ion. This results in emission of a broad spectrum of coherent XUV radiation that encodes within it information on the electronic and nuclear wavefunctions of the molecule. In this presentation I will talk about recent results from my own group using molecular HHG for measuring molecular structure and dynamics and speculate about the future prospects for this method for attosecond reolved atomic scale imaging of matter.

Invited Talk SYDI 2.2 Fr 14:30 E 415

Time-resolved diffraction from selectively aligned molecules — •Ernst Fill[1], Martin Centurion[2], Peter Reckenthäler[1], Werner Fuss[1], and Ferenc Krausz[1] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching — [2]Dept. of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588-0111, USA

The random directions of molecules in a gas result in diffraction patterns in the form of isotropic rings. Their evaluation yields information only on the radial distribution function i.e. on interatomic distances. However, by dissociation with linearly polarized light molecules are partially aligned and the pattern becomes anisotropic. In our experiments the iodide C2F4I2 is dissociated by fs UV pulses and molecular difference intensities and difference radial distribution curves are measured for directions parallel and perpendicular to the direction of polarization. The curves clearly demonstrate transient anisotropy of the diffraction pattern. The anisotropy decays by molecular rotation with a time constant depending on the rotational temperature. In our experiments we measure decay within 2.6 ps. This experiment is a first step towards the determination of the structure of complicated molecules by alignment methods.

Invited Talk SYDI 2.3 Fr 15:00 E 415

Imaging Molecules from Within: Ultra-fast Structure Determination of Molecules via Photoelectron Holography with Free Electron Lasers. — •Joachim Ullrich[1,2], Faton Krasniqi[2], Bennaeur Najjari[1], Alexander Voitkiv[1], Sascha Epp[2], Daniel Rolles[2], Artem Rudenko[2], and Lothar Strüder[3] — [1]Max-Planck-Institut für Kernphysik, Heidelberg, Germany — [2]Max Planck Advanced Study Group, Center for Free Electron Laser Science, Hamburg, Germany — [3]MPI Halbleiterlabor, München

A new scheme is suggested based on (i) brilliant X-ray Free Electron Laser sources, (ii) novel energy and angular dispersive, large-area electron imagers and (iii) the well-known photoelectron holography that shall provide time-dependent three-dimensional structure determination of small to medium sized molecules with sub-Angström spatial and femtosecond time resolution. Inducing molecular dynamics, i.e. wave-packet motion, dissociation, passage through conical intersections or isomerization, by a pump pulse this motion is visualized by the X-ray - laser probe pulse launching keV photoelectrons within few femtoseconds from specific and well-defined sites, deep core levels of individual atoms, inside the molecule. On their way out the photoelectrons are diffracted generating a hologram on the detector that encodes the molecular structure at the instant of photoionization, thus providing femtosecond snapshot images of the molecule from within. The technology allows obtaining time-dependent structure information for classes of samples not accessible otherwise such as aligned, oriented or conformer selected molecules or ultra-cold ensembles.

Invited Talk SYDI 2.4 Fr 15:30 E 415

Ultrafast processes and imaging of clusters — •Thomas Möller — IOAP, Technische Universität Berlin

The understanding of the interaction of high intensity, short-wavelength, short-pulse radiation with matter is essential for virtually all experiments with new superintense X-ray sources [1], in particular for flash imaging of nm sized particles. Clusters as a form of matter intermediate between atoms and bulk solids are ideal samples to study fundamental light matter interaction processes. They are finite systems with the density of bulk solids allowing the investigation of inner- and interatomic phenomena. Very recently, initial experiments have shown that in nm-sized gas phase particles can be imaged by single shot scattering. X-ray lasers and advanced detectors [2] allow improving the resolution and going to smaller particles. This opens new fields in cluster and nanometer-scale science. Ultrafast electron and ion dynamics can be studied with nm spatial resolution by means of time-resolved scattering using pump-probe techniques as well as time of flight spectroscopy [3].

[1] Bostedt, C. et al. Experiments at FLASH. Nucl. Instr. Meth. 601, 108-122 (2009).

[2] Strüder, L. et al. Large-Format, High-Speed, X-ray pnCCDs Combined with Electron and Ion Imaging Spectrometers in a Multipurpose Chamber for Experiments at 4th Generation Light Sources. Nucl. Instr. Meth. A, accepted (2009).

[3] Bostedt, C. et al. Multistep ionization of argon clusters in intense femtosecond extreme ultraviolet pulses. Phys. Rev. Lett. 100 (2008).