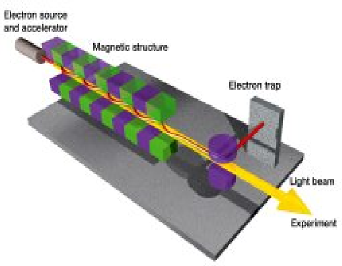
DEMOKRITOS
NATIONAL CENTER FOR SCIENTIFIC RESEARCH

Γεωπονικό Πανεπιστήμιο Αθηνών
Agricultural University of Athens

ΕΘΝΙΚΟ ΙΔΡΥΜΑ ΕΡΕΥΝΩΝ 1958

BE/OPT-XFEL

Δίκτυο για την βελτιστοποίηση της αξιοποίησης του Ευρωπαϊκού X-FEL
από την Ελληνική Επιστημονική Κοινότητα
Network to optimize use of the European X-FEL by the Greek Research Community



WORKSHOP ON XFEL RADIATION & ITS APPLICATIONS

Athens 2010

www.xfel.gr **June 18-19, 2010 NCSR "Demokritos", Aghia Paraskevi, Athens, GREECE**

Program and Abstracts

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WORKSHOP ON XFEL RADIATION & ITS APPLICATIONS

June 18-19, 2010

Main Amphitheater,

NCSR “Demokritos”, Aghia Paraskevi, Athens, Greece

Organized by the National Center for Scientific Research “Demokritos”, the National Hellenic Research Foundation and the Agricultural University of Athens, in the framework of the BE/OPT-XFEL network (www.xfel.gr) funded by the General Secretariat for Research & Technology.

PROGRAM

Friday 18-6-2010

9:00-9:30	***Registration***	
9:30-10:00	***Opening address***, *General Information about the BE/OPT-XFEL*	**Michael Kokkinidis** IMBB & Univ. of Crete , Heraklion, Crete, Greece
1st session	***Introduction: Science***	
10:00-10:40	*The European X-ray Free-Electron Laser in Hamburg*	**Massimo Altarelli** European XFEL, GmbH, Germany
10:40-11:20	*The Linac Coherent Light Source at SLAC: Facility and early science*	**Jochen Schneider** DESY/Hamburg & CFEL, Germany
11:20-11:40: ***Coffee Break***		
2nd session	***Instrumentation***	
11:40-12:20	*European XFEL scientific applications and the related instrumentation*	**Thomas Tschentscher** European XFEL, GmbH, Germany
12:20-13:00	*Undulator systems for the European X-Ray Free Electron Laser*	**Joachim Pflüger** DESY/HASYLAB-Hamburg, Germany
13:00-14:30: ***Light Lunch***		

3rd session	***Time resolved/ high field applications***	
14:40-15:20	*Optical and X-ray studies of the ultrafast molecular dynamics in solutions*	**Majed Chergui** École Polytechnique Fédérale, Lausanne, Switzerland
15:20-16:00	*Time resolved photoemission of highly correlated materials*	**Luca Perfetti** Ecole Polytechnique Palaiseau, Paris, France
16:00-16:20: ***Coffee Break***		
4th session	***More on time resolved***	
16:20-17:00	*Clusters exposed to intense optical and vacuum-ultraviolet laser pulses*	**Josef Tiggesbäumker** Universität Rostock, Rostock, Germany
17:00-17:40	*Non-linear processes in simple atoms and molecules interacting with vuv and xuv short laser pulses*	**Henri Bachau** Université Bordeaux, France

Saturday 19-6-2010

1st session	***Application in Biological samples***	
10:00–10:40	*Diffractive Imaging of Biological Specimens with Intense, Coherent X-rays*	**Changyong Song** RIKEN SPring-8 Center, Harima Institute, Sayo, Japan
10:40–11:20	*Biological Applications at the European XFEL*	**Edgar Weckert** DESY-Hamburg, Germany
11:20-11:40: ***Coffee Break***		
2nd session	***Material Sciences***	
11:40-12:20	*Probing Magnetism by X-Ray Scattering and Holography*	**Stefan Eisebitt** Technische Universität Berlin, Berlin, Germany
12:20-13:00	*The X-ray Correlation Spectroscopy Instrument at the Linac Coherent Light Source*	**Aymeric Robert** Linac Coherent Light Source, SLAC National Accelerator Laboratory, Stanford, USA

13:00-13:40	*Pump-probe XFEL coherent diffraction imaging of femtosecond laser irradiated Au nanocrystals*	**Loren Beitra** London Centre for Nanotechnology, University College London, UK (Prof. I. Robinson's lab)
13:40–14:45: ***Light Lunch***		
14:45–17:00	**Round Table,** **Closing remarks**	**All speakers**

1. The European X-ray Free-Electron Laser in Hamburg. Massimo Altarelli, *European XFEL GmbH, 22607 Hamburg, Germany.*

Synchrotron light sources have contributed in the last decades to a revolution in photon science. The constant improvement in brilliance of storage ring sources is however attaining its basic physical limits.

There is at present a worldwide flurry of activity towards the realization of free electron laser (FEL) UV and X-ray sources to produce spatially coherent, ultra-short (~ *100 fs* or less) pulses with very high peak brilliance (in excess of 10^{28}-10^{32} *photons / s / mm*^{2} */ mrad*^{2} */ 0.1% bandwidth*). These sources overcome the intrinsic limits to the brilliance imposed by the storage ring geometry, where the same electrons radiate millions of time per second, with a single-pass geometry, based on linear accelerators (linacs). The scientific case includes time-resolved studies of dynamics on sub-ps scales, structural studies by imaging of non-periodic systems, and investigation of high-energy density phenomena such as the phase diagram of warm dense matter and non-linear x-ray optics.

The European XFEL project in Hamburg is an international effort, aiming to attain the hard X-ray region, with wavelengths of order *0.1 nm* or less, and with the high repetition rate allowed by the superconducting linac technology. The project is presented and discussed, with reference to the presently operational facilities, FLASH at DESY and LCLS in Stanford.

2. The Linac Coherent Light Source at SLAC: Facility and Early Science. Jochen R. Schneider, *Deutsches Elektronen-Synchrotron DESY Center for Free-Electron Laser Science CFEL,* email: Jochen.Schneider@desy.de.

Already in 1992, at a workshop on 4th Generation Light Sources at SLAC, the suggestion was made to use of the existing SLAC linac equipped with low emittance electron guns to drive 4 nm to 0.1 nm free-electron lasers. Seventeen years later, on April 10, 2009, lasing at saturation at 0.15 nm wavelength was demonstrated at LCLS. Operation for users started in October 2009 providing beam in the spectral range from 0.8 to 2 keV at the AMO station. 11 experiments were scheduled and performed very successfully. Most of the experiments benefited largely from the fact that the pulse duration at LCLS could be varied routinely between ~10 and 300 fsec by changing bunch charge and compression. As a result of the stunning success of LCLS start up the Department of Energy initiated a 380 M& upgrade program.

After a presentation of layout and current performance of LCLS results of the first experiments will be discussed to the extend material is available. A short presentation of the upgrade plans will be followed by a brief comparison of LCLS with the other FEL facilities under construction, planed or discussed in Asia, Europe and the US.

3. European XFEL scientific applications and the related instrumentation. Thomas Tschentscher, *European XFEL GmbH, Albert-Einstein-Ring 19, 22671 Hamburg, Germany.*

X-ray free-electron lasers (FEL) using very small emittance high energy electron accelerators provide intense, ultrashort and high brilliance short-wavelength radiation. FEL radiation is recognized for its transverse coherence, pulse durations approaching 10 fs and pulse intensities of

order 10^{12} – 10^{14} photons per pulse. Applications of FEL radiation have been proposed in a wide range of natural sciences (e.g. physics, geo-sciences, chemistry, life sciences and, of course, interdisciplinary areas). The scientific results from the first years of operation of FLASH show applications in many different fields of physics and have obtained a very high visibility. In addition, important instrumentation developments could be started at FLASH which will enable broadening scientific applications to further areas of science. An overview of some of the most important scientific applications of FEL radiation will be presented. Further it will be emphasized how the scientific applications drive instrumentation needs. Examples of particular interesting instrumentation efforts will be presented.
A further particular aspect is the instrumentation aspects related to the specific time structure of the European XFEL with repetition rates going up to 4.5 MHz. Examples are specific developments that have started in areas such as x-ray area detectors and ultrafast femtosecond optical lasers. Here, the current status will be reported.

4. The Undulator Systems for the European X-Ray Free Electron Laser. Joachim Pflüger, *DESY/HASYLAB-Hamburg, Germany.*

The European X-Ray Free Electron Laser (XFEL.EU) will use the SASE (Self Amplified Spontaneous Emmision) principle to generate radiation in the wavelength range 0.1 to 1.6 nm and even below. A central role in the XFEL.EU play the three undulator systems with lengths up to 220m called SASE1, SASE2 and SASE3 in which the FEL process takes place and the radiation is generated. In the presentation the plans for these undulator systems, their design and properties are described in detail. An overview is given on system requirements and research and development activities. Future plans and schedule are presented.

5. Optical and X-ray studies of the ultrafast molecular dynamics in solutions. Majed Chergui, *Laboratoire de Spectroscopie Ultrarapide (LSU), Ecole Polytechnique Fédérale de Lausanne, Faculté des Sciences de Base, ISIC, Bât. CH, Station 6.* Email: Majed.Chergui@epfl.ch

By combining various ultrafast laser techniques with ps and fs X-ray absorption spectroscopy, we can fully identify the photocycle of solvated systems. We will review some of our recent results on the solvation shell changes around atomic solutes, on binuclear molecular complexes, and on the structural changes induced by electron transfer and spin changes in metal-based molecular complexes.

6. Time resolved photoemission of highly correlated materials. Luca Perfetti, *Ecole Polytechnique Palaiseau, Paris, France*

Albeit most of the experiments are performed in equilibrium conditions, new horizons of condensed matter physics can be explored when a strong perturbation drives the system into a highly exited state. After the absorption of an ultrashort laser pulse, the interatomic forces that bind the atoms can be substantially altered, leading to propagation of lattice waves or to sudden structural changes. Since the pathway to non equilibrium states evolves on the femtosecond timescale, any experimental observation of the nuclei and electrons motion is especially challenging. In our approach, an intense and ultrashort laser pulse perturbs the system, while an ultraviolet source induces the emission of photoelectrons after a variable time delay. Such technique exploits the high potentials of photoelectron spectroscopy for the investigation of ultrafast insulator-metal transitions in Mott insulators, coherent lattice motion in charge density wave materials, and electron-phonon coupling in high temperature superconductors. We will show that time resolved techniques provide novel information on many-body interactions that would not be accessible by standard means.

7. Clusters exposed to intense optical and vacuum-ultraviolet laser pulses. Josef Tiggesbäumker, *Institut für Physik, Universitätsplatz 3, 18051 Rostock, Germany*.
Email:josef.tiggesbaeumker@uni-rostock.de.

The advent of new laser sources like FLASH covering the extended ultraviolet (EUV) spectral range has opened the possibility to explore the electronic properties of size-selected clusters giving direct excess to the geometry through the measurement of their chemical shifts or to optical properties when performing single pulse scattering studies. First successful attempts into this direction will we presented. In addition, short wavelength and strong field conditions can be tackled. With changing the photon energy, the cluster response modifies from the field driven for optical laser pulses to the photon driven regime when EUV pulses are used. In this talk we outline experiments comparing the response of small particles to intense pulses in both scenarios. Finally FLASH radiation will be used to characterize warm dense matter targets.

8. Non-Linear processes in simple atoms and molecules interacting with vuv and xuv short Laser pulses. H. Bachau, *Université Bordeaux, France*.

The development of laser sources like the free electron laser (FEL) or high order harmonic generation (HOHG) provides laser pulses with typical wavelengths ranging from the vacuum ultraviolet (vuv) to the soft x-ray regions with intensities up to 10^{14} W/cm^{2}. These experimental developments have opened up new research areas in non-linear science like two-photon double ionization (TPDI) of atoms and the ionization of simple molecules (H_2,H_2^+ …) through the absorption of few vuv photons. The other important characteristic of these vuv/xuv pulses is their durations, which go from the attosecond for HOHG to the femtosecond regime for the FEL, i.e., the time scales of the electronic and nuclear motion in small molecules, respectively. Therefore we expect that the ionization dynamics of atoms and molecules is strongly affected when the pulse duration reaches the femtosecond and sub-femtosecond regime. We will present recent results for TPDI of helium, with a special focus on sub-femtosecond pulse duration and related correlation effects. Nuclear interference effects occurring during three-photon ionization of H_2^+ in femtosecond regime will be also presented.

9. Diffractive Imaging of Biological Specimens with Intense, Coherent X-rays. Changyong Song, *RIKEN SPring-8 Center, Harima Institute, 1-1-1 Kouto, Sayo, Hyogo 679-5148 Japan.*

X-ray imaging technique has been advanced rapidly as high resolution analytic microscopy. Notwithstanding the inherited benefits with synchrotron x-rays, x-ray imaging of non-crystalline specimens has generally been challenged; difficulty in acquiring crystalline specimens or a focusing lens. These have limited its application in general bio-imaging at near atomic resolution. The x-ray diffractive imaging technique expects to provide a breakthrough. A series of developments has matured the technique to demonstrate noninvasive 3D imaging of whole biological cells and organelles at a few tens of nm resolution. This imaging technique, further with the advent of bright and short-pulse x-ray lasers, aims to bring forth near atomic resolution 3D imaging of single-macromolecules. In this talk, I will introduce our recent progress on diffractive imaging by using hard x-rays and a prototype EUV-FEL of SPring-8 Compact SASE Source. Its perspective as a high resolution and high contrast imaging probe will also be discussed.

10. Biological Applications at the European XFEL. Edgar Weckert, *DESY-Hamburg, Germany.*

X-ray free electron lasers (XFELs) will provide radiation with unique properties such as photon pulse lengths likely below 10 fs, extremely high peak brilliances and intensities, as well as an almost coherent beam in the transverse direction. These properties have opened up totally new options for experiments in life sciences. The transverse coherent radiation allows for diffraction experiments of non translation periodic objects. In conjunction with sufficient oversampling of the diffraction pattern the solution of the phase problem for reconstructing the object is straight forward. This method bears the potential to obtain the structure of larger biological particles like viruses or huge complexes without the need to grow crystals. The actual limits for this technique with respect to the smallest possible particle size and achievable resolution are under investigation at present. First results look very promising. The same method can also be applied to nano and micro crystals of biological molecules if it is not possible to grow larger crystals.
A second possible application in biology will be time resolved studies. XFEL radiation will enable to follow the steps of chemical as well as biological reactions with so far unprecedented temporal resolution enabling deeper insight for example in basic processes like vision and light harvesting.

11. Probing Magnetism by X-Ray Scattering and Holography. Stefan Eisebitt, *Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany.* Email: eisebitt@physik.tu-berlin.de

Coherent scattering techniques encode information on a sample beyond statistical averages. If carried out with x-rays in resonance with electronic transitions, coherent scattering can provide unique magnetic information with high spatial resolution. Images of magnetic nano objects can be obtained by solving the phase problem via holography.
As FELs provide unprecedented coherent x-ray flux in femtosecond pulses, it becomes possible to probe magnetism with nm spatial resolution on a fs time scale via single shot and pump-probe experiments. This combination enables unique studies in the area of Femtomagnetism.
I will give an overview on our recent magnetic scattering work at FLASH in the context of ultrafast demagnetization (single shot / IR-pump X-ray-probe / X-ray pump X-ray-probe) as well as on the methodology and recent advances of magnetic and ultrafast imaging via Fourier Transform Holography (multiplexing, scanning holography, sequential imaging).

12. The X-ray Correlation Spectroscopy Instrument at the Linac Coherent Light Source. Aymeric Robert, *Linac Coherent Light Source SLAC National Accelerator Laboratory, Menlo Park CA-94025, USA.*

The X-ray Correlation Spectroscopy Instrument (XCS) is one of the four hard

x-ray experimental station to be operated at the Linac Coherent Light Source, the world's first hard x-ray free electron laser. The XCS instrument is designed to take full advantage of the unique properties of the LCLS to probe dynamical phenomena in condensed matter systems down to nanometric lengthscales by means of X-ray Photon Correlation Spectroscopy.
The XCS instrument will use the unprecedented coherence and flux properties of the LCLS. It will enable to probe both slow (i.e. with a characteristic time scales larger than 10ms) and ultrafast dynamics (i.e. ranging between hundreds of femtoseconds up to several nanoseconds) in various scattering geometries (SAXS, WAXS, Grazing Incidence). The ultrafast dynamics will use a novel Split and Delay technique.
The design and status of XCS will be presented and the unique science enabling capabilities of XCS will be discussed.

13. Pump-probe XFEL coherent diffraction imaging of femtosecond laser irradiated Au nanocrystals. Loren Beitra[a], Ian Robinson[a], Takashi Matsuura[a], Naonobu Shimamoto[b], Ross Harder[c], Justin Wark[d]
a *London Centre for Nanotechnology, University College, 17-19 Gordon Street, London, WC1H 0AH, UK*
b *Waseda University, Tokyo, Japan*
c *Advanced Photon Source, Argonne, Illinois 60439, USA*
d *Trinity College, Oxford University, UK*

We are interested in the strains that appear in small crystals, considering that these strains are the origin of new and interesting properties of nanomaterials. We intend to use the new XFEL sources to perform a time resolved pump-probe experiment, investigating the effect on nanoscale Au crystals when rapidly heated by a laser. Initially, the nanocrystals will be nearly defect-free so we will be able to observe if large amounts of strain are induced. Using coherent x-ray diffraction imaging (CXDI), it will be possible to determine the time dependant structure of the laser induced strain field using a single XFEL pulse (by varying the probe laser to XFEL pulse timing offset). Using the XPP end station of the LCLS, a Ti Sapphire laser focussed to a spot size of several microns will be used to heat each individual Au nanocrystal. CXDI measurement will then use the specular Au (111) Bragg reflection from each crystal in an array of similarly shaped 200nm size crystals resulting in a snapshot 2d diffraction measurement.
Our group has developed analytical CXDI software which allows pre-determination of the structure of Au crystals to be measured at the LCLS. The CXD beamline at 34-ID C, APS, has an in-situ confocal microscope, which allows selection of a particular 200nm sized crystal. These diffraction patterns are then inverted and phase information (lost during measurement) recovered by oversampling of data and utilising a support based Hybrid-Input-Output algorithm. This recovered phase is a projection of the displacement field onto the direction of the Q-vector which allows visualisation of defects within the crystal. The confocal alignment method also allows for a full determination of the strain tensor provided three or more Bragg reflections from the same crystal. Once the structure is solved in this way, any changes caused by the laser pump in the 2D pattern at the LCLS, can be revealed despite the eventual destruction of the sample. The timing of the pump to probe can be varied across samples, enabling a clear picture of the time evolution of the strain field to be constructed.

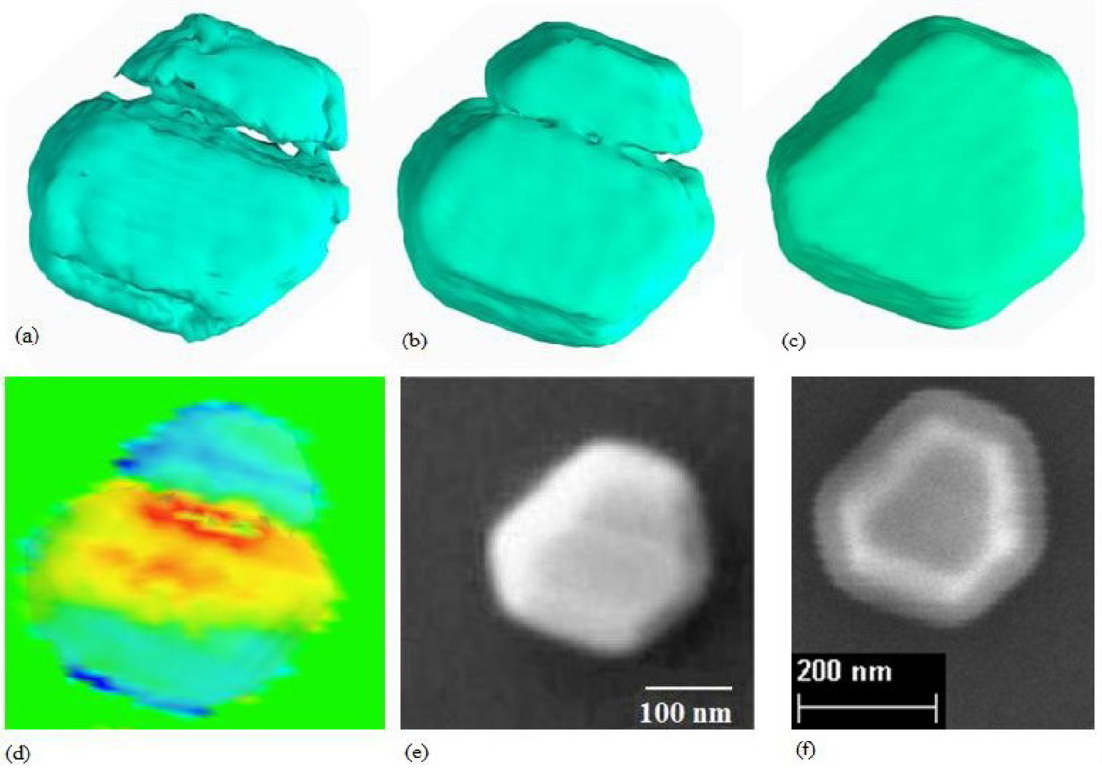

Figure showing: reconstructed complex amplitude from (a) 020 (b) -111 and (c) 11-1 with missing section in (a) and (b) due to twinned crystal. (d) shows recovered phase information from reflection (a). (e) and (d) are Scanning Electron Microscope images of the measured crystal, which show defect on surface.