

## BESSY VSR - WORKSHOP "THE VARIABLE PULSE LENGTH SYNCHROTRON RADIATION SOURCE"

Berlin, 14 – 15 October 2013 - ABSTRACTS

DAY 1 – 14th October 2013	
11:45 a.m.	Registration and informal lunch
01:00 p.m.	Welcome
01:10 p.m.	<p><b>BESSY VSR – Status</b></p> <p><i><b>BESSY VSR: Science opportunities and current developments</b></i> Alexander Föhlisch, Helmholtz-Zentrum Berlin</p>
01:35 p.m.	<p><i><b>BESSY VSR: The accelerator physics of BESSY VSR</b></i> Andreas Jankowiak, Helmholtz-Zentrum Berlin</p>
02:00 p.m.	<p><b>Science Drivers - Session I: Basic Energy Science &amp; Chemistry</b></p> <p><i><b>Ultrafast X-ray absorption spectroscopy of solutions: new avenues</b></i> Majed Chergui, EPFL Lausanne The development of ultrafast X-ray techniques (spectroscopy and diffraction) is opening new possibilities for the study of chemical dynamics in solutions. In terms of temporal resolution, synchrotrons cover the range of 50 ps to infinite time, while the new X-ray free electron lasers (XFEL) can reach 100 fs and less. There is however need for a source of tunable X-rays that would have a time resolution of a few picoseconds. Examples of such studies by X-ray spectroscopy will be presented, mostly pertaining to the important effect of the solvent on the chemical dynamics of solutes.</p> <p><i><b>From Quantum Materials to Solvation Dynamics: Experiments proposed for picosecond x-rays at the Advanced Photon Source</b></i> Linda Young, Argonne National Lab Chicago The Advanced Photon Source at Argonne is a 7 GeV synchrotron source commissioned in 1996 presently operating with 66 beamlines over the soft and hard x-ray regimes. A proposed upgrade to the APS, now undergoing modification to include a low-emittance MBA lattice, included the incorporation of chirped electron pulses in order to produce ultrastable, widely tunable, polarized picosecond x-ray pulses at a repetition rate of 6.5 MHz. I will summarize some of the proposed experiments that utilize the unique characteristics of this source and then compare with BESSY-VSR parameters.</p> <p><i><b>New opportunities in liquid-phase science via picosecond soft X-ray spectroscopy</b></i> Nils Huse, CFEL Hamburg Bridging the 'time-resolution gap' between X-ray free-electron lasers (XFELs) and synchrotrons holds potential for a lot of transient investigations of solution-phase chemistry such as charge migration, spin transitions, and structural changes which happen on few-picosecond timescales. Using high-repetition rate lasers in combination with low-alpha lattices in storage rings would allow for many new detailed studies which are hardly feasible at XFELs given the cost and scarcity of experimental opportunities. I will provide some examples to underscore the prospects of a variable storage ring for transient X-ray spectroscopy of liquid-phase systems</p>

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	<p><b><i>Structural Dynamics in (Bio)chemical Systems</i></b>          Simone Techert, DESY Hamburg, Institute for X-ray Physics, GAU/Max Planck Institute for Biophysical Chemistry</p> <p>Molecular crystals have the potential to be used i.e. in molecular electronics, optoelectronics, as molecular switches, in sensor technology or as pharmaceuticals. In order to optimize their performances, ideally the knowledge of their time-dependent structure - function relation is required. Characteristic for all chemical reactions in molecular solids are bond breaking and bond making processes. Our vision is to optimize these structures towards specific product states by a clever combination of chemical site-specificity, self-assembly and state-selectivity which can be "tuned" from orbital control through the structure of the local environment and selective excitation schemes (heat / optical pulses) to bulk structural changes – or to say it in other words – from the simple to the complex. In the present contribution we will give an overview on our strategy utilizing the pulsed characteristics of x-ray sources, in particular synchrotrons and free electron lasers, to gain such information. On the x-ray methodological side, molecular crystals form the ideal matrix to proof the capabilities of ultrafast radiation generated with Free Electron Lasers (FLASH at DESY or LCLS at SLAC). In the current contribution we will present our studies on the possibility to collect the "molecular movie" with spatial resolution down to electron density distribution on femtosecond time scales. Last are the typical time scales of atomic and charge movements (in particular within the Born Oppenheimer limit). Common for all time-resolved x-ray experiments is the applied pump / probe scheme, where an optical pump-laser initiates a reaction whose structural time evolution is then investigated by x-ray probe pulses at various time delays. The x-ray photon-in / photon-out techniques are based on diffraction or spectroscopic techniques like near edge spectroscopy or x-ray emission spectroscopy. Meanwhile x-ray spectroscopic techniques probe the local environment around specific atoms in a molecule such as orbitals, crystallographic experiments (monochromatic or Laue) reveal the structure of the bulk of periodic systems. (Time-resolved diffuse x-ray scattering experiments give information about the structure of liquids). Finally, we will present our efforts in systematizing the characteristic structural changes in molecular systems during chemical reactions to some kind of "periodic table" of structural dynamics allowing to predict reaction properties in chemistry from a time-dependent structural point of view.</p>
03:50 p.m.	Coffee Break
04:20 p.m.	<p><b>Science Drivers - Session I: Basic Energy Science &amp; Chemistry</b></p> <p><b><i>Electronic structure movies - opportunities with time-resolved x-ray spectroscopy</i></b>          Wilfried Wurth, Universität Hamburg</p> <p>High-repetition rate linear accelerator based light sources such as the superconducting free-electron lasers FLASH at DESY in Hamburg in the extreme ultraviolet, and the European XFEL currently under construction in Hamburg as well as new concepts discussed for storage ring sources such as BESSY VSR can provide ultrashort pulses in the soft and hard x-ray regime with unprecedented properties for time-resolved x-ray spectroscopy. With these new sources it is possible to extend the well-established x-ray spectroscopic techniques for the investigation of the static electronic structure of matter like e.g. photoelectron and x-ray absorption and emission spectroscopy to probing the evolution of the electronic structure after controlled excitation in the time domain. The talk will review recent time-resolved x-ray spectroscopy experiments illustrating the opportunities for the study of ultrafast electron dynamics with high-repetition rate sources.</p>

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	<p><b><i>Opportunities for electron spectroscopy at the VSR source at HZB Berlin</i></b>  Nils Mårtensson, Uppsala Universitet  Photoelectron spectroscopy is a major techniques to study the electronic structure and chemical properties of solids and surfaces. The characteristics of the VSR makes it an excellent source to study ultrafast processes with this electron spectroscopy. Some examples of possible applications will be given.</p> <p><b><i>Development of a time, energy and momentum spectrometer based on angular resolved time of flight measurement</i></b>  Svante Svensson, Uppsala Universitet  A review will be made of the development of a new generation of time, momentum and energy resolving spectrometers with excellent transmission and resolution. These instruments have been used to demonstrate the feasibility of pulse picking (pseudo single bunch) operation for photoemission studies at BESSY II. The fact that the sensitivity allows also for such operation in low alpha mode implies that sub pico second processes can be studied using pump probe techniques.</p>
06:00 p.m.	End of Day 1

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**DAY 2 – 15th October 2013**

09:00 a.m.	<p><b>Science Drivers - Session II: Future Information Technology</b></p> <p><b><i>Studies of Magnetization Dynamics at the Jülich Beamline</i></b>          Claus Michael Schneider, Peter Grünberg Institut, Forschungszentrum Jülich          High-frequency deterministic magnetisation switching and spin dynamics are at the heart of magnetic data storage and spintronics. Tailoring the functionality of spintronic devices requires a control of the magnetic state on the picosecond time scale and a detailed understanding of the underlying physical mechanisms. In order to explore the dynamic behaviour of magnetic systems on short length and time scales FZ Jülich operates an aberration-corrected photoemission microscope at the beamline UE-56/2-SGM. This instrument has recently been modified for pump/probe experiments exciting the sample with ultrashort magnetic field or light pulses. A variable gating mechanism enables the use of complex bunch patterns as envisaged in the VSR concept. We will discuss the opportunities of magnetodynamic imaging experiments in the context of the current challenges in the field.</p> <p><b><i>The Future of Information Technology seen with X-Rays</i></b>          Hermann Durr, SLAC Stanford          The need to establish speed limits for electronic and magnetic switching is clearly important for future technologies attempting to harvest new forms of information processing and storage. However, it also serves fundamental science. It enables us to disentangle competing interactions in the time domain. In addition, at conditions very far from equilibrium often novel electronic and magnetic phases are emerging that promote novel materials properties and functionalities. X-rays are uniquely suited to understand these emerging phases on their natural length and time scales. I will discuss two recent developments aimed at controlling emerging magnetic and electronic order driven by fs optical lasers and intense electric field pulses, respectively. They will point the way towards the use of synchrotron radiation at pulse lengths approaching only few picoseconds duration.</p> <p><b><i>The use of Variable Pulse Length in Magnetism Research: From Skyrmion Dynamics to Ultrafast Magnetization Changes</i></b>          Stefan Eisebitt, Technische Universität Berlin          Intrinsically relevant time scales in magnetism span many orders of magnitude, in particular including the nano-, pico- and femtosecond regimes. Often, it is necessary to understand the dynamics of a system under investigation at several time scales separated by orders of magnitude, in order (i) to be able to carry out well-controlled experiments and (ii) to gain insight into the physics governing the system. I will present examples from recent research in dynamic phenomena in magnetism where the availability of an x-ray source with different pulse lengths would have enabled better experiments and can thus be expected to drive new science in the future.</p>
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10:15 a.m.	<p><b>Session III: VSR Accelerator Physics</b></p> <p><b><i>Short pulse plans for SPEAR3 and PEP-X</i></b>          James Safranek, SLAC Stanford</p> <p>I will start with an update on SPEAR3 low alpha, short pulse operations to date. Then I will discuss our preliminary work investigating the possibility of installing two higher-harmonic superconducting RF systems in SPEAR3 (similar to the BESSY proposal) in order to generate both short and long electron bunches simultaneously. I will also discuss ideas for generating short-pulse, high-peak-current bunches in PEP-X (a proposed diffraction limited light source at SLAC) in order to drive a soft x-ray FEL.</p> <p><b><i>Discussion of Machine Parameters</i></b></p>
11:05 a.m.	Coffee Break
11:35 a.m.	<p><b>Science Drivers - Session IV: Quantum Materials</b></p> <p><b><i>Towards a complete understanding of magnetization dynamics in lanthanides - new frontiers in spin-dependent band mapping at BESSY VSR</i></b>          Martin Weinelt, Freie Universität Berlin</p> <p>Laser-driven ultrafast demagnetization is a continuing subject of intense experimental and theoretical studies, in the itinerant and the rare earth ferromagnets as well as their alloys and layered structures. Being technologically interesting for opto-magnetic devices, e.g., data-storage applications, new experimental results push the limits of our understanding of femtomagnetism. It has been confirmed by several experimental techniques that laser-driven demagnetization occurs in the itinerant ferromagnets within a few hundred femtoseconds. In contrast, for the rare earths Gadolinium and Terbium we find two decay constants of below one and several picosecond. The underlying microscopic processes are still debated. Understanding the origin of the different timescales is crucial because in an FeCoGd alloy magnetic reversal could be achieved upon optical excitation. Switching occurs by ultrafast demagnetization of the Fe sublattice and interaction with the slower decaying Gd moment, which leads to a reversal of the Fe moment. This requires a nanoscale flow of angular momentum between the sublattices in the alloy. We have studied the transient band structure and exchange splitting of Gd and Tb after femtosecond laser excitation by time- and angle-resolved photoemission with VUV radiation from a HHG-source as well as using X-ray magnetic circular dichroism (XMCD) at the BESSY femtoslicing facility FEMTOSPEX. The analysis of the valence band structure is fostered measuring in parallel the linear dichroism in angle-resolved 4f photoemission. Our results indicate that the magnetic anisotropy plays an important role in ultrafast demagnetization. Using in the future the spin-filter momentum microscope that is currently being built for installation at the Russian-German beamline at BESSY II will offer the opportunity to simultaneously analyze the transient, spin-polarized band structure and Fermi surface in 4 dimensions, i.e. for parallel momenta <math>k_x</math> and <math>k_y</math>, at a given binding energy and delay time. At BESSYVSR, the repetition rate of short 1.5 ps pulses in the low MHz regime fits perfectly well to the acceptance of the delay-line detector used in the time-of-flight spectrometer. Together with the highly efficient spin detector, this experiment will make accessible new frontiers in spin-dependent band mapping.</p>



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	<p><b><i>Spin Resonance at Terahertz Frequencies</i></b>            Johan van Tol, Florida State University, National High Magnetic Field Laboratory, Tallahassee            High spin molecules consisting of transition metal ions and/or (increasingly) lanthanide ions can have interesting magnetic properties and have applications in quantum information and quantum storage devices. Also they play a role in various biological reactions like the Mn4 complex oxygen evolving system in photosynthesis. Many of these high spin systems have large zero-field splittings in the range of 4-100 cm<sup>-1</sup> and are not easily accessible by conventional EPR. A variety of techniques can and are used to study these spin systems: high-frequency EPR, frequency swept EPR, FT-IR. A major impediment to the development of magnetic resonance at frequencies above in the terahertz range is the limited source power available, both for single-frequency as well as broadband sources. Relativistic electron sources like Free Electron Lasers could be a avenue for high power THz single frequency sources. BESSY VSR would be a viable broadband source and has the potential of becoming an important instrument in the development of new magnetic (nano)materials with high-frequency spin transitions.</p> <p><b><i>Examples of Ultrafast X-ray Diffraction Experiments: Synchrotron vs. Laser-Plasma Sources</i></b>            Matias Bargheer, Universität Potsdam            This contribution discusses recent experimental studies of ultrafast lattice dynamics in various oxide materials including ferroelectric, ferromagnetic and multiferroic materials. The important role of inhomogeneous excitation and the coupling to domain walls and lattice defects is emphasized. While experiments at the laser-plasma x-ray source in Potsdam already supports a time resolution of about 100 fs, the experimental setup at the XPP-KMC3 beamline at BESSY II provides an excellent test ground for the high repetition rate supported by the VSR mode.</p>
01:00 p.m.	Lunch Break
02:00 p.m.	<i>Plenary Discussion</i>
03:00 p.m.	End of Workshop
03:00 - 04:00 p.m.	<i>Closed Session (for invited speakers)</i>