**Diffraction limited storage rings - how and why?**

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**How?**

During the last few years, new light source magnet lattices open up the possibility to design and build storage rings approaching the diffraction limit in the hard X-ray spectral region. This development opens up the door towards a new class of investigations explained below.

The most common way of achieving the small electron beam emittance necessary is to use the Multi-Bend Achromat (MBA) magnet lattices in the storage rings. The large number of unit magnet cells introduced in this way reduces the emittance in a powerful way, the electron emittance decreases as the number of cells increases to the third power.

The “Chromaticity Brick Wall”, experienced earlier with conventional magnet lattices resulting in a too reduced dynamic aperture, could be broken with the MBA scheme. The miniaturization of the magnet units with the MBA scheme is both a necessity and a possibility. Necessary to keep the cost and size of the facility down, possible since the small dispersion in the rings implies a smaller physical aperture need. Needless to say, this miniaturisation has quite an impact on other accelerator systems like vacuum, heat absorbers, RF etc. Beam dynamic effects, not so pronounced at rings with larger emittances, must also be taken in account to a higher degree.

Today MAX IV and Sirius are the forerunners for the MBA concept being facilities under constructions. Serious MBA preparations are underway at several other facilities as ESRF, APS and SPRING8 to mention a few.

**Why?**

DLSRs will considerably enhance science applications in the area of 3D coherent X-ray imaging and X-ray photon correlation spectroscopy. High-resolution tomography of very large objects or of preselected regions in such objects enables us to bridge the so-called ‘imaging gap’ between the macroscopic world and the nanoworld. DL SRs thus allow us to cover the ‘blind spots’ not only in the spatial domain but also in the time domain. Imaging applications and nanoprobe are highlighted by a number of contributors to this special volume (Thibault et al, Schroer and Falkenberg, Shpyrko, de Jonge et al).

The small beam spots generated by DLSRs also bring significant advantages to protein crystallography, as explained by Fischetti *et al*, as well as to X-ray spectroscopies such as RIXS and ARPES. In RIXS, a substantial gain may be achieved in energy resolution (see contribution by Schmitt *et al*), while in ARPES one can select a small homogeneous part of the sample surface (Rotenberg). Small spots also allow research on micrometer-sized samples under extremely high pressure (McMahon). Clearly, spectromicroscopy in energy, chemical and biological sciences profits from small beam spots and enhanced energy resolution (de Jonge and Jacobsen, Frenkel and van Bokhoven, Toney and Hitchcock).

Extreme requirements are put on the quality of the beam optics, the thermal and vibrational stability of the beam line and the positioning accuracy of the sample environment. These requirements are discussed in the contributions by Yabashi *et al*, Susini *et al* and Siewert *et al*. Detector requirements are the subject of a contribution by Schmitt and Denes.
Lattice design challenges for fourth-generation storage ring light sources

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Third-generation low-emittance storage ring light sources based on double- and triple-bend cells and undulator magnets have been in operation around the world for more than two decades. On the horizon is a new generation based on the multi-bend achromat (MBA) lattice concept [1,2], promising several orders of magnitude higher brightness than is available in today’s sources. In this paper, we describe the challenges inherent in designing MBA lattices, as well as potential solutions. Topics covered include storage ring scaling, lattice concepts, brightness optimization, nonlinear dynamics, beam lifetime, undulator effects, and injection schemes.


Magnet design for a low emittance storage ring

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The MAX IV synchrotron radiation facility, currently under construction, will consist of a 3 GeV storage ring, a 1.5 GeV storage ring, and a full energy linac injector/SPF/FEL driver. The 3 GeV storage ring has a multibend achromat lattice, consisting of 20 identical achromats, each consisting of two matching cells and five unit cells. The magnet elements of each lattice cell is designed as one mechanical unit, a 2.3-3.4 m long solid iron block, with the poles of the different magnet types, dipole, quadrupole, etc, machined out of the iron block. The MAX IV 3 GeV storage ring consists of 140 such magnet block units, each containing 8-13 different magnet elements, with electrical cabling and coil water cooling circuits integrated on each unit. A main feature of this magnet design concept is that the alignment of magnet elements within each unit is given by the mechanical accuracy of the CNC machining of each iron block. Another defining aspect of the MAX IV 3 GeV storage ring magnet design is the relatively small pole aperture of 25 mm. A smaller pole gap means higher field gradients in the quadrupole magnets and shorter distances between the magnet elements, enabling a compact lattice design. The small pole gap is made possible by the use of distributed pumping (NEG coating) in the vacuum system. This is an example on how magnet design and vacuum design considerations interact and sets limits on storage ring lattice design.

At the time of writing, the production of these magnets is ongoing. This article presents the MAX IV 3 GeV storage ring magnet design from the perspective of
Some of the characteristics of Diffraction Limited Storage Rings (DLSR) or ultra low emittance light sources are the compact lattice combined with small magnet apertures. Such requirements present a challenge for the vacuum system design and performance. The vacuum system should provide the required pressure for the machine operation (mainly to reduce the beam-gas scattering and to increase the beam lifetime) and handle the heat load from synchrotron radiation. Taking into consideration that the magnet profiles are small, resulting in that the conductance of the chamber is low, and lumped pumps are ineffective. One way to provide the needed vacuum level is by having distributed pumping which can be realized by the use of non-evaporable getter (NEG) coating of the chamber walls. Lumped absorbers cannot be used to absorb the heat load from synchrotron radiation as an antechamber is difficult to realize with such compact lattice. To solve this, the chamber walls can work as distributed absorbers, if they are made of material of good thermal conductivity and distributed cooling is used at the location where the synchrotron radiation hits the wall. The vacuum system of the 3 GeV storage ring of MAXIV is used as an example of possible solutions for vacuum technologies for DLSR.

First multi-bend achromat lattice consideration

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At the beginning of 1990 three synchrotron light sources of the third generation had been successfully commissioned (ESR, ALS and ELETTRA). All machines reached their target specifications without any problems. At this time we had a lot of discussions with the colleagues at ELETTRA about the next generation, the “Diffraction Limited Light Source (DFL)”, because it should be possible to run light sources with a smaller emittance, higher brilliance and emitting coherent radiation. At this time we performed a first design of a DFL. It is a 3 GeV storage ring with a modified multiple bend Achromat (MBA) optics as a lattice leading to a normalized emittance of $\varepsilon(x) = 0.5$ nmrad. The novel feature of this lattice is the use of horizontally defocussing bending magnets with different bending angles to keep the radiation integrals low. The circumference is 400 m including 12 straight sections with a length of 6 m. the dynamical behavior should allow to store a beam of 100 mA with a lifetime larger 5 hours.

Collective effects in DLSR

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In this paper, we shall give an overview of the collective effects that are likely to appear and possibly limit the performance in a DLSR that stores a high intensity ultra-low emittance beam. With the term collective effects, we aim to cover, both collective beam instabilities and other intensity-dependent effects that may significantly impact the machine performance. The latter include beam-induced machine heating, Touschek scattering, IBS (Intra Beam Scattering), as well as incoherent tune shifts. We shall start from reviewing the generally existing relation that the efforts made on the magnetic lattice to achieve an ultra-low emittance result in increasing the machine coupling impedance. They tend to enhance the beam sensitivity to instability as well. The nature of the resulting coupling impedance shall then be described, followed by reviewing a series of potentially dangerous beam instabilities driven by the former, which are; resistive-wall, TMCI (Transverse Mode Coupling Instability), head-tail and microwave instabilities. In addition to the above, beam-ion instability arising from beam collision to the residual gases existing in the beam duct, as well as CSR (Coherent Synchrotron Radiation)-driven instability shall also be addressed. The
Touschek scattering and IBS are then be discussed as potentially dangerous sources of performance deterioration in a DLSR. Some of the existing and proposed means to fight against the collective effects are then introduced, along with their expected performance, specifically, lengthening of the bunch with passive harmonic cavities and bunch by bunch transverse feedback. Numerical codes developed and used to evaluate the machine coupling impedance, as well as to simulate the beam instability using the former as inputs, shall also be described.

The MAX IV storage ring project

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The MAX IV facility, currently under construction in Lund, Sweden, features two electron storage rings operated at 3 GeV and 1.5 GeV and optimized for the hard X-ray and soft X-ray/VUV spectral ranges, respectively. A 3 GeV linear accelerator serves as a full-energy injector into both rings as well as a driver for a short pulse facility, in which undulators produce X-ray pulses as short as 100 fs. The 3 GeV ring employs a multibend achromat (MBA) lattice to achieve, in a relatively short circumference of 528 m, a bare lattice emittance of 0.33 nm rad, which reduces to 0.2 nm rad as insertion devices are added.

The engineering implementation of the MBA lattice raises several technological problems. The large number of strong magnets per achromat calls for a compact design featuring small-gap combined-function magnets grouped into cells and sharing a common iron yoke. The small apertures lead to a low-conductance vacuum chamber design that relies on the chamber itself as a distributed copper absorber for the heat deposited by synchrotron radiation, while non-evaporable getter (NEG) coating provides for reduced photodesorption yields and distributed pumping. Finally, a low main frequency (100 MHz) is chosen for the RF system yielding long bunches, which are further elongated by passively operated third-harmonic Landau cavities, thus alleviating collective effects, both coherent (e.g. resistive wall instabilities) and incoherent (intrabeam scattering).

In this paper, we focus on the MAX IV 3 GeV ring and present the lattice design as well as engineering solutions to the challenges inherent to such a design. As the first realization of a light source based on the MBA concept, the MAX IV 3 GeV ring offers an opportunity for validation of concepts that are likely to be essential ingredients of future diffraction-limited light sources.

The Sirius project

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We present the lattice design and beam dynamics optimization for Sirius, a new low emittance synchrotron light source presently under construction at the Brazilian Synchrotron Light Laboratory (LNLS) in Campinas, Brazil. The electron storage ring is based on a 5-bend achromat (5BA) design achieving a bare lattice emittance of 0.28 nm.rad for a 3 GeV beam. The circumference of 518 m contains 20 achromatic straight sections of alternating 7-m and 6-m in length. An innovative approach is adopted to enhance the performance of the storage ring dipoles by combining low field (0.58 T) magnets for the main beam deflection with a very short 2 Tesla permanent magnet superbend sandwiched in the center dipole. This superbend creates 12 keV critical photon energy dipole sources with modest total energy loss from dipoles. In addition it also creates a longitudinal dipole field gradient that reduces the emittance by about 10%. The optimized dynamic aperture allows for top-up operation with off-axis injection and the optimized energy acceptance allows for a total beam lifetime around 10 hours at nominal current with third harmonic cavity.

Short bunches in diffraction limited storage rings

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High repetition rate, high brightness short X-ray pulses that may be produced in a diffraction limited storage ring (DLSR) are of great interest to time-resolved photon science experiments. Short bunches in a storage ring can be generated by applying high RF focusing gradient. If high RF focusing is selectively applied to a fraction of the RF buckets, with, for example, a two-color harmonic RF system, the short bunches can be compatible with simultaneous high current long bunch operation.

If a full-energy linac injector is available, short pulses can also be produced in the ring by circulating the injected short-bunch beam for multiple turns with an isochronous ring lattice. Coherent synchrotron radiation can cause significant longitudinal phase space distortion, emittance growth and potentially microbunching instability. The number of turns
the injected beam can circulate in the ring depends on the bunch charge, bunch length and momentum spread of the injected beam.

The multi-turn circulation mode of operation may also be used to produce high brightness X-rays with the low emittance electron beam of the linac injector. This mode provides high repetition rate, high brightness photon beam simultaneously to many beamlines. The disadvantage of the circulating mode is that the beam quality changes with time.

In this article we discuss the performance and challenges of the approaches of generating short bunches in DLSR and the multi-turn circulation mode.

Coherent imaging at the diffraction limit

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Among X-ray microscopy techniques, coherent diffractive imaging (CDI) is widely seen as most promising for dose-limited resolution because it does not require any optical elements between sample and detector. Ptychography, a scanning variant of CDI, is robust to experimental “imperfections,” such as positioning errors, unknown illumination or finite coherence, and thus virtually guarantees successful high-fidelity image reconstruction. The technique, which can be used for three-dimensional imaging when combined with tomography, is offered at 3rd-generation synchrotron sources and is being implemented at multiple facilities worldwide.

While sampling rates of several thousand resolution elements per second have already been demonstrated, comparing well with most other scanning X-ray microscopies, the coherent flux at most of today’s sources may soon prove limiting the image acquisition rate, ahead of other experimental overhead caused by settling times of positioning systems and detector readout.

With coherent flux orders of magnitude higher than at current 3rd-generation X-ray sources, novel sources will allow ptychography to approach imaging speeds that are thus far the exclusive domain of full-field methods. Diffraction-limited sources will also provide the necessary conditions to fully exploit ptychography’s inherently quantitative nature, thus complementing spectroscopic analyses. Yet, exploiting the technique’s potential will necessitate additional technological and analytical advances in such disciplines as sample handling and scan optimization, high-volume data analysis, and ptychography’s very own reconstruction methodologies and measurement strategies. Beyond promises of high-throughput imaging with dose-limited resolution and sensitivity, a higher coherent flux could provide access to sample dynamics, through time-resolved imaging or by a careful characterization of decoherence effects.

Hard X-ray scanning microscopy

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Hard x-ray scanning microscopy enjoys an increasing demand in many fields of science, such as physics and chemistry, biology, materials, earth, and environmental science, and nano technology.

Its key strength lies in the large penetration depth of hard x-rays that can penetrate specialized sample environments, such as chemical reactors, microfluidic or pressure cells. X-ray microscopy is thus ideally suited for in-situ and in-operando studies of physical and chemical processes. By using various x-ray analytical techniques as contrast, such as x-ray fluorescence, absorption, or diffraction, x-ray scanning microscopy allows one to measure quantitatively the elemental composition, the chemical state, or the local mesoscopic or atomic structure, respectively. In combination with tomography the three-dimensional inner structure of a specimen can be reconstructed.

Scanning microscopy is intrinsically a brilliance limited technique, thus greatly benefiting from ever more brilliant x-ray sources. In this article we extrapolate the current capabilities at synchrotron radiation sources of the third generation in terms of sensitivity and both spatial and temporal resolution and explore the opportunities for hard x-ray scanning microscopy at a nearly diffraction limited storage ring. As all nanobeams are intrinsically laterally coherent at these sources, scattering techniques can be naturally extended to lensless real-space imaging techniques with high spatial resolution.

In order to take full advantage of the small irradiated phase space volume of such a source, significant improvements over current beamline instrumentation is required. We give estimates for the required parameters for the various optical components of a microscopy beamline.
XPCS and coherent imaging of fluctuating condensed matter

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Presence of random disorder or defects in materials can be described as random configuration of scatterers, which, when illuminated by coherent x-rays, gives rise to far-field scattering pattern decorated with so-called speckle field. The particular speckle field is a result of complex interference pattern describing local configuration of scatterers, and temporal evolution of speckle intensity profile can be used to characterize the equilibrium, or non-equilibrium fluctuations in the system, using approach known as X-ray Photon Correlation Spectroscopy (XPCS). The basic premise of XPCS is to calculate the temporal intensity-intensity auto-correlation function, with the decay of the correlations describing the fluctuation rate of the system at a given wavevectors, or characteristic length scales.

XPCS has become an increasingly important technique for the study of dynamical phenomena in a wide range of materials, ranging from the study of atomic diffusion and magnetic domain motion, to that of fluctuations at surfaces and interfaces, colloidal glasses, soft solids, quasicrystals, biological membranes, liquid crystals, charge and spin density waves and other complex materials.

Until recently XPCS has been limited to study of slow, glassy dynamics, limited in part by the relatively low coherent content of the third generation light sources. Availability of Diffraction Limited Storage Rings, present an increase in available coherent x-ray flux over third generation source by a factor of several hundred, thereby expanding the time window accessible to XPCS by 5 orders of magnitude. Such a dramatic increase in the range of measurable timescales would have dramatic effect on experiments aiming to understand the nanoscale dynamics and fluctuating order parameters in a variety of soft and hard condensed matter physics, materials science, biophysics, chemistry, environmental sciences and other disciplines. It would also make it possible to expand the application of XPCS to higher order temporal and spatial correlation functions that reveal further, often “hidden” details of nanoscale fluctuations in complex materials.

X-ray nanoprobes and diffraction limited storage rings: opportunities for fluorescence tomography of biological specimens

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Abstract
X-ray nanoprobes require coherent illumination to achieve optic-limited resolution, so that they will benefit directly from diffraction-limited storage rings. Diffraction limited storage rings offer opportunities to rethink beamline and instrument design in more compact directions, and opportunities to fully exploit lower-level, indirect signals such as fluorescence and inelastic scattering. We focus on the example of high-resolution x-ray fluorescence tomography as one of the most demanding applications of coherent flux. Addressing metal distributions in biological and environmental specimens involves detected signals that are a fraction of the incident flux, complexity in sample handling due to diffusible ions and radiation sensitivity, and in analysis due to minimum dose requirements and self-absorption. By understanding the requirements and opportunities for nanoscale fluorescence tomography, one gains insight into the R&D challenge necessary in optics and instrumentation needed to fully exploit the source advances that diffraction limited storage rings offer.

Summary
The two optics figures of merit for an x-ray microprobe are the spatial resolution and the sensitivity per unit time of measurement. If nothing else is changed, DLSR upgrades will result in dramatic gains to the x-ray intensity in a given size of focus (directly addressing sensitivity), and perhaps factor of 3-5 gains in spatial resolution. With current technologies this would result in perhaps an order of magnitude gain in output. Several concomitant technical challenges must be overcome in order to realise signal gains of several orders-of magnitude, to preserve specimen integrity, and to fully exploit the rich data that will be provided.

1. Introduction
   a. Why are trace elements important? Play crucial roles in biology and environment (metal diseases, therapeutic agents, biotic limiters but also toxins in the environment)
   b. Why fluorescence? Best sensitivity at minimum damage.
   c. Why tomography? The real world is heterogeneous at the nanoscale, and 3D

2. X-ray nanoprobes
   a. General principle: we don’t have detectors which simultaneously offer high spatial resolution, high collection angle, and energy resolution. Therefore must scan.
   b. Optics for nanofocusing
c. Illumination for nanofocusing: coherence and spatial filtering lead one to prefer diffraction limited storage rings.
e. X-ray nanoprobe instruments: scanning, cryo, detectors

3. Handling the data
   a. Pixel mode and fluorescence event mode
   b. Alignment and reconstruction
   c. Refined reconstructions: self-absorption, alignment refinement, pattern recognition

4. Examples today and tomorrow
   a. Examples today
   b. Challenges for tomorrow

5. Summary and conclusion

Structural Biology in the 21st Century
or
Structural Biology at 4th Generation Storage Ring X-ray Sources

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Structural biology has undergone a revolution in the past 20 years due to the availability of intense, highly parallel X-ray beams from insertion devices on second and third generation storage rings. Now we are on the precipice of another major advance with the development of near diffraction limited storage rings. New storage rings being developed in Lund, Sweden (Max IV) and San Palo, Brazil (SIRIUS) will increase the brightness to record levels. Major upgrades at facilities like the APS, ESRF and SPring-8 will exploit the large diameter of the storage rings to reduce the beam emittance towards the diffraction limit, resulting in X-ray beams of high coherence and brightness.

High brightness sources and advanced beamline designs have proven critically important for solving some of the most important biological structures in the past 10 years. However, with current sources, the smallest crystal from which useful data can be collected is limited by the maximum intensity that can be focused to a micron-sized beam with low convergence. The increased brightness from diffraction limited sources will enable smaller beams of unprecedented intensity to probe submicron crystals.

This paper will summarize some of the anticipated advances of the new sources and their potential impact on structural biology. The ability to examine submicron crystals may significantly reduce the time from "first crystals" to a solved structure. The intense, micron-sized beams will allow one to obtain data of high signal-to-background from weakly scattering crystals of membrane proteins and complexes, and may allow one to "out-run" secondary radiation damage at room temperature. Finally, we will compare the benefits of these new sources and X-ray free electron lasers for structure determination. Improvements in beamlines, detectors and sample handling will also be discussed.

High resolution resonant X-ray inelastic scattering studies of materials, liquids and gases

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The spectroscopic technique of Resonant Inelastic X-ray scattering (RIXS) will particularly profit from immensely improved brightness of diffraction limited storage rings (DLRS). In RIXS, one measures as a function of momentum transfer $q$ excitations of an electronic system as the difference between the energies of the incident and scattered X-rays, $h\nu_{\text{out}} - h\nu_{\text{in}}$. DLRS will allow pushing the achievable energy resolution, signal intensity and the sampled spot size to new limits. With RIXS one nowadays probes a broad range of electronic systems reaching from simple molecules to more complex materials displaying phenomena like peculiar magnetism, two-dimensional electron gases, superconductivity, photovoltaic energy conversion and heterogeneous catalysis. In this article we envision for several of these scientific cases what kind of improved RIXS studies will in the future be possible employing in some cases also coherence and time structure of the X-ray beam from DLRS.

For small molecules vibrational resolution will give access to fine details in the scattering dynamics and the involved states. One will be able to study consequences of the dipole selection rules and their limits in small symmetric systems.
For larger molecules electronic-vibronic coupling will be in the focus of research, and one vision is to use detuning to control the nuclear wavepacket in complex potential surfaces, which is relevant for the understanding of chemical reactions. For liquids (and molecular materials) the opportunity to map the local potential surfaces of the electronic ground state is a new unique tool. Analyzing the natural line shapes associated with electronically excited states will give important information about the intermolecular interactions.

For solid state materials one can study with RIXS all elementary excitations within spin-, orbital-, charge-, and lattice degree of freedom of the solid. In case of transition metal oxides (TMOs) with a single electron or hole in the valence band one can understand magnetic, dd- and charge transfer excitations in a straight forward way. For systems with 2 to 8 occupied d states, multi-electron interactions modify the description of the ground states and the respective excitations are more complex to describe. This requires further progress in first principle and model Hamiltonian based theory descriptions.

TMOs possess functional properties like ferro- and antiferromagnetism, metal-insulator transitions and superconductivity. Oxide heterostructures made of layered TMOs are constantly gaining in research interest as their special functionalities can be used for the design of device components in advanced technologies based on the electronic and magnetic materials properties. In the future, artificially designed electronic systems providing complex or coupled functionalities will be indispensable. Unconventional superconductors within TMO and related material families are another important class of materials that is of high relevance for future improve of energy generation, transmission and storage. Increased energy resolution in RIXS at DLRS will allow, e.g., probing the relevant energy scale of the superconducting gaps. Furthermore, one would be able investigate coupling effects between lattice and spin degree of freedom that might be intimately related to their superconducting properties. For all of these materials it will be essential to understand their low-energy properties at a sub-μm to nm length scale as electronic inhomogeneities and intrinsically heterogeneous materials need to be understood. Higher signal intensities will for the case of DLRS allow analyzing the polarization conditions of scattered beam in RIXS allowing thereby assessing the character of the detected excitations.

In the spectra of covalent and metallic transition metal solids dispersional effects and local correlation effects are competing giving thereby rise also to strong fluorescence contributions. Coordination complexes, transition metal ions in solution and transition metals in proteins share the dominant effects of dd- and charge transfer excitations with transition metal oxides. Improved resolution of RIXS has the potential to reveal in these areas details on the differences in electronic structure as well as the related excitation and decay mechanisms in coincidence detection with non-radiative decay channels. The spectra of rare earth systems are dominated by ff-transitions. Improved resolution will reveal more details regarding the crystal field effects on the ff-transitions, an important field in luminescent and photon-capturing applications.

**NanoARPES investigations of heterogenous correlated electron systems**

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The article will address the application of the ARPES and nanoARPES techniques at diffraction limited light sources. The most important consideration is the space-charge broadening which limits energy and momentum resolution and depends crucially on the flux, spot size, and pulse duration of the light source. In previous studies these effects were calculated in one regime or another, but not all at once. Calculations will be presented over a wide range of parameters, and optimum parameters for ARPES will be discussed.

In case the NanoARPES beamline at ALS is operational before the submission deadline, then some first data will be presented.

**X-ray spectroscopy for chemical and energy sciences**

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Nanometer size beams produced by the Diffraction Limited Storage Ring source will carry the same flux as the beams used at today’s synchrotrons. Catalytic activity and selectivity of supported metal catalysts depend strongly on their shapes, sizes, support orientations and the states of order and disorder. Hence, catalysts possess inherent structural heterogeneity due to the distributions of cluster sizes and shapes. Studies of the architecture and electronic properties of nanocatalysts by X-ray absorption are hindered by ensemble averaging nature of this technique, posing a real challenge when its results are compared with first principles theories. Operando studies at the single nanoparticle level will allow to directly evaluate the structure and electronic properties and their relation to catalytic performance as probed in real time, in the same spectroscopy experiment. These studies will enable the determination of the structural properties of
single particles. Using nanobeams in monochromatic or dispersive modes, EXAFS experiments will provide the size and shape of individual particles in real time, with 10ms time resolution or better. Secondary emission and high energy resolution experiments (HERFD, RIXS, HEROS) will be possible at the single particle level as well. These experiments will complement EXAFS by providing information about local chemistry of particle-adsorbate-support interaction through the measurement of the electronic structure of the individual catalyst during the catalytic reaction. Time-resolutions at the macrokinetic time scale, using e.g. gas switching, and at the ultrafast scale, using pump probe, will yield relationships between performance on the one side and structure and structural changes that occur during individual reaction steps on the other.

Reciprocal and real space spectromicroscopy and imaging with diffraction limited X-ray sources with focus on energy materials applications

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This article will discuss those types of spectromicroscopy and reciprocal space imaging methods which will benefit from the increase in brightness expected from a diffraction limited storage ring (DLSR). These include mainly advanced scattering techniques and nanoprobe based systems using Fresnel zone plates or other diffractive optics. [Coherent diffraction imaging (CDI) is being dealt with in a separate chapter – we will make connections]. The current capabilities and important scientific themes will be outlined and the potential performance improvements of a DLSR estimated. Several examples of energy sciences research problems which are out of reach of current instrumentation, but which might be solved with the enhanced DLSR performance will be outlined.

Sections
1. the spectromicroscopy, scattering and reciprocal space imaging landscape as it pertains to energy sciences
2. performance of state-of-art instruments relying on coherent X-ray probes
3. predicted improvements with DLSR
4. examples of ‘impossible’ or dream experiments that may be do-able on a DLR
   a. organic photovoltaics – quantitative visualization of their operation
   b. 1 nm hard X-ray tomography
   c. sub-nm soft X-ray imaging as applied to energy storage
   d. in-operando single particle imaging

High pressure science on diffraction limited storage rings

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The advent of the ESRF, APS and Spring-8 synchrotron sources in the early 1990’s heralded a new, and extremely productive, era of high-pressure science. While diffraction studies have been performed at previous generations of storage rings as early as the mid 1970’s, the level of structural information available was limited by the energy-dispersive powder-diffraction techniques employed. The development of angle-dispersive diffraction techniques utilizing 2D detectors in the early 1990’s was perfectly timed with regards the start-up of the 3rd generation synchrotrons. As a result, high-pressure science was immediately able to reap the benefits of the extremely intense, monochromatic, micro-focused beams available from such machines to extend detailed structural studies to pressures comparable with the centre of the Earth. This research has revealed that the structural behavior of high-pressure matter is very much more interesting than previously believed, with a multitude of extremely complex (and often non-periodic) structures in even the simplest systems. Simultaneously, the development of dynamic compression methods on large laser platforms, utilising laser-plasma x-ray sources, has enabled structural studies of dynamically-compressed matter to be pushed to ever higher pressures. This too has revealed previously unimagined structural complexity.

High-pressure studies necessarily involve the use of extreme small samples. A new generation of diffraction limited storage rings that offer smaller, higher-brightness x-ray beams will engender the next generation of high-pressure diffraction and scattering studies. Studies can be pushed to high pressures – perhaps as high as 1 TPa (10 megabars) by utilizing micron-sized samples, while weaker scattering materials such as hydrogen can be studied with x-rays to extremes for the first time. But it is perhaps in the field of dynamic time-resolved experiments where such sources can be utilized to their best, either by using dynamic compression methods to pressurise the samples, or dynamic heating methods to attain P-T conditions previously inaccessible. In this paper I will summarise the present stat-of-the-art achievable with current x-ray sources, and then describe what new science can be achieved with diffraction-limited sources.
Pixel detectors for diffraction-limited storage rings

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Dramatic advances in synchrotron radiation sources produce ever-brighter beams of X-rays, but those advances can only be used if there is a corresponding improvement in X-ray detectors. With the advent of storage ring sources capable of being diffraction-limited (down to a certain wavelength) advances in detector speed, dynamic range and functionality is required. Diffraction-limited sources do not increase flux, but they do increase brightness – a key advantage for microscopies and photon correlation spectroscopy. In addition, the dramatically reduced horizontal emittance means that more photons can be effectively focused on to a sample for any given experiment. The temporal resolution of X-ray photon correlation spectroscopy (XPCS) scales as Brightness², which means that detectors must become significantly faster: ideally as very fast-framing pixel detectors or ultimately as time-stamping pixels with ns (or even ps) resolution. For coherent imaging, higher brightness pushes not only framing speed, but also dynamic range. For example, in ptychography the dynamic range scales as (probe size / ultimate resolution)⁴ – so that higher resolution requires much higher dynamic range detectors.

While many of these improvements in detector capabilities are being pursued now, the orders of magnitude increases in brightness of diffraction-limited storage ring sources will require challenging, non-incremental advances in detectors. This article summarizes the current state of the art, developments underway worldwide, and challenges that diffraction-limited storage ring sources present.

Optics for coherent X-ray applications

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Development of optics for coherent X-ray applications and their roles in DLSR are described. For manipulating coherent X-ray beam, high-quality optics should be employed for preserving wavefront and suppressing unwanted speckles. For this purpose, advanced technologies on preside processing and metrology, as well as characterization of optical elements using propagation-based coherent X-rays from an undulator source, have been developed. It was found that a Beryllium window produced with a physical-vapor deposition (PVD) method gives ideal speckle-free property. An elastic emission machining (EEM) method was utilized for developing reflective mirrors with excellent figure shapes that can sufficiently suppress distortion of the wavefront. This method was further applied to production of diffraction-limited focusing mirrors, which include a device enabling the smallest spot size of 7 nm. As an example, optical systems installed for an X-ray free electron laser are introduced. Characterization of coherence properties are another important issue for utilization of coherent X-rays. X-ray Hanbury Brown and Twiss experiments and their applications to evaluate transverse coherence, longitudinal coherence, and higher-order coherence are presented. Based on these works, we discuss further evolution of X-ray optics and their contribution to development of DLSR applications.

New challenges in Beamline instrumentation for Diffraction Limited Storage Rings

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Although beamline instrumentation is by nature driven by science, some recent examples serve as reminders that new technologies also enable new science. Indeed, exploiting the full scientific potential of forthcoming DLSRs will, in many cases, require the development and implementation of novel instrumentation. In comparison to present SR facilities, the majority of beamlines should reap immediate performance benefits from the improved source characteristics (principally through increased flux and/or horizontal beam size reduction at the sample), and instrumentation will have to develop along similar quantitative and qualitative trends. More speculative and more challenging is anticipating new science, driven by unprecedented source and beam properties (in terms of transverse and longitudinal coherence). This is where clear opportunities exist today for synergetic developments with the new X-ray FEL sources.
Beamline instrumentation for specific issues will likely be addressed in other science-related articles, and so this article targets, in more general terms, the major challenges to be addressed in order to fully exploit DLSRs, covering specific issues like optics, or needs for a more integrated instrumentation (including detector and other elements of the acquisition chain). To illustrate, the ESRF’s impending Upgrade Programme - Phase 2 is expected to explore many aspects of instrumentation developments that will closely resemble, if not mirror what is expected for DLSR.

Increased brightness and fully coherent beams will foster applications aiming at very high time- and spatial-resolutions, effectively impacted by both static and dynamic performances of all beamline components. DLSRs will enable more complex experiments, with much higher data rates, to cope with ever-increasing numbers of combined measurements. In this context, two aspects will be further elaborated:

1. Improved strategies for beam transport beamline optics
2. Toward fully-integrated experiments, which take into account a full optimization of sample environment and the acquisition chain.

On the characterization of ultra-precise X-ray optical components – advances and challenges in ex-situ metrology

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To fully exploit the ultimate source properties of the next generation light sources, such as Free-Electron Lasers (FEL) and Diffraction Limited Storage Rings (DLSR) the quality requirements for gratings and reflective synchrotron optics, especially mirrors have increased significantly over the last few years. These coherence preserving optical components for high brightness sources will feature nanoscopic shape accuracies over macroscopic length scales up to 1000 mm. Today, planar grating blanks with 0.1 µrad rms residual slope error of 150 mm length are state of the art whereas the acceptable residual slope error for e.g. future gratings at the European XFEL will be 50 nrad rms over a length of 500 mm. It is also intended to install 800 mm long plane mirrors for the beamlines at the European XFEL – these plane mirrors will feature radius of curvature larger than 1000 km and 50 nrad rms slope error, which is corresponding to a 0.5 nm rms / 2 nm peak-to-valley residual figure error. To enable high efficiency in terms of photon flux such optics will be coated with application-tailored single or multilayer coatings. Advanced thin-film fabrication of today enables to synthesize layers on the sub-nm precision level over a deposition length of up to 1500 mm, like at HZG.

Specifically dedicated metrology instrumentation of comparable accuracy has been developed to characterize such optical elements. Second generation slope measuring profilers like the Nanometer Optical component measuring Machine (NOM) at the BESSY-II-Optics Laboratory allow to inspect up to 1500 mm long reflective optical components with an accuracy better than 50 nrad rms. Besides measuring the shape on top of the coated mirror, it is of particular interest to characterize the internal material properties of the mirror coating, which is the domain of X-rays. Layer thickness, density and interface roughness of single and multilayer coatings are investigated by means of X-ray reflectometry.

In this publication we will show recent achievements in the field of slope measuring metrology and demonstrate the characterization of different type of mirror coating. Furthermore we discuss upcoming challenges in the inspection of ultra-precise optical components designed to be used in future FEL- and DLSR-beamlines.