Working group 7
Undulators, Beamlines, X-ray Optics, and Detectors

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Future x-ray source development is driven by scientific needs (working group 1), and employs advances coming from accelerator physics and from novel source concepts. The x-ray sources and their infrastructure of beamlines and x-ray optics have become essential tools across the sciences, medicine and engineering. Working group 7 considered a different aspect of future light source development: what is required to connect future light sources to the science? That is, what is needed from beamlines, x-ray optics, and detectors? What should accelerator physicists know about developments and needs for beamlines, optics, and detectors to maintain the rapid pace of advance in these fields to capture ultra-fast phenomena and probe materials with atomic resolution, for instance?

The ICFA workshops do not typically draw experts in the area of beamlines, x-ray optics, and detectors, so our summary of the workshop drew from a smaller number of participants. Even so, we have attempted to capture the key developments in this area through conversations with x-ray experimentalists worldwide. At most facilities the development of undulators is undertaken by the accelerator physicists rather than the photon scientists due to the intimate relationship between key undulator parameters and electron beam characteristics, so commentary on undulators was provided by one author (JNG).

Radiation Sources, Undulators

The capabilities and limitations of planar permanent magnet undulators, in terms of period, field and field quality are well-understood; they will of course be in widespread use in future light sources. However, advances in short-period undulators based on cryocooled permanent magnets and superconducting undulators can have very significant impact on the performance of existing storage ring sources as well as future light sources. Present efforts to produce performance enhancements are aimed primarily at

- Producing high-brightness sources of few-Å wavelength x-rays with lower-energy electrons
- Producing high-brightness sources in the 0.1 Å range in the higher-energy storage rings
- Improved polarization control

Cryocooled hybrid permanent magnets offer the possibility to extend the limits of performance (in terms of peak field) for permanent magnet technology by 20% or more. Superconducting undulators can also produce higher peak fields in shorter-period undulators. Nb_3Sn conductor offers a significant performance advantage over NbTi. New high-Tc conductors, in thin-film geometries appropriate to their mechanical properties, could produce performance even further beyond the state-of-the-art. The very good and highly reliable performance of traditional-design permanent magnet undulators, combined with the need for synchrotron facilities to operate with extreme reliability, have slowed the implementation of novel superconducting IDs (SCIDs) in storage ring light sources. In-vacuum cryocooled hybrids and SCIDs pose additional challenges, such as measurement within a restricted bore, precision trimming of the field and management of heat load from synchrotron radiation and image currents. These problems must be completely solved prior to installation to ensure no adverse impact on storage ring operations. Both active (trim coil) corrections and passive (Meissner effect) correction schemes have been explored. Several prototype superconducting undulators will be tested in the next few years. It is reasonable to expect superconducting devices will have greater tolerance of ionizing radiation, which causes demagnetization of hybrid small-gap insertion devices after extended exposure to beam losses in top-up operation.

ERLs and FELs (as well as “on-axis injection” storage rings) have no need for large horizontal aperture for injection. This will enable the use of quite different and more (magnetically) efficient insertion devices producing circular polarization. Helical-motion undulators based on electromagnets and “delta” geometry undulators will, when perfected, offer distinct advantages for on-axis injection “ultimate” storage rings, ERLs and FELs:

- higher field strength at arbitrary polarization setting,
- shorter gain lengths (making practical shorter tunnels or shorter linear accelerators)
- higher SASE power at saturation in an FEL
- higher output power in a seeded FEL.

In terms of impact on the design of future light sources, it is quite likely that these new undulator technologies will materially change the design rules for FELs, ERLs and “ultimate” storage rings much as “top-up” operation has done for storage ring sources.

Spatial coherence and incoherence in x-ray experiments

A common motivation for many future source developments involves ever-increasing source brightness. This is important for many experiments, but not all.

One way to look at this question involves speaking not of brightness, but of total flux and phase space area. As in accelerator physics, phase space area in a photon beam refers to the product of source size multiplied by divergence at a focal waist. As was pointed out by Kondratenko and Skrinsky [*Optics and Spectroscopy* **42**, 189 (1977)], Krinsky [*IEEE Trans. Nucl. Sci.* **NS-30**, 3078 (1983)], and Winn *et al.* [*J. Sync. Rad.* **7**, 395 (2000)], the full-width/full-angle phase space area that can be accepted for experiments requiring spatial coherence or, equivalently, requiring a diffraction limited focus is approximately equal to the photon wavelength squared, so that the spatially coherent flux is the brightness (photons per phase space area, such as per mm^2•$mrad^2$) B divided by wavelength squared, or B/λ^2. One can also speak of the number of coherent modes in a beam as the phase space area of the beam divided by λ^2.

It is straightforward to separate out the mutually spatially coherent flux from the total flux. One approach is to place a pinhole at the focus of a beamline optic with a pinhole diameter given by the beam convergence angle divided by the wavelength; in visible light optics labs a microscope objective/pinhole pair called a "spatial filter" routinely provides this function, while in a x-ray beamline a focusing mirror or crystal can be combined with a pinhole or a slit to serve this purpose. Using this approach, experimenters have been generating coherent beams from incoherent 2nd and 3rd generation light sources for decades; one does not need a storage ring with 0.1 nm•radian emittance (or a FEL source) to do coherence experiments or to achieve a high resolution focus, although increased source brightness leads directly to increased flux in coherence-based experiments.

Who needs coherent flux versus incoherent flux? There are as many particular answers as there are experiments, but here are some glittering generalities:

- Most x-ray experiments do not require coherence at all; they just want raw flux on the sample, with rather unstringent requirements for the phase space in which the flux is contained.
- Coherence in fact can be detrimental to many experiments; in that it translates disturbances in the phase across a beam into intensity variations further downstream (known as speckle). Just as one prefers to use thermal lamps rather than lasers in conventional, full-field microscopes, one prefers incoherent flux for many x-ray experiments including full-field imaging.
- In the area of imaging, one does *not* need a fully coherent beam in order to exploit phase contrast. Frits Zernike's 1953 Nobel Prize in physics demonstrated how one could split and recombine beams on a pixel-by-pixel basis in a microscope to obtain phase contrast with a thermal lamp source. In other words, one can use as many spatially coherent modes (or source phase space/λ^2) as pixels in the image – a number that exceeds a million! If one uses propagation methods to achieve phase contrast, the coherence requirement goes up somewhat, but since most experiments use only 0.5 or 1 fringe for turning phase shifts into intensity variations one divides the number of image pixels by only a small number of order 10.
- Experiments that use high resolution optics for beam nanofocusing, such as in scanning microscopy or microprobe/nanoprobe analysis, certainly do need coherent flux even if one is subsequently using an incoherent process (like fluorescence) to yield the final image.
- Experiments that attempt to reconstruct an object's optical disturbance from far-field intensity measurements, such as coherent diffraction imaging experiments, need coherence [although advances in phase reconstruction are allowing one to deal with not just single-mode but several-mode illumination; see e.g., Whitehead *et al.*, *Phys. Rev. Lett.* **103**, 243902 (2009)].
- It is easier to design high energy resolution monochromators that need to work with only small beam étendue or phase space area. With large étendue, one might be forced to work with difficult-to-manufacture aspherical optics or with bent crystals.
- Experiments that combine crystalline diffraction (with its narrow rocking curve) and small beam spots do not strictly require coherence, but they can require source phase space areas that approach λ^2. In inelastic x-ray scattering, each separate wavelength-dispersive crystal monochromator might collect a signal from a small beam spot and "image" it to a small pixel on a one-dimensional detector. However, one needs a small source phase space area to achieve a small focused beam spot anyway; this does not usually lead to an additional requirement on the source. A more demanding example

involves crystallography from micro-crystals. The ability to crystallize membrane proteins (which control transport of many pharmaceutical agents into cells, and which are notoriously hard to crystallize because of their structural adaptation to ever-rearranging membranes) has advanced tremendously in recent years, yet one might have crystals that are only a few micrometers across with modest mosaic spread on the diffracted beam thereby requiring small-phase-space illumination.

Monochromaticity or temporal coherence

The length over which radiation from a source is mutually coherent is determined by the source monochromaticity times the wavelength, or $\lambda^2/\Delta\lambda$. Most experiments do not by themselves require much in the way of temporal coherence, and just as spatial filters are used to isolate spatially coherent flux from incoherent sources, one uses monochromator optics to isolate the desired degree of temporal coherence or monochromaticity at a loss in flux. What then sets the desirable level of monochromaticity?

- Chemical bonds involve energies of a few eV per molecule, so energy widths of order 0.1 eV are important for many spectroscopy experiments. This is routinely achieved with crystal monochromators for multi-keV X rays, or grating monochromators at lower photon energies although the energy range of about 2-3 keV is in a somewhat awkward in-between zone.
- A smaller class of phenomena requires the understanding of phonon modes in solids, where an energy resolution of 0.01 eV or even below 0.001 eV is demanded.

Continuous, stroboscopic, and one-shot experiments

The demands on a light source vary tremendously between continuous, stroboscopic, and one-shot experiments. Even though most accelerator-based light sources involve microbunched beams, the duty cycle and bunch repetition rates are fast compared to thermal relaxation times as well as signal integration times of the detectors in the experiment, so they are best thought of as continuous-in-time sources. Most experiments are continuous, in that the specimen under examination must “survive” unchanged over the course of the experiment. Consider the example of tomographic imaging of a cell; the cell should remain unchanged as it is imaged from 10^2-10^3 viewing angles [while Raines *et al.*, *Nature* **463**, 214 (2010) have proposed that 3D imaging can be done with a single viewing angle, most researchers feel that this is only possible for very small and sparse objects such as simple molecules]. Consider the example of using a 10 nm focused x-ray beam for scanned imaging with a temperature increase of no more than 1 K; a simple calculation shows that for an ice-embedded thin specimen imaged using 500 eV photons one cannot handle a flux higher than 4×10^{10} photon/sec while a silicon-embedded thin specimen imaged at 10 keV cannot tolerate a flux higher than 2×10^{10} photons/sec. As a result, in conventional rocking-curve crystallography, tomography, and also spectromicroscopy (where one acquires spectrum-per-pixel data to study chemistry at the nanoscale), one cannot use more flux than a certain value so that heating does not alter the specimen while data acquisition proceeds.

Stroboscopic measurements such as pump-probe studies are more forgiving. One can "turn down" the beam intensity and repetition rate to prevent specimen heating, or in the case of reproducible phenomena in fluids or gases one can use specimen flow to provide a continuous source of ambient temperature "specimens" for study.

The opposite extreme involves one-shot experiments. If one is studying nonlinear phenomena, high irradiance (photon flux per area, which translates into oscillatory electric field strength or equivalently multi-photon overlap) is essential. Another example is the solution to the simultaneous limit of low flux rate to avoid heating and low cumulative exposure to avoid the decline in data quality set by radiation damage: collect data with an intense pulsed beam so that the required information is obtained before damage processes take their toll. A now-classic example is the proposal of Neutze *et al.* [*Nature* **406**, 752 (2000)] to collect diffraction patterns from single molecules before both thermal and ionization-driven Coulomb "explosions" can take place. This frontier is rich with important experiments, but it is important to keep sight of the fact that these are not representative of *all* exciting experiments.

Beamline optics and nanofocusing optics

Generally, discussions covered state-of-the-art techniques extrapolated to the higher average and peak brightness of future sources. Damage to optics from heating and ablation (in the case of FELs) must be taken into consideration in the design of optics. In the next few years, the new x-ray sources facilities will provide valuable data on damage thresholds. As described earlier in this working group summary, coherence is not necessarily a desirable property of an x-ray beam if it results in undesired intensity fluctuations within the sample volume. Preservation of coherence (or control of detrimental coherence effects) will be a consideration of growing importance for design of beamline optics. The effect of collimators, attenuators, lenses and mirrors on a coherent beam will be an integral part of beamline design.

Temporal coherence and time-domain properties of ultrashort pulses must also be taken into account in optics design. This issue was touched upon in Michael Klopf's presentation of JLAMP beamline concepts. A double-diffracting monochromator was proposed as a means of producing "transform limited" x-ray pulse.

Detectors

Presentations and discussions addressed array detectors for imaging and energy-resolved scattering measurements, with heavy emphasis on the challenges posed by the need to read out frames of data on a shot-by-shot basis from high repetition rate sources such as storage ring slicing sources, FELs or ERLs. The full dynamic range of signals from single photon sensitivity to 1,000 x-rays per pixel must be spanned in a single shot and read out at the pulse rate of the source. Frame readout rates of 100-200 Hz are a present-day challenge; future sources will require the readout of many megapixels of data at average rates of 10-100 KHz or higher. In order to do this, detectors must have, at the single pixel level, dedicated amplifiers with adjustable gain, a high degree of parallelization of the digitization and readout process. Dedicated readout for each row or even each individual pixel is required. Onboard data storage for each pixel is required to collect data from x-ray sources with “burst” time structure (e.g. the European XFEL) can be used to best advantage.

It is clear that advances in detector performance (especially in readout rate) will amplify one of the most significant challenges associated with present-day FELs: processing raw data at a rate of terabytes per day for a single experiment. At present, FEL users are coming to grips with the need for real (or perhaps “human”) time data analysis to be certain that the experiment is working properly. In the future, experimenters will likely need to develop automated “post-triggering” or rejection of bad data frames and perhaps real-time post-processing of raw data.

Perspective on Future X-ray Experiments with New Sources and Beam-line infrastructure

The impact of new x-ray sources is considerable and is building nicely from the success of the current generation of storage rings. New sources such as ERLs, ultimate light sources and XFELs are now driving the demand for further improvements in all the associated beamline technologies of insertion devices, optics and detectors and methods used to collect the x-ray data.

For the XFELs, the many orders gain in high peak brightness and ultra-short pulse capability is revolutionizing pump/probe experiments, particularly in the nano-crystallography area just to mention one example. With future ultimate storage and ERL possibilities, there will be new opportunities to extend the synchrotron x-ray techniques now practiced at 3rd generation storage ring sources to continuously follow the time-evolution of many dynamic processes 100 to 1000 times faster than can be done now without destroying or significantly altering samples during their examination. This will be of great benefit, for example, for following the change in structure of a catalyst during the life-cycle of it activity.

In summary, the accelerator and x-ray science communities are still in an exciting period of development with lots of new instrumental developments to be made and many new scientific directions yet to be explored.