3 Accelerators for Synchrotron Radiation

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3.1 Introduction

The explosion in synchrotron-based research over the last two decades can be attributed to dramatic advances in accelerator technology, but these advances have been to a large degree driven by the demands of an expanding, highly diverse user community. This intense light source covers most of the electromagnetic spectrum. The polarization of the light and the pulsed time structure are being utilized more and more as more complex studies are carried out. These machines have developed from "parasitic" operation during colliding-beam experiments to dedicated machines (TESLA in Hamburg, Germany) where highly coherent pulses of X-rays can be produced.

3.1.1 Dipole Radiation

According to Liénard [1] and Wiechert [2], the electric field originating from a moving charge (see Fig. 3.1) can be written as

$$\mathbf{E}(x,t) = \frac{e}{4\pi\epsilon_0}\left[\frac{\mathbf{n}-\boldsymbol{\beta}}{\gamma^2(1-\boldsymbol{\beta}\cdot\mathbf{n})^3R^2} + \frac{1}{c}\frac{\mathbf{n}\times[(\mathbf{n}-\boldsymbol{\beta})\times\boldsymbol{\beta}]}{(1-\boldsymbol{\beta}\cdot\mathbf{n})^3R}\right]_{ret}. \qquad (3.1)$$

The first term describes the near (velocity) field, which we shall not treat here, while the second term describes the far (acceleration) field (the notation used in the equations are defined in Table 3.1). The latter term refers to the synchrotron radiation (SR) produced when the acceleration is perpendicular

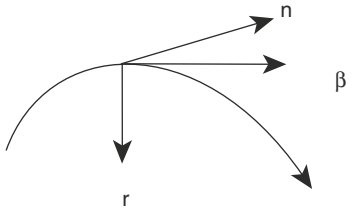

Fig. 3.1. A schematic diagram indicating the relevant vectors for synchrotron radiation produced in a dipole magnet

Table 3.1. Notation and definitions used in the equations

Parameter	Definition
β	Particle velocity in units of c, the speed of light
R	Distance from point where light is emitted to observer
ϵ_0	Permittivity of free space
γ	Lorentz factor
ρ	Bending radius of an electron moving in a magnetic field
$\mathbf{n}$	Unit vector from particle to observer
λ_u	Undulator period length
θ	Angle between particle velocity and radiation direction
$K_u = eB\lambda_u/(2\pi m_e c)$	Undulator parameter
B	Undulator peak magnetic field
N	Number of poles in insertion device
ω_c	Critical frequency for bending-magnet radiation
e	Electron charge
m_e	Electron mass

(when the charge is deflected in a bending magnet) to the velocity β. The far-field radiation has the following characteristics for relativistic particles:

1. The electric vector is in the plane of acceleration.
2. The total power emitted is given by

$$P = \frac{2e^2 c\beta^4\gamma^4}{3\rho^2} \,. \tag{3.2}$$

3. The power is highly focused within an angle

$$\frac{1}{\gamma} \,. \tag{3.3}$$

4. The radiation is emitted in a *broad spectral range* up to the critical frequency

$$\omega_c = \frac{2c\gamma^3}{3\rho} \,. \tag{3.4}$$

3.1.2 Undulator Radiation

When a relativistic electron passes through a periodic magnet device (period length λ_u), known as an undulator (see Fig. 3.2), we can see from (3.1) that an electromagnetic (EM) wave with the following properties will be generated.

The wavelength of the EM wave is given by

$$\lambda_i = \frac{\lambda_u}{2\gamma^2 i}\left(1 + \frac{K^2}{2} + \frac{\theta^2\gamma^2}{2}\right) \,. \tag{3.5}$$

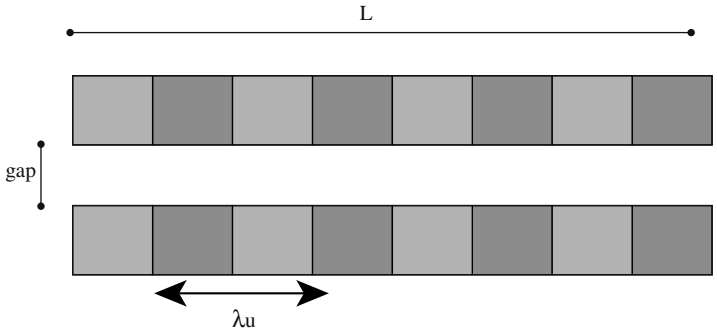

Fig. 3.2. A schematic diagram of an insertion device. The period of the device, λ_u, is indicated

The wavelengths produced are described by $\lambda_i N_u$. The bandwidth of this wave is Fourier transform limited to $1/(nN)$, where n is the harmonic number and N is the number of poles in the magnetic undulator array. Modern storage rings implement insertion devices as the primary source of radiation. See Fig. 3.3 for a diagram comparing the brightness of a bending-magnet

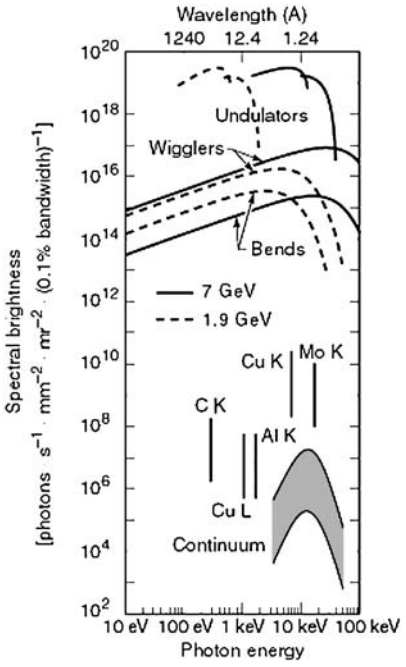

Fig. 3.3. A comparison of the brightness of undulators, wigglers and bending-magnet sources. Metal-anode sources are also indicated in the plot

source with two insertion device sources. It should be mentioned that the full exploitation of the characteristics of undulator radiation puts stringent demands on the electron beam quality in terms of emittance and energy spread in order to preserve the narrowest natural line width. The measures of photon intensity have developed from flux (photons/s) to brightness (photon flux per unit source area per unit solid angle) and brilliance (photon flux per unit phase space volume), where the source size and the small opening angle of undulator radiation are taken into account.

Another variant of the magnetic insertion device is the "wiggler". The wiggler spectrum is the incoherent superposition of the spectra from N poles, and is generally used as a wavelength shifter which can produce a dipole-like spectrum at a shorter wavelength.

3.1.3 Coherent Radiation

When (3.1) is integrated over all space, it can be seen that for wavelengths larger than or similar to the bunch dimensions, the EM waves add in phase and the power emitted is proportional to the number of particles squared. We now have a coherent radiation source. This is a very important characteristic of undulator radiation and is currently the focus of new developments in machine design.

3.1.4 Synchrotron Radiation Facilities

These radiation characteristics have proved to be quite useful for the study of matter; we have now some 60 dedicated synchrotron radiation facilities in operation around the world, and new ones are being planned and built. The first generation of synchrotron radiation research took place at existing high-energy physics accelerators such as DORIS (Germany) and SPEAR (US). These are called the "first generation" of synchrotron light sources. The second-generation sources were specially built machines with small, intense electron beams dedicated to SR research: SRRC (UK), MAX I (Sweden), and BNL (US), to name a few. The introduction of special insertion devices, undulators and wigglers, increased the brilliance by several orders of magnitude. The third-generation sources take full advantage of undulator radiation. Some examples of X-ray sources are ESRF (France), APS (US), and Spring8 (Japan). Some examples of soft-X-ray sources are ALS (US), MAX II (Sweden), Ellettra (Italy), SLS (Switzerland), and BESSY (Germany). The fourth generation of light sources could very well produce mainly coherent light. The two X-ray coherent sources being designed today are XFEL (Germany) and LCLS (US). The perfomance development of synchrotron radiation sources is demonstrated in Fig. 3.4.

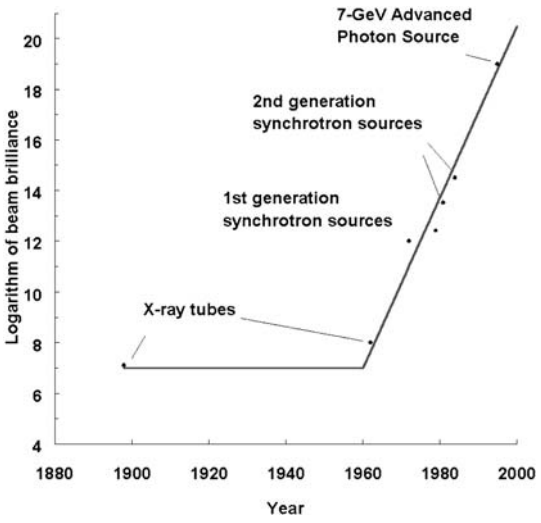

Fig. 3.4. Development of light source performance

3.2 Instrumentation for Synchrotron Radiation Experiments

Although some early experiments used the entire continuous spectrum of light from relativistic electrons more or less directly in, for example, absorption spectroscopy, nearly all modern experiments rely on specialized optical systems to extract the radiation to the experiment in an efficient way. The optical scheme can be designed for a particular purpose, such as high flux throughput, polarization, or high spectral resolution. Microscopy experiments require a highly focused beam, while lithography demands a stable beam of parallel X-rays for accurate imaging. In addition, most experiments require a single, narrow-bandwidth (BW) photon energy, which should be tunable over a wide range of energies. A number of different optical systems have been developed in response to the varied needs of the user community. All of the properties which are important for experiments can be optimized by designing optical systems together with the design of the ring lattice. Achieving the highest performance at the experiment depends upon having the correct emittance, polarization, stability, and pulse structure in the electron beam. These *monochromators* should be able to operate in a laboratory environment where conditions are constantly changing, and they should work with a variety of different kinds of experiments.

A short overview of some common monochromators will be given here. The long-wavelength regions (*visible* and *infrared*) have traditionally been the domain of lasers, but recently synchrotron radiation has proven to be a useful tool even in the infrared region. In the *ultraviolet* region, an unprecedented photon-energy resolution of 150 000 has been obtained in the

10–30 eV region, and new variable-polarization undulators, where the polarization vector at the sample can be rotated by tuning undulator parameters, open up new possibilities for experiments. Dramatic improvements in insertion devices and beam emittance have pushed the performance of *soft-X-ray* monochromators to unprecedented resolution; finally, it has been possible to resolve vibrational levels in molecules even for inner shells. A photon BW substantially smaller than the lifetime broadening of inner-shell levels in light elements (40 MeV BW at 500 eV) is routinely available at many SR laboratories. More information on soft X-ray monochromators can be found in [12].

The quality of the light at the sample depends on all of the optical elements between the source and the experiment. The primary mirror generally images the source at a point several meters from the storage ring. The mirror may also magnify the source, and it functions as a coarse filter owing to the reflection properties of the mirror surface coating. Generally, the mirror has a high-energy cutoff determined by the angle of incidence and the surface material. The mirrors may be subjected to enormous thermal loads, which lead both to deformation of the mirror surface and to photocatalysis, resulting in carbon buildup on the mirror. The former may be handled by cooling schemes, while the latter is more difficult to remedy. Keeping in mind that the storage ring and the optics associated with each beam line are installed in an interconnected vacuum system (see Fig. 3.5), all operations involving movements of mirrors or other optical elements must be designed for ultra-high vacuum (better than 10^{-7} Pa). The vacuum constraints require reliable security systems to guard against accidents in any part of the experiment affecting the operation of the monochromator or storage ring.

The task of the monochromator is to extract a single wavelength from the continuous spectrum after the primary optics. The task is accomplished by a series of mirrors and a dispersive element such as a diffraction grating, which focus the dispersed radiation on an exit slit. See Fig. 3.6 for a schematic diagram of a monochromator for soft X-rays.

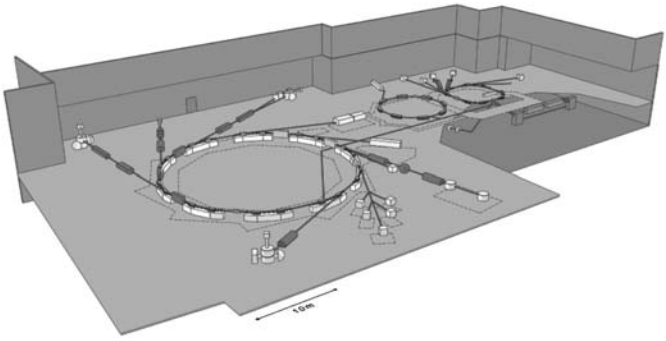

Fig. 3.5. A diagram showing the MAX electron storage rings. The *beam* lines are indicated in the figure

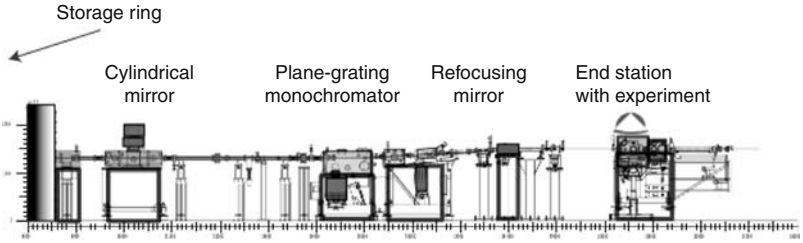

Fig. 3.6. A diagram of a beam line with a grazing-incidence plane-grating monochromator

The final stage in the beam line is the refocusing optics. The purpose of these optics is to make it possible to place an experiment at the final focus of the light. Several meters are needed after the monochromator exit for diagnostic instruments, differential pumping stages, and filter systems and for large experimental vacuum chambers.

The monochromators can be divided into several classes: the dispersive elements can be diffraction gratings, which can be ruled on a focusing mirror surface (spherical or toroidal grating), or crystal diffraction can be used to disperse X-rays. Some common monochromator designs are listed in Table 3.2.

Table 3.2. A list of common monochromator classes used at synchrotron radiation sources. A few typical parameters are given

Monochromator Type	Spectral Range (typical)	Energy Resolution	Energy at which Used (eV)	Applications
FTIR	Infrared	1000–10 cm^{-1}		
NIM	Ultraviolet	5–40 eV	10^5	Chemical dynamics, valence band
SGM, PGM	Soft X-ray	30–2000 eV	10^5	Inner-shell electrons, NEXAFS
Crystal mono. chromator	Hard X-ray	3–20 keV		Protein crystallography, diffraction, EXAFS

3.3 Research with Synchrotron Radiation

The primary characteristics of synchrotron radiation can be found in short form in [4]. The most important properties are:

1. High brightness.
2. Variable energy.
3. Polarization: linear to circular.
4. Pulsed time structure.
5. Highly focused (monochromator).
6. Narrow bandwidth (monochromator).

Most of these properties depend upon the characteristics of the electron beam, and on the design of the monochromator and beam line optics.

3.4 Experiments

It is impossible within the scope of this chapter to do justice to even a small fraction of the research which is presently being done using synchrotron radiation. The light source is used for spectroscopic studies of atoms, molecules, solids, molecular materials, and hybrid systems; angle-resolved photoemission is a standard tool for studying band structure; and hard X-rays are used for a variety of experiments, including protein structure studies, angiography, and lithography. A short summary of some of these research areas where synchrotron radiation has played a particularly important role is given here, and a few key references are listed at the end of the chapter. In Chap. 2, about "Accelerators for Medicine", the application of synchrotron radiation in medicine is outlined.

3.4.1 Atomic and Molecular Physics and Chemistry

Early studies exploited the broad spectrum of synchrotron radiation for absorption measurements of atoms and molecules [5]. Angular distributions of photoelectrons can be studied using the highly linearly polarized light from bending magnets or undulators [9]. Fundamental quantities such as total and partial ionization cross sections can be measured using SR if careful measurements of the sample and source fluctuations are made during the spectral measurement. In molecules, it is important to know fragment yield cross sections and to identify the thresholds for dissociation pathways in order to understand photochemical processes taking place in the atmosphere, for example. A series of studies has been made at LURE (France) and Astrid (Denmark) where photoionization cross sections for singly charged atomic ions were measured. Photoionization induced by SR of several hundred eV energy was recently used to study inner-shell photodetachment of negative-ion clusters [11]. Most of these studies are carried out on VUV or soft-X-ray beam lines. A typical end station setup is shown in Fig. 3.7.

The tunability of SR allows selective excitation of electronic states when the photon energy is tuned to a resonance energy. For valence electronic

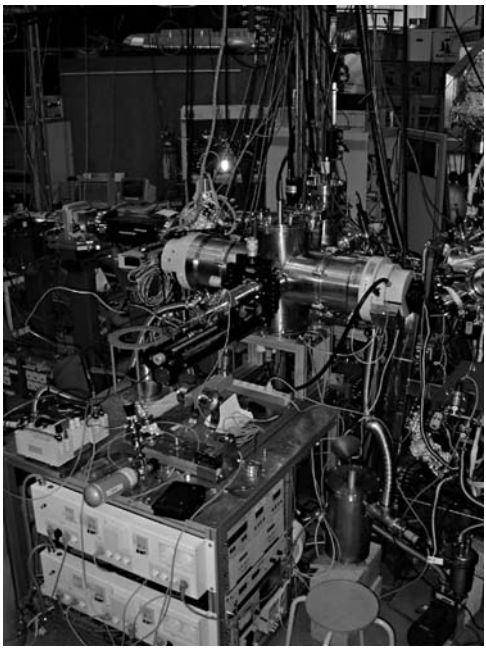

Fig. 3.7. A photograph of the end station at BL I 411 at MAX-Lab. There are a hemispherical electron analyzer, a time-of-flight ion mass spectrometer, and a cluster source mounted on the beam line

levels, this makes it possible to determine the energies of atomic and molecular Rydberg and valence states with high accuracy. The high density of states in the 5–40 eV region often leads to overlapping states, so the narrow bandwidth available from normal-incidence monochromators is necessary to perform selective excitation. For inner-shell states, the electronic states are well separated in energy. In molecules, the molecular orbitals associated with core-excited states are generally localized on a particular atom. Thus selective electronic-state excitation is equivalent to a spatial selectivity in the molecule. Combining the site selectivity of the excitation with spectroscopies such as electron spectroscopy, ion fragment spectroscopy, and fluorescence emission spectroscopy has provided insight into the nature of core molecular orbitals [10]. Another important aspect of core-excited states is the very short lifetime of these states. A core hole in an oxygen molecule will be filled via an Auger transition in a few fs. Since the spectroscopic information pertains to the final states, it is possible to follow the development of core-excited states on the fs timescale by comparing the populations of static and dynamic states in the spectrum. The concepts used in this type of analysis were developed in close collaboration between quantum chemists and experimental groups studying atoms, molecules, and molecular adsorbate systems [6, 7].

3.4.2 Materials Science

The method mentioned in the previous section has been used to study charge transfer between substrates and adsorbates, and between different subunits in a molecule [8]. Although the method probes these dynamical effects in an indirect way, it is one of the few methods able to probe such fast processes. Catalytic materials can be studied by using X-rays for photoelectron spectroscopy, and surface-sensitive methods can illuminate bonding geometries. Near-edge X-ray absorption spectroscopy (NEXAFS) is element-specific, and can provide information about electronic states and bonding. The chemical composition of materials ranging from geological samples to blood and engine exhaust can be obtained. Dynamic information can be obtained by combining XAS with pulsed laser excitation. The degradation of the wood in the excavated Swedish warship *Vasa* has been studied using these methods. In cleaner systems, the bonding of molecules to metallic surfaces can be determined by performing such measurements at different angles with respect to the polarization plane of the SR.

An important tool for structure determination of periodic and semiperiodic solids is extended X-ray absorption fine structure (EXAFS). An inner-shell ionization processe produces an electron, which can scatter from ligand neighbors. The scattering is dependent on the distance and on the momentum of the electron. EXAFS can provide distances, coordinations, and even atomic displacements in alloys and under extreme conditions.

Another emerging area exploits the novel polarization properties of SR. Circularly polarized X-rays can be extracted, with the proper optics, from bending-magnet or undulator sources. Magnetic materials can be characterized using circular dichroism, and magnetic domains can be studied in layered systems, for example.

3.4.3 Microscopy

Microscopy is one area which is developing rapidly at synchrotron radiation sources. In photoelectron microscopy schemes, the operation of the ring must be highly stable, and schemes where the ring current is replenished continuously are optimal. The small source size combined with high brilliance makes highly focused beams in the soft-X-ray region possible to achieve. The focused beam is scanned in a raster pattern over the sample surface. Photoelectron spectra are measured at each point in the raster. The surface may be treated by heating or by dosing with reactive agents. More recent spectromicroscopes utilize circularly polarized light for studies of magnetic circular dichroism. Magnetically induced circular dichroism (MCD) is the differential absorption of left and right circularly polarized light in the presence of a magnetic field. Electron detectors which are sensitive to electron spin are employed for spin-resolved photoemission studies. Presently the resolution achieved is 30 nm, but developments in zone plates produced using synchrotron radiation

should push this limit to below 20 nm. Future work will exploit two-photon excitation, where lasers are combined with synchrotron radiation to extract time-dependent information about surface reactions. The coherence of undulator light will also be used for interference lithography.

X-ray microscopy is also used for imaging of biological cells in frozen or aqueous environments. Phase contrast imaging using interferometers for hard X-rays is also used to study medical samples. X-rays penetrate farther into the sample than do electrons; thus X-ray microscopy is able to image thicker samples, and there are no vacuum requirements for X-ray studies, making measurements in realistic enviroments feasible in many cases. More information on microscopy schemes can be found in [13].

3.4.4 Crystallography

Crystallography is the most important area in synchrotron radiation research in the life sciences. Crystallographic studies provide structural information about macromolecules and complexes [14]. Although it is possible to carry out crystallographic studies using standard rotating-anode sources, the brilliance and small cross section of the beam (microfocused to 10^{-6} m) have allowed determination of much smaller crystals (down to $\sim 10^{-6}$ m) and of samples which are easily damaged by radiation. The multiwavelength anomalous diffraction technique (MAD) requires tunable wavelengths, which is only possible at synchrotron radiation sources. In short, SR permits structural determination of larger, more complex samples than is possible otherwise.

At the frontier of crystallography lie time-resolved studies. There are a number of time ranges of interest for imaging biological processes in action. In some cases it is possible to slow down a process by thermal control, so working on the picosecond timescale will be sufficient for many applications. Conformational changes on the ps timescale in biological macromolecules are highly interesting, since such changes are closely related to function. Enzyme activity in biological systems can change the structure of a macromolecule in several steps; these developments could easily be followed using shot-to-shot imaging methods. Even chemical reactions on the fs–ps scale could be followed using combined spectroscopic and structural studies. Since these experiments require three-dimensional structural information in addition to temporal resolution, the requirements on the light source are stringent.

3.4.5 Summary

The symbiotic development of SR sources and experiments has made the synchrotron radiation laboratory a unique facility. Research is highly cross-disciplinary; experiments in materials science and the life sciences are performed side by side with basic research in atomic and molecular physics and quantum chemistry. Important advances in imaging techniques and crystallography have led to a veritable explosion within biological science at SR

facilities. Future machine developments will focus on short pulses on the fs scale, and on the production of coherent radiation.

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Part II

The Electrostatic Accelerator