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A plane-grating monochromator for circularly polarized undulator radiation at BESSY II

F. Senf,[a]* K. J. S. Sawhney,[b] R. Follath,[a] M. Scheer,[a] F. Schäfers,[a] J. Bahrdt,[a] A. Gaupp[a] and W. Gudat[a]

[a]BESSY GmbH, Lentzeallee 100, D-14195 Berlin, Germany, and [b]Centre for Advanced Technology, Indore 452 013, India. E-mail: senf@exp.bessy.de

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At BESSY II, a third-generation 1.7 GeV storage ring is under construction. A planar elliptical undulator will be installed as a source of X-rays that have a high degree of circular polarization. Radiation in the first, third and fifth harmonics will cover the energy range 87–1330 eV. The beamline will essentially consist of a plane-grating monochromator working with collimated light in the dispersion plane. A single set of optical elements can be used to handle the two angularly separated beams of opposite helicity from the double undulator. The degree of circular polarization ranges from 73 to 100%, and a flux of up to 5×10^{13} photons s^{-1} $(100\ mA)^{-1}$ can be achieved. A maximum spectral resolution of about 13 000 will be possible at 100 eV using a 20 μm slit.

Keywords: circular polarization; undulators; monochromators.

1. Introduction

Circularly polarized synchrotron radiation has become an important tool in the investigation of circular dichroism (CD), mainly of the transition and rare-earth elements. Circularly polarized off-plane synchrotron radiation from bending magnets, which has been extensively used for experiments in the past, is now being substituted by a more intense coherent radiation from insertion devices. At BESSY II, a third-generation 1.7 GeV storage ring under construction, a planar elliptical undulator of the Sasaki type (Sasaki *et al.*, 1992) will be installed. A device of this type offers high-brilliance synchrotron radiation with a high degree of circular polarization. The insertion device at BESSY II (Bahrdt *et al.*, 1996) essentially consists of two undulators which can be steered, similarly to an undulator at the ESRF (Elleaume & Chavanne, 1991), to produce two angularly separated beams of opposite helicity. Because of expected interference, at BESSY II it has been decided not to switch helicity by changing the path of the electrons in the storage ring; instead the helicity switching will be performed in the beamline. Thus, for the design of the beamline the following criteria had to be fulfilled:

(i) The product of the square of the degree of circular polarization and the flux, *i.e.* the appropriate figure of merit, should be as high as possible.

(ii) The spatial overlap of the two beams at the sample should be large to avoid incorrect data interpretation in case inhomogeneous samples are investigated.

(iii) In order to be relatively insensitive to thermal drifts and misalignments, only one set of optical elements should be used to handle the two separated beams.

(iv) The chopping of the two beams should occur in a section with large separation and low heat load.

(v) Nevertheless, the expected performance of the beamline with respect to resolution and flux should be comparable with that of monochromators at other undulators.

Comprehensive simulations of the expected performance of the undulator-beamline combination have been carried out (Sawhney *et al.*, 1997) to derive quantitative information about the above design goals. The undulator source characteristics are briefly discussed in §2. The design of the beamline will be described in §3, and in §4 quantitative results of calculations of the undulator-beamline system are presented.

2. The source

The planar elliptical insertion device at BESSY II essentially consists of two undulators in one straight section of the storage ring, which can be either steered to produce two angularly separated beams of opposite helicity, or combined to emit one central beam of one helicity. The system can also be used to produce linearly polarized light of different orientation. The horizontal angular separation of the two beams has been set to a minimum value of ± 0.2 mrad necessary to avoid overlapping of the two cones at their largest extension (*i.e.* at lowest energy). Each undulator consists of 31 periods with a length of 56 mm each. The centres of the two undulators are separated by 2 m, hence providing space for steering magnets. The maximum k parameter ($k = 3.0$) corresponds to a vertical peak magnetic field of 0.63 T. The maximum horizontal field is 0.38 T. For tuning the first undulator harmonic from 116 to 436 eV the horizontal and vertical magnetic field components can be kept equal. Thus completely circularly polarized light is emitted and no intensity is found in the higher odd harmonics. For scans above 436 eV the third and fifth harmonics are needed, which will only provide intensity for unequal fields. Below 116 eV a scan with the first harmonic can only be made with unequal fields since the vertical magnetic gap will be limited to 20 mm. In these cases the emitted radiation is elliptically polarized still with a high content of circular polarized light (between 73 and 88% for photon energies from 360 to 1330 eV).

3. Design of the beamline

Because of the small separation of the two beams of opposite helicity, a single set of optical elements can be used to steer and monochromatize the synchrotron radiation. The advantage of this 'monolithic' design is that it will be relatively insensitive to thermal drifts, mechanical misalignments, *etc*., which often limit the performance of beamlines if separate optics are employed. Moreover, our beamline design can be used without changes if the two undulators are coupled to a single undulator emitting one central beam. The first optical element in the beamline, a horizontally deflecting toroidal mirror, M1, of 300 mm length at 17 m distance from the source, is large enough to accept the two angularly separated beams and to horizontally focus them to the sample position at 35 m distance from the source. For further details of the beamline, see Sawhney *et al.* (1997).

The requirement of high resolution over a large scanning range from 87 to 1330 eV led to the decision to use a plane-grating monochromator (PGM) with variable included angle (Kunz *et al.*, 1968). The monochromator employs a rotatable plane mirror in front of the plane grating. Compared with spherical-grating monochromators, which would require about twice the number of gratings to cover this energy range, it also offers a more effective higher-order suppression. This is of advantage if faint differences, *e.g.* in circular dichroism, are investigated. As in other PGMs at BESSY II (Follath *et al.*, 1998), the grating works in collimated light in the dispersion plane (Hunter *et al.*, 1982), which is provided by M1. This enables the monochromator to be operated in either the higher-order suppression mode or the high-energy resolution mode without rearranging slit or optical elements in the beamline. Gold-coated 400 l mm^{-1} and 1200 l mm^{-1} laminar gratings have been chosen to optimize the full energy range coverage of the beamline. The gratings and the first two mirrors (M1 and a rotatable plane mirror) are made of SiC with water-cooled side plates. A horizontally deflecting cylindrical mirror, behind the grating, focuses the diffracted light vertically onto the exit slit at 9 m distance. A UHV-compatible chopper for fast switching (>100 Hz) has been placed about 1 m behind the horizontally deflecting cylindrical mirror. At this position the heat load is already below 1 W and the separation of the two beams is still large enough to allow for clear switching. Behind the exit slit a horizontally deflecting conical mirror refocuses vertically the monochromatic image at the slit onto the sample position with a 1:1 magnification.

4. Calculation and results

Comprehensive simulations of the performance of source and beamline have been performed by using the undulator code *WAVE* (Scheer, 1995) and the ray-tracing code *RAY* (Schäfers, 1996). The angular intensity and polarization distribution generated by *WAVE* have been used as input for *RAY*, which has been modified to trace and visualize contributions of different helicities of the double undulator. *RAY* also calculates reflectivities, polarization characteristics and, due to the inclusion of a code developed by Neviere *et al.*, (1974), grating efficiencies and higher-order contributions. Fig. 1 shows the photon flux expected at the sample position from one of the double-undulator modules. At the sample a maximum flux of 5×10^{12} photons s^{-1} (100 mA)$^{-1}$ can be achieved by a 400 l mm^{-1} grating and 200 μm slit size, which corresponds to an energy resolution of

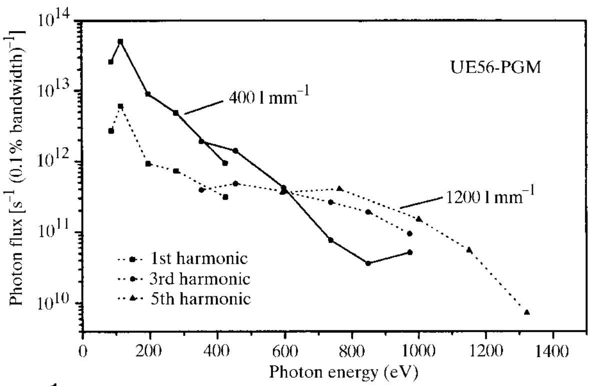

Figure 1
Photon flux at the sample from each of the undulator modules for a 200 μm slit.

more than 2000. With the 1200 l mm^{-1} grating the full energy range of the first, third and fifth harmonics of the undulator can be covered. The large drop in intensity at higher photon energies can be mainly attributed to the reduced reflectivity of the optical elements and about one order to the undulator. However, a relatively high energy resolution ($E/\Delta E$) of more than 13 000 at 100 eV and still 6000 at 1300 eV can be reached by using the 1200 l mm^{-1} grating and a slit width of 20 μm, with a flux ten times smaller than presented in Fig. 1. The energy resolution is mainly limited by the fact that none of the two undulator beams is focused at the slit position. The first undulator is focused in front of the slit, the second behind. At the slit position they must have the same broadening to provide the same intensity at the sample. If the double undulator is steered as one long device, the resolution increases to more than 20 000, since the focus is in the right position. The simulations show that in the first harmonic above 116 eV the degree of circular polarization is 100%. For the above reasons, in the third and fifth harmonics, and below 116 eV in the first harmonic, the radiation is elliptically polarized. The depolarization caused by the beamline is very small. Moreover, for the 400 l mm^{-1} grating even a significant increase of the degree of circular polarization can be observed. Only below 90 eV is the degree of circular polarization reduced (−5%) by the beamline. The overlapping of the two beams at the sample position is relatively good; the maximum difference in the photon density is about 3%. Analytical and ray-tracing studies showed a deterioration of the overlap of the two beams if demagnifying optics are applied. The spot size at the sample for a 200 μm slit is 900 (H) × 180 (V) μm. The higher-order content of the beamline is, due to the possibility of the high-order suppression mode of the plane mirror and plane grating in collimated light, lower than 1% for the full energy range.

5. Conclusions and outlook

In the design study presented here, we provide quantitative data about a beamline optimized for a high degree of circular polarization and flux. An important feature is the fact that only one single set of optical elements is used to condition and monochromatize the undulator radiation. The advantage of the 'monolithic' optics is a more forgiving behaviour of the beamline with respect to thermal and mechanical misalignment. Finally, it can be used without changes if the two undulators are coupled together to one single device, and achieves the same high performance as other state-of-the-art undulator beamlines elsewhere. As a matter of fact, three beamlines of this type are already being built at BESSY II, underlining the multiple applications of such an undulator-beamline combination, not only for circular polarization experiments. A minimum magnetic gap of 16 mm, available with smaller vacuum chambers in the near future at BESSY II, will extend the range of 100% circular polarization to about 80 eV with corresponding lower limits for the onset of elliptically and linearly polarized light.

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