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Design of a Four-Crystal Monochromator Beamline for Radiometry at BESSY II

Michael Krumrey

Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, D-10587 Berlin, Germany. E-mail: krumrey@ptb.de

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A four-crystal monochromator beamline will be part of the radiometry laboratory that the Physikalisch-Technische Bundesanstalt will install at the new storage ring BESSY II. The most important design criteria for the beamline are the tunability of the photon energy in a wide spectral range from 1.75 to 10 keV, the high spectral purity of the radiation, as well as the good reproducibility of the absolute photon flux.

Keywords: four-crystal monochromator; radiometry; X-ray optics.

1. Introduction

The Physikalisch-Technische Bundesanstalt, the national metrology institute of Germany, has been operating a radiometry laboratory at the electron storage ring BESSY I since 1982. Major tasks performed in this laboratory are the calibration of detectors and radiation sources in the VUV and soft X-ray range as well as the investigation of optical components (Ulm & Wende, 1995). A similar laboratory will also be installed at the third-generation storage ring BESSY II that is currently under construction in Berlin-Adlershof. This laboratory will not only allow the use of undulator and wiggler radiation for radiometry, but will also extend the usable spectral range into the X-ray region because the critical energy of the bending-magnet radiation will be 2.5 keV compared with 0.65 keV at BESSY I. One of the first three beamlines of this laboratory will therefore be a crystal monochromator beamline to cover the spectral range from 1.75 to 10 keV.

The reproducibility of the ratio of the monochromatic photon flux to the stored electron current is a key feature for the design of the beamline because one of the most demanding applications will be the calibration of detectors, based on a cryogenic electrical substitution radiometer (ESR) as primary detector standard (Rabus, Scholze, Thornagel & Ulm, 1996). For this purpose photon energy scans will be performed for different detectors which can require extremely different photon fluxes [*e.g.* 10^{10} photons s^{-1} for the ESR, 10^3 photons s^{-1} for an Si(Li) detector]. These fluxes will be realised by varying the stored electron current, which is already possible at BESSY I, over 12 orders of magnitude.

The other main requirement, the high spectral purity of the radiation, is not only important for detector calibrations but also for reflectometry, where the reflectance of mirrors or multilayers and the transmittance of filters has to be determined with low uncertainties.

2. General beamline design

The main optical components of this beamline will be a four-crystal monochromator and two 1 m-long grazing-incidence mirrors (Fig. 1). Monochromatization and focusing are completely decoupled in order to achieve the required reproducibility of the photon flux in photon energy scans. The first mirror is located at 13.5 m from the source point close to the radiation protection wall. It has a toroidal shape to focus the beam in the horizontal plane and to collimate it in the vertical plane. Usually, the imaging errors of a toroidal mirror are minimized if the source-to-mirror distance is equal to the mirror-to-focus distance. For a focusing and collimating mirror as required here, it could be shown that the imaging errors are minimized if the distance to the horizontal focus is almost twice as long as the distance to the source. This results in a total beamline length of 38 m. The long radius of the mirror (4.3 km) is larger than the ideal radius for a perfectly collimated beam in order to obtain a vertical divergence of 40 µrad (8 arcsec), which is a good match for the acceptance of the four-crystal monochromator. The mirror acceptance is 3.2 mrad (horizontal) and 0.5 mrad (vertical). It is made from monocrystalline silicon and is coated with platinum. Active cooling is not foreseen because only up to 10 W are absorbed due to the small grazing angle of 7.5 mrad (0.43°).

The second mirror, located behind the monochromator, will be flat but can be bent down to a radius of 2.5 km to focus the beam in the vertical plane if a small vertical beam size is required, *e.g.* for detector calibration, instead of a small vertical divergence, *e.g.* for reflectometry. This mirror is made from Zerodur and has two different coating stripes, platinum and magnesium fluoride, which can be selected by horizontal translation of the entire mirror chamber. At the grazing angle of 7.5 mrad the cut-off energies are ~10.5 and 4.5 keV, respectively, making higher-order suppression possible also at lower photon energies. For the mirror chambers and the bender the HASYLAB design has been copied and modified according to our needs (Hahn & Gürtler, 1995).

3. Four-crystal monochromator

For the monochromator the four-crystal configuration first proposed by DuMond (1937) has been adopted for several reasons: (i) fixed exit without crystal translations; (ii) high reproducibility of the photon flux in photon energy scans (only two precisely controllable rotations are required); (iii) high spectral purity (low higher-order content and suppression of the rocking-curve tails); (iv) high spectral resolution, only determined by the crystals. The high spectral resolution of this configuration was the reason for the recent installation of four-crystal monochromators at other synchrotron radiation facilities (Tolentino, Durr, Mazzaro, Udron & Cusatis, 1995; Kraft, Stümpel, Becker & Kuetgens, 1996).

To cover the energy range from 1.75 to 10 keV, two crystal reflections will be used: Si(111) and InSb(111). The latter is required to reach the technologically important Si K-edge at 1.84 keV Thc mechanics of the four-crystal monochromator consist of two main rotary tables, each carrying a wheel on which two crystals of each kind are mounted (Fig. 2). The first and fourth crystals are mounted in the centre of the wheels so that the beam always hits the central position. The second and third crystals are relatively long, 145 mm for Si and 50 mm for InSb, so that the beam travels on the surface when the energy is scanned.

Both rotary tables are mounted onto a single cast-iron block that is supported by slides on a massive synthetic granite block. This slide mechanism is also used to bring either the Si or the InSb crystals into the beam without breaking the vacuum. To scan the energy, one rotary table will rotate clockwise, the other counter-clockwise. Because the second and third crystals are in a dispersive arrangement, the energy resolution is determined only by these two crystals and the transmittance depends on the divergence of the incident radiation. For a perfectly collimated beam the transmittance would be high, but a small angular error between the wheels would drastically affect the transmittance, especially at the high end of the photon energy range (10 keV) where the crystal reflection curve width is only ~6 arcsec. With a divergence of 8 arcsec as defined by the first mirror, the transmittance at 10 keV is reduced by a factor of three compared with a perfectly parallel beam, but the flux reduction caused by an angular error of 1 arcsec between the two rotations is reduced from 12% to 1%. For comparison, in a double-crystal monochromator, where the transmitted photon flux does not depend on the beam divergence, the same angular error between both crystals

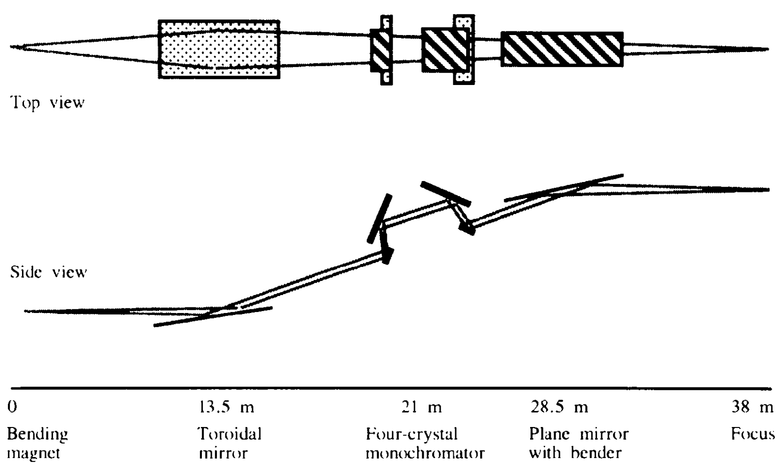

Figure 1
Schematic view of the four-crystal monochromator beamline.

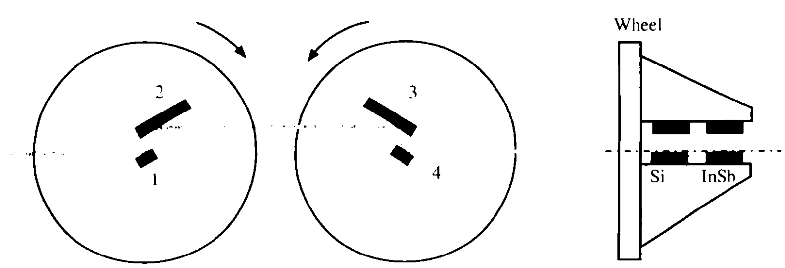

Figure 2
Schematic view of the four-crystal monochromator.

reduces the photon flux by 7%, and here even a translation is required for fixed-exit operation.

The desired reproducibility also requires high thermal stability of the first crystal. The incident radiant power can be controlled by insertion of water-cooled filters. In the worst case (low energy limit of 1.75 keV, only 25 µm Be filter, current 500 mA), 25 W are absorbed by the first crystal. For thermal effects the power density is more important than the total power. Thus, the monochromator position in the converging beam has to be a compromise between small crystal size (important for InSb, which is difficult to obtain defect-free in large sizes) and low power density, corresponding to large crystal sizes. To achieve the required reproducibility the monochromator is positioned at 21 m from the source where the beam is still relatively wide (about 40 mm). A maximum irradiance of 8 W cm^{-2} is obtained, which is several orders of magnitude below the values for insertion-device beamlines at third-generation sources. For the 1.75 keV case described above, a thermally induced distortion of a few arcseconds would be small compared with the broad crystal reflection curve with a width of more than 200 arcsec. At higher photon energies where distortions would have a greater effect because the crystal reflection curves are much narrower, the irradiance is further reduced by the small Bragg angle and the absorption in additional filters. Thus, indirect water cooling has been shown to be sufficient (Krumrey, Herrmann, Müller & Ulm, 1998). The cooling pipes will be fixed in the centre of the first rotary table. As the complete beamline is windowless, the monochromator has to be operated under UHV conditions (low 10^{-8} mbar range).

4. Calculated performance of the beamline

The program *REFLEC* has been used to calculate all relevant properties of the beamline (Schäfers & Krumrey, 1996). The crystal reflectance curves are calculated within this program according to formulae based on the dynamical theory (Batterman & Cole, 1964), and the atomic scattering factors are based on a recent compilation (Henke, Gullikson & Davis, 1993). Fig. 3 shows the photon flux and the radiant power assuming a mirror surface roughness of 0.5 nm. In the whole spectral region the radiant power at an electron current of 100 mA exceeds 5 µW allowing the ESR to be operated with low uncertainties. The corresponding spectral resolving power, which is completely determined by the crystals, is shown in Fig. 4.

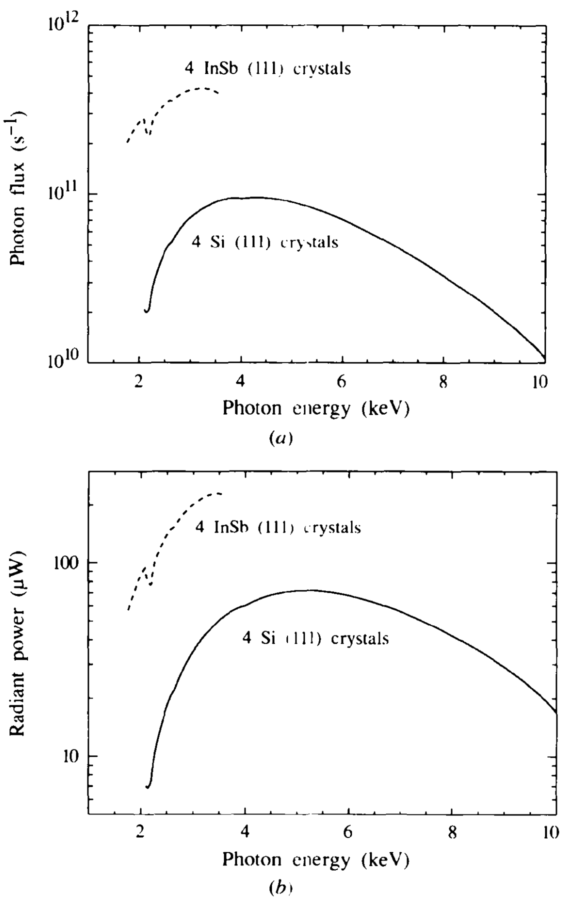

Figure 3
Calculated photon flux (*a*) and radiant power (*b*) of the monochromatic radiation for a stored electron current of 100 mA.

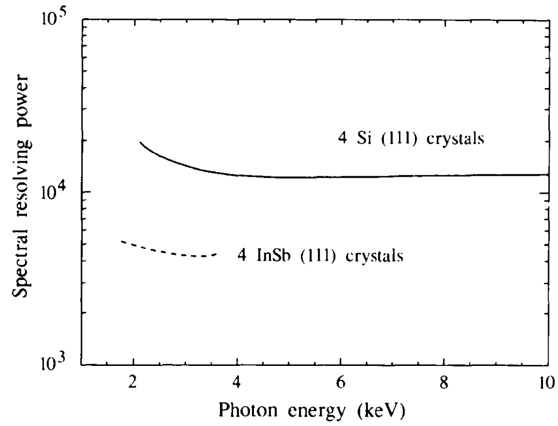

Figure 4
Calculated spectral resolving power.

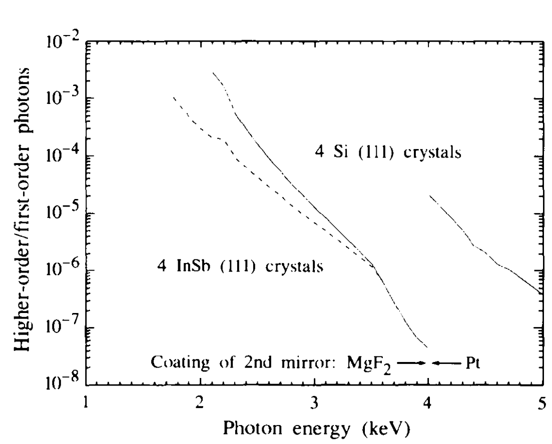

Figure 5
Calculated ratio of the number of photons in higher orders to the number of photons in the first order.

The ratio of the number of photons in all higher orders to the number of photons in the first order is shown in Fig. 5 using the MgF_2 coating of the second mirror below 4 keV and the Pt coating above 4 keV. If scans are performed in limited photon energy ranges, a further suppression can be achieved by detuning the crystals.

By bending the second mirror to a radius of 2.5 km, a circular spot with a diameter of 0.25 mm FWHM can be produced at a distance of 9.5 m behind this mirror. Larger areas can also be illuminated by reducing this distance. The beam divergences are 1.6 mrad in the horizontal and 0.5 mrad in the vertical plane. With a flat second mirror the vertical beam divergence can be reduced by an order of magnitude, *e.g.* for reflectometry.

5. Conclusions

The four-crystal monochromator beamline will be one of the first beamlines that will be ready for the start of operation of BESSY II in 1998. Most components have already been delivered and performance tests have been started. The beamline will allow the extension of absolute radiometry based on an electrical substitution radiometer as the primary detector standard into the X-ray region. Owing to the four-crystal monochromator design achieving a monochromatic beam at a fixed position without crystal translations, very good reproducibility of the photon flux in photon energy scans should be reached, combined with high spectral resolution and a very low higher-order content. A major goal is the calibration of X-ray detectors with relative uncertainties as low as 1%.

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