Performance of the Compton Spectrometer at HARWI/HASYLAB *

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Performance, resolution and spectral throughput both of the sagittally focusing monochromator and of the alternately installed two analysing systems, a Cauchois-type cylindrically bent crystal analyser for Compton-profile measurements, and a spherically bent crystal analyser for $S(q, \omega)$-measurements, of the new Compton spectrometer at the HARWI (harter Röntgen Wiggler) of the DORIS storage ring are presented together with two typical applications.

Key words: X-ray spectrometer; Inelastic X-ray scattering; Focusing X-ray optics; Compton profile; Dynamic structure factor.

1. Introduction

Since the advent of strong sources of synchrotron X-rays, a new generation of inelastic X-ray scattering experiments became feasible [1]. This applies not only to experiments with ultrahigh energy resolution [2] but also both to Compton-profile measurements with a momentum-space resolution of the order of 0.1 a.u. and to experiments performed in order to determine the electronic dynamic structure factor $S(q, \omega)$ with an energy resolution of the order of 1 eV. The Compton spectrometer installed at the HARWI (harter Röntgen Wiggler) of the DORIS storage ring at DESY, Hamburg, is devoted to the latter type of experiments. In what follows the outline of the spectrometer and its main components are described together with two typical examples of its application.

2. Source

The X-ray source for the Compton spectrometer is the 20-pole wiggler of the DORIS storage ring at DESY, Hamburg, whose permanent-magnet structure provides a field of 0.9 Tesla at the electron beam position. When the so-called HASYLAB optics of the storage ring is employed, and the ring is working at 3.7 GeV and 60 mA, the horizontally and vertically integrated spectral flux is $2.0 \cdot 10^{13}$ photons s^{-1} in 0.1% band width for 32 keV photons (Compton-profile measurements) and $1.1 \cdot 10^{14}$ photons s^{-1} in 0.1% band width for 13.7 keV photons ($S(q, \omega)$-measurements). The wiggler emits photons of the desired energy range within a horizontal divergence of 4.2 mrad.

3. Outline of the Compton Spectrometer

An outline of the whole Compton spectrometer is shown in Figure 1. A more detailed description is given elsewhere [3]. The X-ray beam from the HARWI is monochromatised by means of a fixed-exit double-crystal monochromator composed of a water-cooled plane (511) Si crystal (PCM), which has to handle a heat-load of more than 100 Watts, and a cylindrically bent sagittally focusing (511) Si crystal (SFMC). The second crystal consists of ribs monolithically connected with a thin triangular-shaped base, as sketched in Fig. 1, in order to minimise anticlastic bending [4]. 2.8 mrad of the incident beam are horizontally focused onto the position of the scattering sample (SS), where the beam dimension is 8×8 mm^2 with $7.0 \cdot 10^{11}$ photons s^{-1} for Compton-profile measurements (primary energy 32 keV, energy band pass 60 eV) and $6.2 \cdot 10^{11}$ photons s^{-1} for $S(q, \omega)$-measurements (primary energy 13.7 keV, energy band pass 7 eV). Both monochromator crystals exhibit an artificial mosaic spread of 9 arc sec., owing to SiO$_2$ precipitation [5],
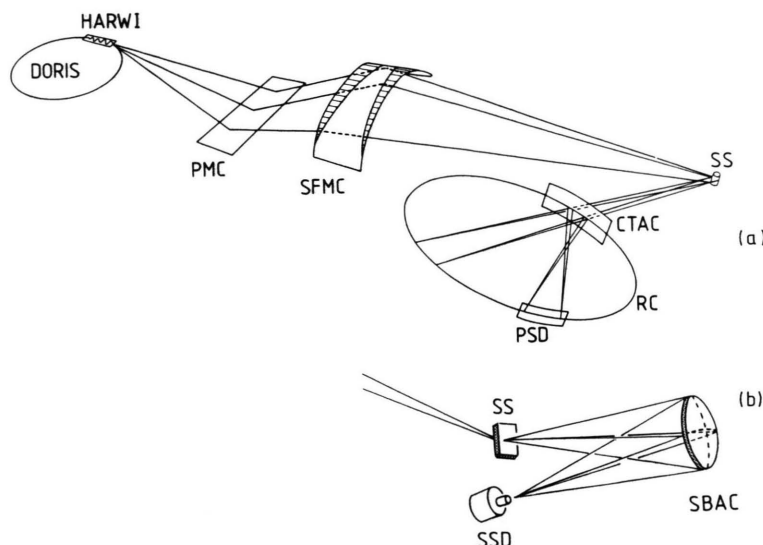
Fig. 1. Outline of the Compton spectrometer.
(a) With the Cauchois-type analyser attached to the monochromator.
(b) The spherically bent crystal analyser.

PCM   Plane monochromator crystal,
SFMC   sagittally focusing monochromator crystal,
SS   scattering sample,
CTAC   Cauchois-type analyser crystal,
RC   Rowland circle,
PSD   position-sensitive detector,
SBAC   spherically bent analyser crystal,
SSD   solid-state detector.

which helps to increase the spectral throughput appreciably.

The scattered radiation can be analysed either in backscattering geometry (Fig. 1 a) by means of a cylindrically bent Cauchois-type (331) Si crystal (CTAC) in combination with a position-sensitive detector (PSD) on the Rowland circle (as proposed for a first time for Compton-profile analysis by Loupias et al. [6]) or in transmission geometry (Fig. 1 b) by means of a spherically bent (12 0 0) Si crystal (SBAC) and a solid-state detector (SD) on the Rowland circle for $S(\boldsymbol{q}, \omega)$-measurements. In this case the analyser is set to a certain energy, so that the energy analysis of the scattered photons is done by changing step by step the energy of the incident photons (inverse geometry as proposed for the first time by Schülke and Nagasawa [7]).

The energy resolution $\Delta E/E$ of the Compton spectrometer working with the Cauchois-type analyser can be calculated to be $1.8 \cdot 10^{-3}$, which corresponds to a momentum-space resolution for Compton-profile measurements of 0.12 a.u. The energy resolution is mainly determined by the 250 μm linear resolution of the PSD, which is a Ge detector with 200 independently working strips, each 200 μm wide and 250 μm apart, where each strip is connected with a complete chain of preamplifier, amplifier and discriminator as described in detail elsewhere [8]. For a 1 mm thick Si sample the count rate within the whole Compton profile is calculated to be $240\,\mathrm{s}^{-1}$. Since the scattering power s of the sample for backscattering geometry is

given by [1]

$$s = (\mathrm{d}\sigma/\mathrm{d}\Omega)_{\mathrm{Th}}\, \varrho \, \sin(\vartheta/2)$$
$$\cdot \{1 - \exp[-\mu(E)\, D/\sin(\vartheta/2)]\}/2\mu(E)\,, \quad (1)$$

where $(\mathrm{d}\sigma/\mathrm{d}\Omega)_{\mathrm{Th}}$ is the Thomson scattering cross-section, ϱ the electron density, $\mu(E)$ the linear absorption coefficient, ϑ the scattering angle, and D the thickness of the sample, the corresponding count rate of any other sample can be calculated easily.

For calculating the energy resolution of the spherically bent crystal analyser we have to take into account its use in combination with the monochromator, since the geometrical parameter of monochromator and analyser are chosen to fulfil the requirements of the so-called dispersion compensation [1, 9]. Dispersion compensation means that the linear wavelength distribution in vertical direction at the sample position (on the Rowland circle of the analyser), produced by the monochromator due to the vertical divergence of the wiggler beam, is simultaneously Bragg-reflected by the spherically bent analyser crystal. Thus the spectral throughput of the spectrometer can be increased, since the band pass of the monochromator may be much larger than the energy resolution of the whole spectrometer. The latter is mainly determined by the vertical height of the source (electron beam) and by the reflection width of the monochromator crystals. We calculate with 13.7 keV primary energy a band pass of 7 eV, an energy resolution due to dispersion compen-
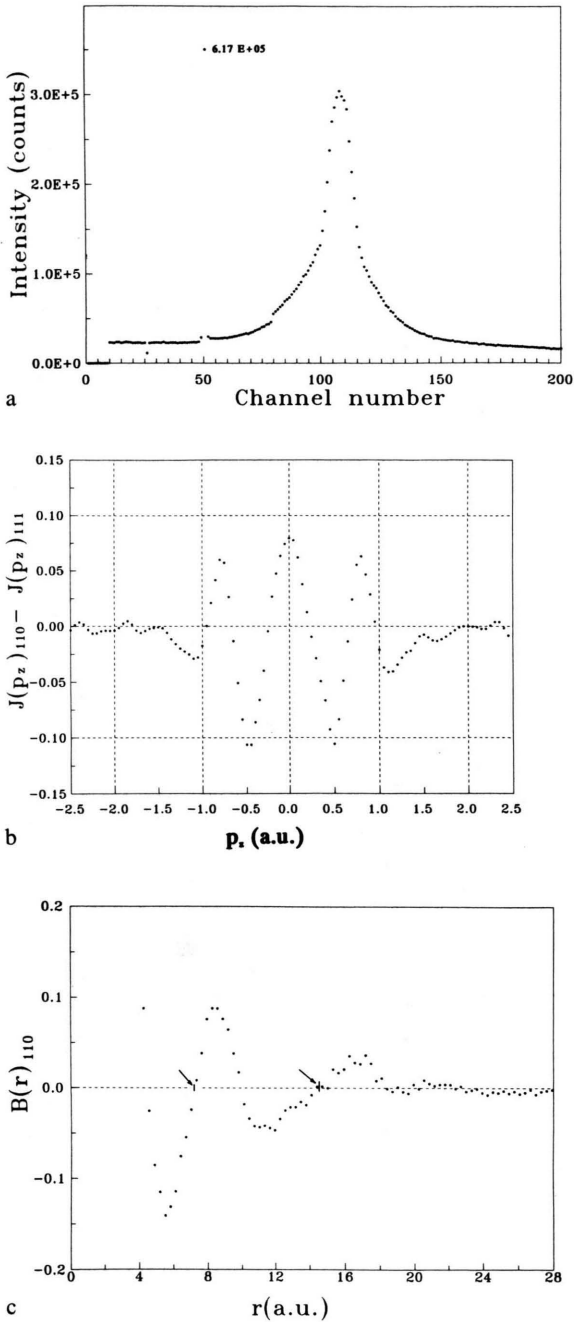
a

b

c

Fig. 2. (a) Experimental data of a [100] Si Compton profile. The data are corrected for the individual strip efficiency of the PSD, (b) [110]–[111] difference Si Compton profile. (c) Fourier transformed [110] Compton profile. The arrows mark the lattice translations in [110] direction.
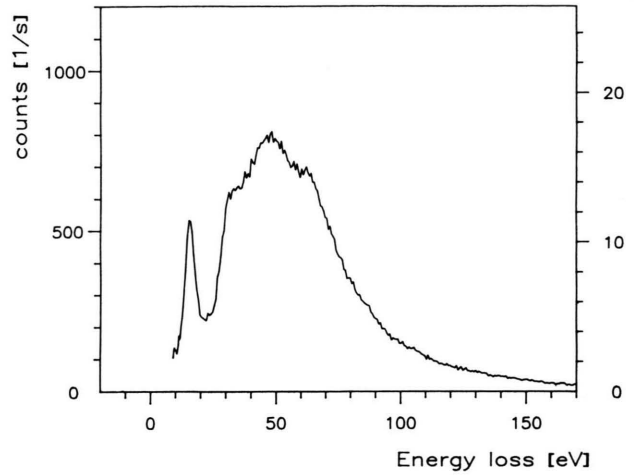

Fig. 3. Raw experimental data (after subtraction of the quasi-elastically scattered line) of an $S(q, \omega)$-measurement on highly oriented pyrolytic graphite (HOPG) with $q \parallel c$-axis; $q = 1.45$ a.u. The left-hand ordinate scale refers to this experiment (wiggler source, sagitally focusing monochromator optics). The right-hand scale refers to a previous experimental setup with a bending-magnet source and nonfocusing monochromator optics.

sation of 1.4 eV and an average count rate of 290 s^{-1} within one resolution element for a 2 mm thick graphite sample and a scattering angle of 25°. Again the count rate for any other sample in transmission geometry can be calculated by means of the following expression for the scattering power s [1]:

$$s = (d\sigma/d\Omega)_{\text{Th}} \varrho D \exp[-\mu(E) D/\cos(\vartheta/2)] . \quad (2)$$

4. Examples of Application

The first example of an application refers to Compton-profile measurements using the Cauchois-type analyser.

Figure 2a shows the raw data of a [100] Si Compton profile (sample thickness 1 mm), where the data are only corrected channelwise for the variation of the individual strip efficiency of the PSD as described in detail in [8]. We found in the whole Compton profile a count rate of 200 counts s^{-1} with the storage ring working at 3.7 GeV and 60 mA. This count rate is not far from that we have calculated in Section 3. The total energy resolution of the experiment can be estimated by the width of the quasielastically scattered line, which essentially consists only of one point,

marked within Fig. 1 a by its number of counts, so that one can deduce an experimental $\Delta E/E = 1.95 \cdot 10^{-3}$, which corresponds to a momentum-space resolution of 0.135 a.u., not far from the one predicted in Section 3.

After having performed the standard correction and evaluation procedures [10], namely energy calibration of the detector channels, correction with respect to energy-dependent absorption and scattering cross-section, correction with respect to energy-dependent reflectivity of the analyser, transformation of the energy scale into a p_z-scale, subtraction both of the quasielastically scattered line and of the background, normalization, and multiple-scattering correction by using data of scattering samples of different thickness, we obtained Compton profiles of Si for the [100], [110] and [111] direction of the scattering vector. Figure 2 b presents the profile difference [110]–[111], and Fig. 2 c the Fourier-transformed [110] profiles. Note the high degree of symmetry with respect to $p_z = 0$ in the directional differences of the Compton profiles, and the exact positions of the zero-passages of the Fourier-transformed profile (indicated by arrows) at the Si lattice translations in [110] direction [11], namely $R = 7.26$ a.u. and $R = 14.52$ a.u.

The second example of application refers to $S(\boldsymbol{q}, \omega)$-measurements using the spherically bent crystal analyser. Figure 3 presents the raw data (after subtraction of the quasielastically scattered line) of an $S(\boldsymbol{q}, \omega)$-measurement on a 2 mm thick sample of highly oriented pyrolytic graphite (HOPG) with $\boldsymbol{q} \parallel c$-axis, $q = 1.45$ a.u. The count rate obtained in this experiment can be read from the left-hand ordinate scale, and is in good agreement with the predictions of Sect. 3, the right-hand ordinate scale refers to a previous setup, where only the emission of a bending magnet and no focusing monochromator optics have been utilized. The energy resolution, which can be read from the width of the quasielastically scattered line, is near the predicted value of 1.4 eV, provided the vertical beam position of the HARWI is stable within 20% of the vertical electron-beam height during the whole measurement. $S(\boldsymbol{q}, \omega)$-measurements of the kind shown in Fig. 3 have been used to obtain information about electronic excitations in graphite and alkali metal intercalation compounds of graphite [12, 13].

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