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Carbon K-edge polarimetry with Cr/Sc multilayers

A Gaupp[1], F Schäfers[1], M MacDonald[2], S Uschakow[1], NN Salashchenko[3] and PK Gaykovich[3]

[1] Helmholtz-Zentrum Berlin, Institute for Nanometer Optics and Technology, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany
[2] Canadian Light Source Inc. Saskatoon, Canada
[3] Institute f.Physics of Microstructures IPM-RAS, Nizhny Novgorod, Russia

E-mail: gaupp@bessy.de

Abstract. We investigate the polarization changes simultaneously occurring with intensity changes due to carbon contamination of optical components at two plane grating beam lines PGM-1 and PGM-2 at BESSY II. The two beam lines are very similar to each other and connect to the same APPLE II type undulator UE56/2. The spectra measured with initial horizontal and vertical polarization differ for the two beam lines. For polarimetry measurements the BESSY 8-axis polarimeter is equipped with a Cr/Sc multilayer in transmission as phase retarder and a Cr/Sc reflecting multilayer operating near the Brewster angle as analyzer. The polarimetry results also differ for the two beam lines. Only at PGM-2 we observe no decline of the degree of polarization within experimental errors i.e. the degree of polarization at PGM-2 is always found P > 0.96. We find big changes of the polarization which rapidly vary across the carbon edge. A tentative interpretation predicts the orientation of the dipoles in the contaminating carbon layers. Circular polarization is largely recovered (80% and higher) at PGM-2 thru out the carbon edge by setting the undulator shift to approximately compensate the polarizing properties of the beam line.

Synchrotron radiation investigations in the spectral range around the carbon K-edge (270 eV - 300 eV) are scarce (see e.g. [1]) because of the strong and rapidly varying intensity reduction due to the omnipresent and practically unavoidable carbon contamination of beam line optical components. In this contribution we concentrate on polarization changes occurring simultaneously with intensity changes.

During two measuring campaigns in September 2011 and April 2012 data have been collected at two almost identical beam lines, PGM-1 and PGM-2 [2] fed by the same APPLE II type [3] undulator UE56/2 at the 1.7 GeV electron storage ring BESSY II. The undulator can not generate any inclined linear polarisation, i.e. there is no S_2 from the source. An aperture located 13 m downstream of the source is set to $0.15\,mrad \times 0.15\,mrad$ optimized for flux (PGM-1) and to $0.08\,mrad \times 0.08\,mrad$ matched to the high brilliant central radiation cone (PGM-2). The first, horizontally deflecting toroidal mirror M_1 vertically collimates and at PGM-2 horizontally focuses the radiation onto the sample. The plane monochromator mirror M_2 and the plane grating deflect vertically. A horizontally deflecting cylindrical mirror M_3 in the dispersive section vertically focuses onto the exit slit. The horizontally deflecting refocusing mirror M_4 is a toroid at PGM-1 leading to a horizontal focus size of 90 μm, and a conus at PGM-2 leading to a horizontal focus size of 900 μm. At PGM-1 the stronger focusing and the larger acceptance of the front aperture lead to a signal 3.5 times stronger than at PGM-2. The deflecting angle of all

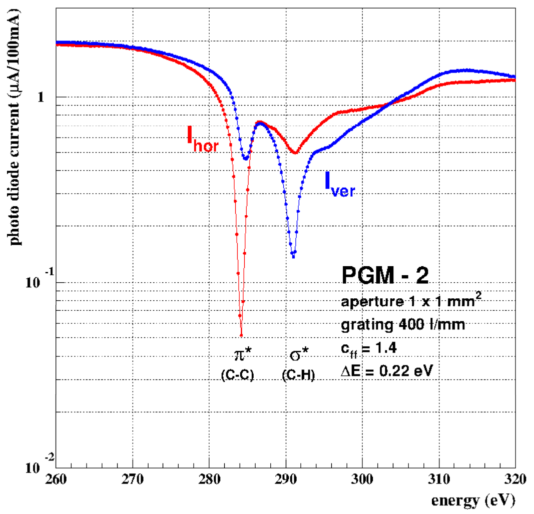

Figure 1. Intensity of beam line PGM-2 normalised to ring current.

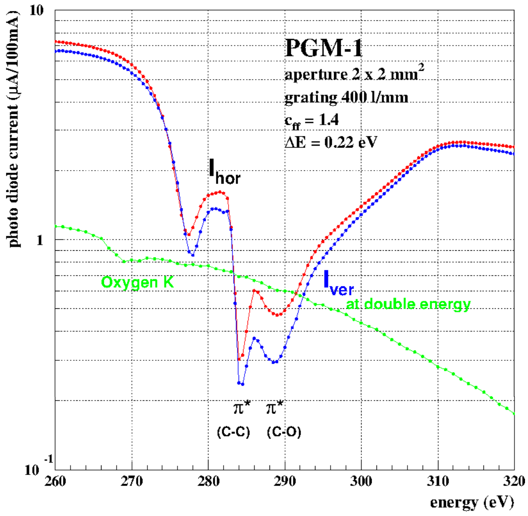

Figure 2. Intensity of beam line PGM-1 normalised to ring current.

mirrors except the monochromator mirror is 174 degree. All mirrors are platinum coated and the gratings are gold coated. We use the 400 l/mm gratings, a fix-focusing constant of $c_{ff} = 1.4$ [4], and an energy resolution of ΔE = 0.22 eV. The monochromators are in service for more than 10 years. At PGM-2 the refocusing mirror has been replaced about one year prior to data taking. All data are normalized to ring current but not corrected for detection efficiency.

The transmission spectra taken with horizontally and vertically linearly polarized radiation I_{hor} and I_{ver} differ significantly for the two beam lines. The minima at 284 eV and 291 eV observed at PGM-2, fig. 1, are tentatively assigned to unoccupied π^* and σ^* orbitals as in C-C and C-H bonds, respectively [5]. There is a strong dependence on polarization as if a horizontally deflecting mirror is covered with vertically oriented hydrogenated graphitic carbon. Assuming similar oscillator strengths there seems to be three times as many unoccupied horizontally oriented π^* orbitals than unoccupied vertically oriented σ^* orbitals. There is no indication of oxygen. The intensity of the dip at 284 eV represents a reduction of a factor of about 35.

The minima at 284 eV and 289 eV observed at PGM-1, fig. 2, are tentatively assigned to unoccupied π^* orbitals as in C-C bonds and chemically shifted as in C-O bonds, respectively [5]. Both π^* features show little dependence on polarisation i.e. the asymmetry $\frac{I_{ver}-I_{hor}}{I_{ver}+I_{hor}}$ is at most 0.24. There is a 10% dip at the oxygen edge around 530 eV. The feature at 277 eV is presently not understood. A possible scenario is a contamination by mostly amorphous carbon with traces of oxygen and/or contamination of several orthogonally oriented mirrors. - Further modelling of the spectra has not been attempted.

The principle of the polarimeter [6] is based on the independent rotation of two optical elements around the light axis by the angle α and β, respectively, while the transmitted intensity is recorded by a polarization insensitive detector. The first optical element is to shift the phase by Δ_1 between two orthogonal polarisation directions and is realized by a transmission multilayer with the glancing angle of incidence Θ_P. The second optical element is to analyze linearly polarized radiation and is realized by a reflection multilayer with the Bragg angle near the Brewster angle with the glancing angle of incidence Θ_A. The optical components are Cr/Sc multilayers [7] with several hundred layers and are used off-resonance of both constituents [8]. The detector is a window-less GaAs Schottky photo diode [9]. Manufacturing tolerances and

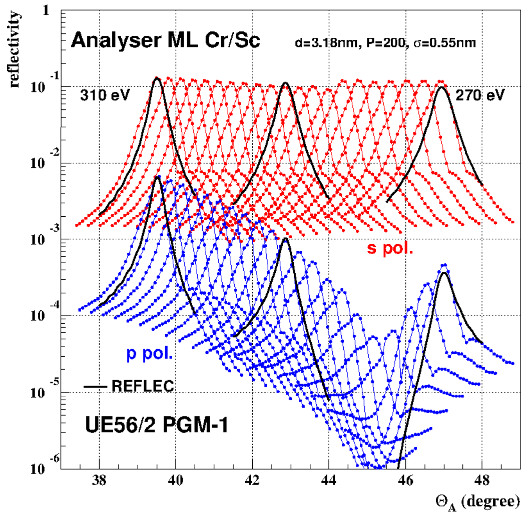

Figure 3. Reflectivity of Cr/Sc multilayer analyser. Model calculations are included for three energies.

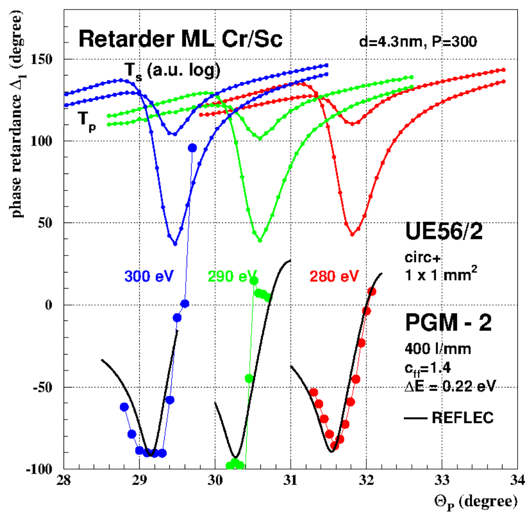

Figure 4. Phase retardation of Cr/Sc multilayer retarder. Simulation using REFLEC resembles the phase shift.

systematic alignment errors cause angular changes of 0.2 mrad at most. This set-up allows distinguish unpolarized radiation from circularly polarized radiation. A fit of the intensity at the detector versus α and β simultaneously determines the normalized Stokes parameters S_1, S_2, and S_3 [10] and the parameters describing the polarization effects of the optical elements [6]. Redundant measuring i.e. α and β between 0 and 2π reduces the influence of systematic errors.

The reflectivity in s- and p-geometry of the analyzer multilayer together with model calculations are shown in fig. 3. The s-reflectivity is constant thru out the region, i.e. there is no 2^{nd} order radiation which introduces features at half the Cr L-edge energy of 574eV. The analyzing power $(R_s - R_p)/(R_s + R_p)$ varies between 0.998 at 278 eV and 0.82 at 310 eV. The phase shift Δ_1 shown in fig. 4 together with transmission spectra and model calculations is large and up to 90^o thru out the carbon K-edge region. Both spectra fig. 3 and 4 show no indication of carbon within the multilayers. The modeling using the computer code REFLEC [11] is adequate. The experimental structures on both sides of the Bragg peaks are attributed to different d-spacings within the ML stack. The shape of the measured phase shift fig. 4 differs from the model calculation in particular at and above the carbon edge which presently is not understood. In the following we present polarimetry data from measurements with linear polarisation and with circular polarisation which are simultaneously fit. For the measurements at PGM-1 the undulator shift is opposite to the shift at PGM-2 measurements. Therefore we reverse the sign of S_2 and S_3 in fig. 6 to match the presentation in fig. 5.

At PGM-2, fig. 5, S_1 closely follows the asymmetry of the Io measurements of fig. 1. S_2 caused by the phase shift within the beam line is proportional to the derivative of S_1 and thus changes sign at the extrema of S_1. S_3 is strongly reduced at the absorption edges. At PGM-1, fig. 6, a strong reduction of the degree of polarization P is observed at the carbon edge in contrast to PGM-2, fig. 5. We speculatively relate this finding to the different acceptances of the beam lines in combination with inhomogeneous contamination of the optical surfaces.

Further polarimetry data (not shown) show the horizontal and vertical linear polarization to be conserved in the beam line.

When the degree of polarisation is preserved in the beam line as in PGM-2 the circular

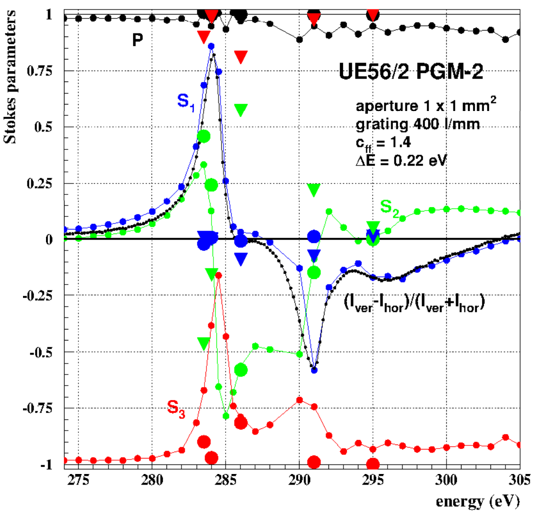

Figure 5. Polarimetry data of PGM-2 measured with negative shift of the undulator. Large marks indicate polarisation data with the undulator shift set to compensate the polarizing effects of the beam line.

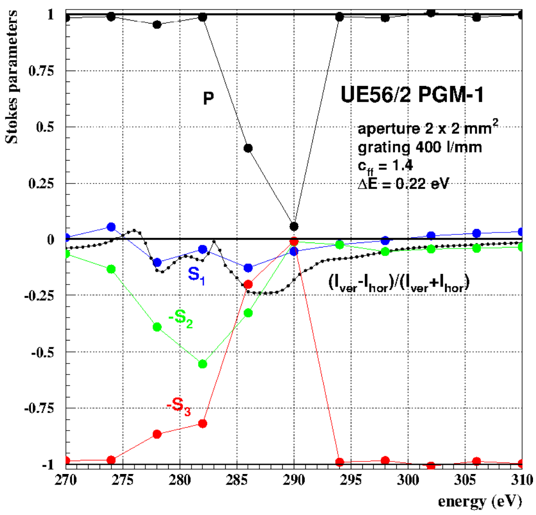

Figure 6. Polarimetry data of PGM-1 measured with positive shift of the undulator. There is a strong decline of the degree of polarisation at the carbon edge. This data set is less complete than the one of PGM-2.

polarisation is mostly recovered by tuning the undulator. This is indicated by the large dots for $S_3 < 0$ and by triangles for $S_3 > 0$ in fig. 5 [12]. Note the S_2 component is not modified.

Summarizing we measured polarization effects due to carbon contamination of beam line components. We investigated two very similar beam lines, PGM-1 and PGM-2 which however differ with respect to the intensity spectra and with respect to polarization. Only at PGM-2 the degree of polarization is preserved above $P \geq 0.96$ and the circular polarization is mostly recovered by tuning the undulator to compensate for polarization effects of the beam line. To identify the reason of the decrease of the degree of polarization around 284 eV only at PGM-1 requires further investigations.

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