Technical developments at HASYLAB

3. Experimental options of DORIS III Beamlines
The beamline W3 for VUV – Spectroscopy

P. Gürtler

On a first glance one could think that VUV spectroscopy on a large high energy storage ring like DORIS mainly used for X-ray studies doesn’t make sense, because most of the radiation is useless and only heats up the optical elements. But a closer view to the properties of such a machine shows that it has even advantages compared to small storage rings built especially for VUV spectroscopy. First of all a large high energy ring means large bunch separation and short bunches so that time resolved measurements can be done with superior performance. And if a proper magnetic configuration with a critical wavelength in the VUV range is used to produce the radiation, the divergence of the beam can be very small because of the high $\gamma$-value of the ring. In such a configuration, the first optical element can be far away from the source and can strongly demagnify the beam, so that a good resolution with full flux can be achieved. These considerations led to the construction of the beamline W3 in the years 1986 – 1987. In the following years, the beamline and especially the experimental setups were continuously upgraded so that the performance was always and is still state of the art in VUV spectroscopy. This is documented by the large number (over 100) of scientific publications produced by many groups at these experiments.

The Light Source

To produce the light for the beamline W3, a periodic permanent magnetic array with long periods and weak field is installed in a 50 cm long straight section between two DORIS bending magnets. The field is so weak, that it is comparable with the fringe field of the bending magnets. Therefore the light is produced by a complicated electron trajectory induced by the periodically varying magnetic field of the permanent magnet array and the varying fringe field of the bending magnets. Measurements have shown, that the divergence of the beam at 10 eV is only 0.9 mrad vertical by 1.5 mrad horizontal FWHM. That corresponds to a critical energy of 500 eV compared to 16.5 keV in a normal DORIS bending magnet. Because of this low critical energy in combination with the high electron energy, the vertical divergence is much smaller than at other Synchrotron Radiation sources (e.g. BESSYI: 5 mrad, DORIS bending magnet: 3.5 mrad). Figure 1 shows the flux into 1.5 x 0.9 mrad at the W3 beamline compared to other sources (DORIS bending magnet, BESSY I bending magnet and the 4 m long BESSY II undulator U-125). One can see from the figure, that about a factor of 10 more flux is available at the W3 beamline compared to a normal DORIS bending magnet and even more compared to a BESSY I bending magnet. Of course, the undulator beamline at BESSY II has much more flux available. This is mainly due to the fact, that it is a factor of 8 longer.

![Flux into 1.5 x 0.9 mrad](image)

Figure 1: Photon flux into the acceptance of the W3 beamline compared to other sources
Layout of the Beamline

To use the beamline in an efficient way, two experimental stations are attached to it and can alternatively use the beam. The W3.1 HIGITI station is a modified wadsworth mount optimized for high throughput using the source as entrance slit. Station W3.2, the HONORMI is a high resolution setup with a 3 m normal incidence monochromator reaching a resolving power of 50000. Both setups have beneath all advantages an inherently small acceptance and are therefore well suited for this beamline.

The first optical element in the beamline, a plane mirror, is placed 19 m apart from the source. This mirror is used to deflect the beam upwards by 26 degree to the HONORMI experiment. It can be moved out of the beam so that the light is brought to the second experiment at this beamline, the HIGITI. They will be briefly described.

**HIGITI (W3.1)**

This setup uses a monochromator of the modified Wadsworth type, where the grating is the only focussing element. The normal disadvantage of such a monochromator – its small acceptance – does not play a role here because the beam is so well collimated and therefore fully accepted. A plane mirror in front of the monochromator is used to get rid of the X-rays, so that the setup does not need any shielding. The source spot serves as an entrance slit and is focussed by the grating onto the exit slit with a demagnification of 1:40. The reflectance angle is close to normal incidence (6.5°) and is chosen in such a way that the image is stigmatic at a wavelength of 150 nm. That means the spot size at the exit slit is only 23 x 80 microns and a minimum resolution of 0.03 nm can be achieved without loss of intensity. A refocusing optic consisting of a plane and an ellipso-toroidal mirror is used behind the exit slit to focus the beam into the center of the experimental chamber. A minimum focus of 100 x 100 microns can be reached. Such a small focus is very important for the detection of secondary processes. The photon flux measured behind the exit slit amounts to $6 \times 10^{12}$ photons/sec for a resolution of 1 nm and 100 mA current.

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**Figure 2: The setup for luminescence spectroscopy at HIGITI**
The Luminescence Setup at the HIGITI
The experimental chamber at the HIGITI station is optimized for luminescence measurements from the VUV to the IR spectral range after VUV excitation. For this purpose, two secondary monochromators are attached to the chamber. Fig. 2 shows the whole setup.

The VUV-luminescence monochromator is a Seya-mount using the illuminated spot on the sample as entrance slit and covers a spectral range from 110 to 500 nm. The luminescence light is detected with a channelplate detector. With a MgF2 lens, the visible and infrared part of the luminescence is focused onto an ordered optical fiber which led the light to a commercial SPEX monochromator. The two exit slits of this device are equipped with a CCD-camera (PI-instruments) and a cooled infrared-sensitive photomultiplier. With the CCD-camera, the luminescence from 250 to 1100 nm can be detected in one shot. and with the photomultiplier, time dependent measurements can be carried out. The primary and Seya secondary monochromator are controlled by a MicroVAX computer. By scanning the primary monochromator and taking emission spectra with the CCD-camera for each excitation wavelength an array of all emission/excitation spectra is derived. This is realized by use of a Macintosh computer which controls the CCD-camera and the CAMAC-crate via IEEE 488 and a combination of a commercial CCD-Software with a LabVIEW-program communicating via Appletalk-scripts.

In addition, the experiment is equipped with an Argon ion laser as a second light source and with a time of flight electron spectrometer to do photoemission and zero kinetic energy electron (ZEKE) spectroscopy. The whole system can be baked, so that ultrahigh vacuum in the 10^{-10} mbar range is reached. The samples are attached to a continuous flow He-cryostat and can be cooled down to 4 K.

Several groups with different scientific programs are using the setup. First of all there is a community studying luminescence properties of rare earth doped crystals (Meijerink et al, Utrecht, Schwarz et al, Greifswald and Tröster, Paderborn). This is an interesting basic research field but has also applied aspects on the development of new materials for luminescent lamps and radiation detection. Another community studies photochemical reactions of molecules and clusters in matrices (Gürtler and Laasch et al. Haseylab, Krätschmer et al. Heidelberg and McCaffrey et al. Dublin). Also high precision transmission measurements on optical filters were carried out (Stephan et al, Garching). Some publications from these groups are listed:


HONORMI (W3.2)
The heart of the HONORMI setup is a 3m normal incidence monochromator in UHV technique from Mc. Pherson Ltd. It covers the energy range from 5 to 40 eV and with the smallest slit of 10 microns, a resolution of 0.03 Å is achieved. Larger slits give less resolution but higher intensity. An ellipsoidal mirror in front of the monochromator focuses the beam onto the entrance slit. This mirror is demagnifying the source by a factor of 11 so that the spot size at the entrance slit is 80 x 300 microns. Therefore part of the intensity is blocked at the entrance slit below a slit width of 80 microns, and the intensity varies quadratically with resolution.

Behind the monochromator a combination of a plane and an ellipsoidal mirror refocuses the beam into the center of the experimental chamber. This 1:1 imaging is slightly astigmatic so that the final focus is symmetric with a diameter of about 200 microns at a distance 600 mm apart from the mirror.
The **A SPHERE** Setup at the HONORMI

The instrument used at the HONORMI experimental station is the *A SPHERE* (*Angular* Spectrometer for *Photoelectrons with High Energy Resolution*) setup which is a central instrument for the community requiring high resolution angle resolved photoemission spectroscopy in the VUV. It was built by the university of Kiel and is now used by different groups including those of joint BMBF-projects No. 05 and 22.

The arrangement is shown in fig. 3. It consists of a large UHV-chamber with a He-cryostat (T ≥ 20 K) as sample holder, which can be aligned by a manipulator. The central part is a spherical electron energy analyzer, which is mounted on a two-axes goniometer and can be precisely rotated around the sample with computer controlled stepping motors. Large pumps are able to maintain a vacuum in the 10⁻¹⁰ mbar range after bakeout. Attached to this chamber is a configuration of chambers for sample preparation and diagnostics. Also a docking port is available, so that samples can be prepared elsewhere and then brought to the station under UHV-conditions. Under computer control energy distribution curves (*EDC*), constant final state (*CFS*), and constant initial state spectra (*CIS*) and photoelectron angular distributions at fixed kinetic energy (*PAD*) can be measured. The resolution in energy is better than 10 meV and in angle better than 0.5°.

![Figure 3: The A SPHERE setup at the HONORMI experimental station](image)

The physics program covers measurements of valence band structure of metals, semiconductors, superconductors and layered materials, phase transitions in the electronic structure, and resonant photoemission of core levels. Some related publications are listed below:


Improvements of Absorption Spectroscopy Beamlines
A1, E4, X1.1 at HASYLAB


Physikalisches Institut, Am Hubland, 97074 Würzburg

In 1998, the major updates of HASYLAB absorption beamlines A1, E4 and X1.1 were mostly completed. A1 is now fully operative for high-resolution and magnetic applications reaching down to the sulfur K edge. E4 is equipped with a new experimental stage including ionization and vacuum chambers. New computer hardware and software is operating. At X1.1, the reconstruction of the HASYLAB 2 building and chemistry laboratory was finished. Several improvements concerning the monochromator were installed.

In this updating process, care was taken to unify as much as possible the equipment used at the three beamlines and design it following a modular principle. This facilitates the (typical) user operation at more than one of these beamlines and largely helps servicing them. The vacuum systems in the experimental hutches of E4 and A1 are fully compatible. New, identical ionization chambers are now operating at E4 and A1 (please see the separate report herein). Software and data format of A1 and E4 are identical. Adopting of X1.1 with respect to ionization chambers and software will be performed in early 1999. A photon beam position monitor for white and monochromatic light is in fabrication and will be installed at all three beamlines. Especially for XAFS applications, stabilization of the monochromatic x-ray intensity is essential during energy scans. The present analog electronic unit MOSTAB serving this purpose has some weaknesses so that a new, more flexible, digital unit called IMOSTAB was developed (please see the separate report herein).

In the following, the developments of absorption beamlines A1, E4 and X1 are discussed in more detail.

Beamline A1 – Absorption Spectroscopy between 2.4 keV and 28 keV

After completing the planned improvements during 1998, the A1 is now an versatile XAFS beamline, which allows standard XAFS experiments as well as the class of experiments requiring a high energy resolution. Within less than half an hour, the beamline can be switched between high-resolution four-crystal operation and higher-intensity two-crystal monochromatisation. Besides focusing on XAFS, near edge spectroscopy in combination with high resolution and X-ray Magnetic Circular Dichroism is the main purpose of the beamline. Using different monochromator crystals, its extended energy range of 2.4 keV to 28 keV covers most of all XAFS applications, so that A1 offers additional capacity for the XAFS community.

The actual energy range available on A1 strongly depends on the monochromator crystals. Because of the monochromator vacuum and the following adjustments, a change of crystals takes about 36 hours. In consequence the scheduled beamtime is divided in different blocks, in which all users can measure with the same crystals. Until now only Si (111) crystals with an energy range of 2.4 keV to 18 keV can be used. One channel-cut crystal is mounted on each of the two goniometers in the monochromator; both are counter rotating against each other during change of energy. A Si (311) pair is already cut and its commissioning is planned in early 1999. Its expected energy range is 4 keV to 28 keV. In contrast to the monochromator crystal change, switching between four- and two-crystal monochromatisation is fast and can be handled by the user himself in about half an hour.

A key improvement of A1 in 1998 is the extended energy range down to the Sulfur K edge. In order to reach Sulfur, the beamline is now designed to measure under HV-conditions (Fig. 1). To further reduce absorption, the Be-window was replaced by a 20 μm thick C-foil, separating the UHV of the beamline from the HV of the monochromator. To be sure that no oxidation affects the precision of the mechanics, the pressure inside the monochromator is specified to 10⁻⁷ mbar. In combination with a totally oil-free pumping system one can avoid Si–C reactions on the surface of the reflecting crystals, which enlarges the life time of the crystals. Because of the easier handling the vacua of sample and reference chamber are separated from the monochromator vacuum by the first ionization chamber and can be choosen between normal pressure and 10⁻⁷ mbar.
This allows the use of cryotechnique without a further window. Especially in the low energy regime up to 7 keV the four crystal mode is essential. Because of the emission characteristic of the DORIS bending magnets the third harmonic is in that case more intense than the first. In addition the small absorption thickness results in a critical sample preparation. In contrast to E4, where higher harmonics rejection can be obtained by the mirrors, using the strong energy dependence of the critical angle, at A1 it can only be achieved by detuning the crystals. For example, in the two–crystal mode at 7 keV and a monochromator transmission of about 50%, the ratio of first to third harmonic is $10^{-3}$. In the four–crystal mode, however, an improvement up to $10^{-6}$ can be achieved. The lower energy regime opens an interesting field of high resolution near edge spectroscopy because of smaller core hole broadening.

For planning an absorption experiment on diluted systems, however, the important quantity is the signal–to–noise ratio and the long time stability of the complete experiment. Because the energy and divergency distribution in the beam is not directly correlated to the incoming beam in a four–crystal monochromator, both aspects can be probably improved in the four crystal mode. In practice, this can only be achieved in a mechanically well–stable system. For this purpose we have performed the following steps:

- **Reducing the vibrations between the monochromator crystals.** For getting the optimal flux and energy stability, the angle mismatch between each crystal has to be adjusted to at least 1/10 of the natural rocking curve, which is in the case of a Si (111) $2^\circ 10^{-4}$ deg. This can only be achieved by decoupling the stainless steel slab, which supports the monochromator interior, from the outer monochromator vacuum tank and by making the channel–cuts as stiff as possible. In the case of A1 the 400 kg inner box, on which the goniometers are mounted, is supported by three bearing applications. The moving parts are reduced to the vertical movement, the goniometer and one cradle per channel–cut. The mechanical resonance frequence of the channel–cut itself is at 400 Hz. The mismatch of each channel–cut is adjusted by a piezo system, detuning the second crystal.

- **Thermal stability of the crystals.** With respect to the high angle–accuracy and the increasing DORIS ring current, the solution of the cooling problem is essentially. A very stiff crystal support, combined with a heat exchanger and a special design of the channel–cuts results in a temperature change of the first crystal of 1°C during a run with 150 mA to 60 mA. Typically, one can start with measurements in a four–crystal mode about four minutes after filling. A further adjustment of the piezo system is not necessary, so that the energy stability is not lost. Using a cooling–machine (Lauda), the temperature of both channel–cuts can be chosen between -15°C and +25°C.

- **Long–time stability.** Especially in the case of samples which are not homogeneous like powder samples, the quality of the spectra is extremely dependent on a stable, non–moving beam on the sample.
Figure 2: Absorption spectra around the Sulfur K edge.

Because of the low angular acceptance of the four–crystal monochromator in combination with a well defining slit system, beam instabilities result in an intensity fluctuation in contrast to usual beam movements. To get a fixed optical axis, the exit slit system, the ionization chambers, the fluorescence–detectors and the sample chambers are anchored to a 3000x1000x200 mm$^3$ 2000 kg granite plate, which is adjustable on an accuracy of 50 $\mu$m in each direction. The number of degrees of freedom is 5, so that the optical axis of the whole experiment can easily be adjusted using scanning techniques to better than 50 $\mu$m to the beam direction. The huge mass of the plate in combination to the large dimensions makes experiments easy in handling (even with heavy equipment) and results in a system insensitive to vibrations and mechanically stable on a time scale of weeks.

• Suppression of background. A reduction of the background scattering improves directly the signal–
to–noise ratio. The technical realisation at A1 was done using three different approaches. Firstly, the scattered white beam light of the first monochromator crystal was strongly reduced by capsulating the first channel–cut crystal in a tungsten box with an emission window (stray light slit) of only 30x3 mm$^2$, moving with the energy. The 5 mm thick vacuum stainless steel tank is a second radiation shield. Furthermore, the scattering of the monochromatic beam on gas was avoided by using vacuum between the ionization chambers. Another improvement was achieved by the high mechanical accuracy of the lifting table and the slit systems, which allows an adjustment by scans of the exit slit system down to 50 $\mu$m. This reduces the diffuse scattering from the monochromator itself.

For scanning the energy, the quality of the spectrum is directly related to the accuracy of the movements of both goniometers. Because of the wide energy range of the beamline it is necessary to adjust absolutely each goniometer to $1 \times 10^{-4}$ degree in a range of about 90 degrees. This is only possible when a feedback system is used with an incremental system for measuring the angular position is used. In the actual mode
the stepper motor is moving without any backlash to the nominal position, then the position is measured 40-
100 times for getting an accurate value and an estimation of the error by evaluating the mean–square. The
statistical errors are measured by this means within 5x10^{-6} deg. Typically, depending on the step size of the
spectrum, three to six iterations are necessary to get a precision of 1x10^{-4} deg. The whole procedure takes
between 10 s and 20 s, so that this is determing the time of one spectrum. Alternatively to this relatively slow
mode, for energy scans over several hundred eV, a faster scanning mode can be used: The movement of the
piezoelectric crystal of the second channel–cut crystal is stabilized to constant photon intensity in the first
ionization chamber (feedback by (I)MOSTAB). The experience of the last six weeks shows that short–time
fluctuations of the beam position typically do not represent problems. Long–time fluctuation of the beam,
which can amount to up to 1x10^{-5} deg (max. 0.7 mm movement at a distance of 40 m during a synchrotron
run) result in a reduced transmission of the monochromator. For the Si(111) a reduction of about 10% of
the maximum peak value was observed. In consequence highly indexed reflections like a Si(511) can not be
used because of the small width of the rocking curve.

Fig. 2 shows an example for Sulfur K edge spectra of two different samples measured at beamline A1 in
the four–crystal mode. As the most pronounced peaks in both spectra, the two different valance states of
Sulfur (+6 and -2) are easily recognized. The spectra exhibit a lot more fine structure. As another result,

La_{0.7}Ca_{0.3}MnO_3 – Mn K–XMCD

![Graph](image)

Figure 3: A transmission XMCD spectrum of a La_{0.7}Ca_{0.3}MnO_3 powder sample at the Mn K–edge; the L_2
and L_1 edges of La are influencing the pre–edge structure. The noise is about 2*10^{-4}.

in Fig. 3 a Mn K–edge Xray Magnetic Circular Dichroism spectrum is exemplarily shown. In the XMCD
mode the difference in absorption between parallel and antiparallel alignment of the absorbing spin–system
to the helicity of the photons is measured. The difference is the dichroic signal, which should only show
effects in and behind the edge. In this respect a dichroic spectrum in the pre–edge region reflects the noise of the spectrum. The signal is the corresponding absorption. In Fig. 3 the measuring time per point was 16 seconds. The signal–to–noise ratio is close to $1 \times 10^{-4}$ even in a wide range of absorption thickness. We want to emphasize, that a further improvement can be expected by enlarging the counting time and improving the statistics, so that a signal–to–noise ratio of far below $1 \times 10^{-4}$ can be accomplished. In consequence this means that, if you plan a experiment with a < 1% noise, you should be able to measure diluted samples with an absorption jump of $1 \times 10^{-2} \mu m$ on a background of $2 \mu m$. In the feedbacked four–crystal mode a spectrum with 300 points and about 15 seconds counting time per point can take a few hours. Using a 0.6 mm vertical slit size and the Si (111) crystals, the photon flux in the two– as in the four–crystal mode is comparable to that of the X1 beam line.

Besides the principle adjustment and the limits of a beamline, the handling of the total experiment is an important quality which determines the results of the users. Therefore, all important adjustments on the lift table can be done now by scanning routines instead of taking photographs. During that procedure a typical beam size is 0.1x0.5 mm$^2$, so that in a short time all positions can be measured on a precision better than 100 $\mu$m. Fast SPECTRA routines are available for each degree of freedom of the lift table and scans can be performed in less than 5 minutes.

The improvements of the beamline and the resulting stability of the complete system offers the opportunity to use the technique of XMCD in a user mode. In collaboration with the group of Prof. Schütz a fast switching normal conducting magnet with 0.6 T maximal field has been made available. The circular polarisation of the photon beam is obtained by using photons above or below the positron orbit. Specifying the off–plane–angle, the adjustment of the complete beam line is automatically done by a routine. A special XMCD modus of the computer program SPECTRA offers all necessary tools for such measurements. The implementation of routines to operate with quarter wave plates or other instruments like special magnets is possible in the computer program. The combination of high resolution with a good signal–to–noise ratio allows for measurements of $10^{-3} \mu m$ effects (Fig. 3). Depending on the photon energy a dramatic reduction of the degree of polarisation occurs. In the case of a Bragg angle of 45 deg the polarisation is vanishing. In that case measurements can only be done by using a quater wave plate.

**Beamline E4**

In previous years several components of beamline E4 have been renewed and modified to improve beam focusing and rejection of higher harmonics. The remaining parts in the upgrade of beamline E4 implied a reconstruction of the experimental stage and a replacement of the beamline soft– and hardware.

The vacuum and ionization chambers were redesigned under special consideration of an easy change of the desired experimental setup. It is now based on 160 ISO–K vacuum parts, the assembly is illustrated schematically in Fig.4. The experimental chamber with 400mm length and 160 mm diameter ports offers sufficient space to mount user specific equipment like ovens, in–situ cells or especially designed sample holders, for instance. In the normal setup a step motor driven horizontal stage is mounted on top of the sample chamber to particularly simplify the sample positioning at grazing x–ray incidence. For a conventional setup in transmission geometry motorized four–fold sample holders are mounted at the sample and reference chamber. While the sample chamber is under high vacuum by means of a turbomolecular pump, the reference chamber is pumped by a rotary pump only. For installation of user specific parts either the experimental chamber or all components behind the first ionization chamber can easily be removed in short time. The experimental stage is equipped with three of the new ionization chambers (please see the separate report herein).

Within the last year both the computer hardware and software for the experimental control were renewed. The old microvax 3200 has been substituted by a Linux PC (two 333 MHz processors) and the EXAFSF program has been replaced by SPECTRA. This is the first case where SPECTRA running on a Linux PC was sucessfully used to control an experiment via Camac; for details on this recent development please see a separate report herein. SPECTRA creates various very valuable graphic outputs during measurement which
Figure 4: Experimental stage at beamline E4

the PC can easily handle without causing any considerable dead time. XAFS dedicated SPECTRA features as well as beamline–specific macros are designed to represent a flexible and user friendly tool for the individual experimental approaches. So far, all user groups were very pleased about this software upgrade.

**Beamline X1.1**

Beginning of April 1998, beamline X1.1 went into user operation after the complete reconstruction of the HASYLAB 2 building. Please see the HASYLAB annual report 1997 for details of the reconstruction. Briefly, the lowered floor level with easy access to the entrance sluice of HASYLAB 1 facilitates movement of heavy experimental equipment to the beamline. The new building has comfortable space for experimental control and electronics and a well–equipped bench for mechanical work just outside the experimental hutch. Users can connect their computers to the net for on–line data analysis at the beamline.

Besides covering high energy XAFS applications (see below), the station is devoted especially to in–situ and chemical applications. Therefore, a chemistry lab was installed only 10 m apart from the experimental hutch containing a fume hutch, chemistry working area, ventilated cabinets for the storage of acids, lyes and poisonous chemicals, a balance and a press for XAFS pellets. We are very grateful for financial support from Haldor Topsøe. HASYLAB does not provide chemicals in this chemistry lab. All chemicals needed by the users must be brought by them on arrival, as well as, on departure, all chemicals including the chemical waste must be taken home. This enables us to handle the rapid turnovers of the chemistry lab. Possibilities for gas in–situ treatment of samples are unique at beamline X1.1. A powerful three–stage ventilation system of experimental hutch and/or chemistry lab is available. An additional, actively pumped exhaust gas line for toxic gases allows in–situ experiments with poisonous gases provided that the experiment is in accordance with HASYLAB safety regulations. Besides five permanent gas lines for inert ionization chamber gases, six permanent gas lines are led from a gas house outside the building directly to the experimental stage in the hutch. To the latter ones (diameter 3 mm) users can connect their own gas bottles (e.g., CO₂, CO, H₂, O₂,
H₂S). Although users are requested to bring their own safety equipment, two additional gas detectors for CO and flammable gases are available from HASYLAB. During experiments with those gases they will be connected to the central DESY alarm system. Three special gas lines leading from the gas house directly into the fume hutch of the chemistry lab enable preparations using (poisonous) gases in the fume hutch also prior to the x-ray measurements.

As an example, Fig. 5 shows a catalytic in-situ measurement after the reconstruction. The Mo/Al₂O₃ catalyst is nitrided in pure ammonia in a temperature programmed fashion from room temperature to 550 °C with a 5 °C/min ramp. Fig. 5 clearly shows the transformation from molybdenum oxide into a molybdenum nitride phase. This pretreatment appears to be quite beneficial for the resulting catalyst activity.

In September 1998, the double-crystal monochromator RÖMO 2 of beamline X1.1 has been upgraded. The former two pairs of Si(311) and Si(111) crystals were replaced by three pairs of crystals, Si(511), Si(311) and Si(111), situated next to each other on the crystal holders. The additional Si(511) crystals extend the energy range of the beamline to around 70 keV. Fig. 6 shows the Ta K edge XAFS measured with the Si(511) crystals. Since the new crystals are still 28 mm wide, no limitations for XAFS applications will occur. As before, crystal exchange between two adjacent crystal pairs horizontal movement of the whole goniometer is very fast (three minutes). Equally important, as their slight misorientation with respect to each other can be
determined once and corrected for in the crystal change procedure, horizontal beam movements with photon energy at the position of the sample are less than 0.2 mm over the whole energy range of 6 - 70 keV.

Furthermore, the 1000 V piezoelectric crystal adjusting the first crystals has been substituted by a 150 V piezo, which, as before, is controlled by the (I)MOSTAB. Its 0 - 10 V output signal drives a subsequent 150 V power supply. This reconstruction allows to flush the monochromator tank with helium gas instead of nitrogen, thereby reducing the background absorption at low energies. Helium flushing is now the standard mode of RÖMO 2, although in order to save helium (during the cleaning cycles after opening the monochromator tank) it is necessary to maintain nitrogen flushing as well. It was observed that at 7 keV, the photon flux at the sample was increased by a factor of 3.5 using helium instead of nitrogen flushing. Water cooling of the copper holder of the first monochromator crystals has been installed using a stabilized, closed cooling circuit. When operating the beamline with monochromator stabilization (MOSTAB), cooling of the first crystals is not essential because the MOSTAB will follow the thermal drifts easily. However, it is now possible to perform long scans with stable intensity without having to use a MOSTAB (typical intensity drifts of less than 2% during 10 minutes). This allows to perform measurements with unchanged spectrometer function.

**Future Developments**

Further developments are in progress for all three XAFS beamlines, a few points are listed below. Because excellent experience with largely automated routines (macros) for beamline adjustment and measurements has been made at A1 and E4, further development in this direction is aspired. The reliable white beam monitor under fabrication is part of this goal and the last component needed for fully automated beamline adjustment of all three beamlines to user specified parameters.

The computer system at beamline X1.1 will be changed to a Linux PC running SPECTRA in early 1999. SPECTRA is already able to run beamline X1.1. By next year, the QEXAFS option will be fully implemented in SPECTRA. It allows to perform quick scans with improved accuracy and at least the same speed.

**Figure 6:** K edge absorption spectrum of a 0.1 mm thick Tantal foil.
as currently the EXAFSF program. All user options of the QEXAFS mode remain. It is planned to addi-
tionally install a motorized yz–table on the experimental stage at beamline X1.1 which will allow more flexible 
positioning of samples and equipment in the beam.

The increasing demand for fluorescence yield (FY) detection makes it desireable to have available appro-
priate detectors beyond the performance of the scintillation counters. A five–element Ge detector has been 
specified for maximum throughput rather than for brilliant energy resolution, i.e. it is especially designed 
for investigating highly diluted systems. It will be available in early 1999. This detector can be handed to 
those user groups who have detailed experience in FY detection. Non–expert users are recommended to 
collaborate with skilled groups to achieve the required experience. Furthermore, a multi–cell Silicon drift 
diode detector is under development (please see the separate report herein).

As the present He cryostat does not cover the general demand for low temperature measurements it is the 
goal to provide an alternative. According to the experiences with the present flow cryostat the new one 
should be a closed cycle model particularly outlined for easy use and handling, to the debit of a somewhat 
worse minimum temperature of approximately 20 K.
Magnetic Diffraction of Ferro- and Antiferromagnets at W1

W. Caliebe
IFF, FZ-Jülich

In the last decade, magnetic x-ray diffraction developed into a standard technique at synchrotron radiation sources. Also at HASYLAB several experiments using resonant magnetic x-ray diffraction of antiferromagnets have been successfully performed [1, 2, 3], and magnetic diffraction of high-energy x-rays was developed and established as a method to investigate antiferromagnetic structures, and to separate the spin and orbital momentum [4, 5]. So far, the experiments were restricted to the study of antiferromagnets in zero field.

In order to study ferromagnets, a different approach has to be taken as the magnetic lattice and the charge lattice coincide. In order to separate the magnetic contribution, which is several orders of magnitude smaller than the charge contribution, an interference term of both scattering events is studied. This can be done in two different ways: (i) In non-resonant magnetic x-ray diffraction, circularly polarized x-rays are diffracted at a scattering angle $2\theta$ of 90°, and the sample is magnetized in the scattering plane. (ii) In resonant magnetic x-ray diffraction, linearly polarized x-rays are diffracted in the polarization plane with the magnetization of the sample perpendicular to the scattering plane. In the first experiment, either the spin of the incident x-rays (left – right circularly polarized) or the magnetization of the sample (north – south) is flipped. In the second experiment only the magnetization is flipped. The difference between the signals with opposite polarization or magnetization, respectively, is proportional to the magnetization.

![Figure 1: Absorption (top) and XMCD (bottom) spectra of Gd at the Gd L edge. The data were collected for a fixed polarization by flipping the magnetization of the sample.](image)

The first approach was taken in August 198 at beamline W1 RÖWI. A quarter-wave-plate QWP was inserted in the beam before the sample to convert the linearly polarized x-rays partly into circularly polarized x-rays. The principle of an x-ray QWP may be explained with dynamical theory: The rocking width of $\sigma$- and $\pi$-polarized radiation is different, so a phase shift between $\sigma$- and $\pi$-polarized x-rays occurs for small deviations from the Bragg-peak. In order to have $\sigma$- and $\pi$-polarized x-rays of equal intensity, the scattering plane of the QWP is rotated by 45° out of the polarization plane of the synchrotron. A phase difference of the transmitted beam between the $\sigma$- and $\pi$-polarized components of $\pi$ is obtained by rotating the QWP slightly of the Bragg-condition. The deviation in angle depends on the thickness of the QWP. The polarization is easily...
flipped by turning the QWP to the other side of the Bragg-peak. As the transmission QWP partly absorbs the incident x-rays, it is advantageous to use low-Z materials like diamond or Be. The beamsize of the wiggler is quite large despite focussing, so diamond could not be used, but a Be-single crystal of very good quality and an appropriate thickness was available. The Be crystal was mounted on a small Eulerian cradle with the \( \chi \)-rotation to turn the scattering plane by 45° and the \( \Phi \)-rotation to rotate the QWP. The reflected and transmitted intensities were measured with standard ion chambers.

The performance of the QWP was tested by measuring the x-ray magnetic dichroism (XMCD) of Gd at the Gd \( L_{II} \)-edge. This edge has been extensively studied and it is well characterized. The performance was measured in two different ways: (1) The polarization was kept constant and the magnetic field was flipped. (2) The magnetic field was kept constant and the polarization was flipped. Both methods give identical results but the data collected with method (1) have less noise due to some stability problems with the monochromator. From an experimental point of view, method (2) has the great advantage that the magnetization is constant, which is quite important for the study of hard ferromagnets which take a long time and high fields for flipping the magnetization. The experimental data are shown in fig. 1.

The circularly polarized radiation was used for non-resonant magnetic x-ray diffraction of the ferromagnet EuO. The experiment and the results are described in detail in this report [6]. The cryostat, which was used to magnetize the sample in the absorption and non-resonant diffraction experiments has a magnetic field in the horizontal plane, and it is equipped with three windows with an opening of approximately 10° each for transmission and for a scattering angle \( 2\theta = 90° \). This cryostat is property of the University of Würzburg, Lehrstuhl Prof. Schütz.

For resonant magnetic diffraction, a cryomagnet with an asymmetric vertical field of up to 5 T and a temperature range of 1.8 K to 310 K with three windows in the horizontal scattering plane with an opening of 110° each was ordered by the institute for x-ray and neutron scattering (group of Prof. Brückel at the IFF), FZ Jülich. It will be applied for resonant magnetic x-ray diffraction of ferro- and antiferromagnets in a magnetic field, where several interesting aspects will be studied on an atomic scale, e.g. the influence of the magnetic field in the incommensurate antiferromagnetic structure in MnP, or the magnetization of different sublattices in mixtures of anti- and ferromagnetic substances which are separated with resonant x-ray diffraction. This cryomagnet will increase the area of scientific topics which may be studied with x-rays at Hasylab.

References


Most commonly, crystalline interfaces and surfaces are studied in surface scattering geometries (Grazing Angle Diffraction (GAD) and Crystal Truncation Rod Diffraction (CTRD)) at typical photon energies around 10keV. These techniques are not applicable in the case of deeply buried solid-liquid interfaces for several reasons: Conventional x-ray scattering geometries are unable to separate the scattering signals from a structurally modified thin liquid layer at an interface from the large background of bulk-like liquid scattering signals. Another problem is the strong absorption of the incoming and scattered beams within the solid and the liquid producing very weak scattering signals on top of a large background from the penetrated solid.

We have developed a new approach for the investigation of solid-liquid interfaces using high energy photons. In order to achieve the necessary interface sensitivity the geometry of GAD has been modified in such a way that total internal reflection occurs at the solid-liquid interface. This produces evanescent waves in the liquid closest to the interface. In the following we discuss the requirements for such a scattering experiment exploiting total internal reflection.

The geometry of our experimental setup is shown in Fig.1. A monochromatic and highly collimated high energy x-ray beam impinges on a flat and mirrorlike interface. The beam is passing almost normal to the wall of the solid with negligible refraction effects and gets subsequently reflected at the interface. For this scenario the electron density of the solid must be smaller than the liquid electron density. By chosing the incidence angle smaller than the critical angle for total internal reflection an evanescent wavefield is transmitted into the liquid (see Fig.2) which is then subject to a kinematic scattering process at density fluctuations in the liquid parallel to the interface.

Intrinsic sources of background scattering are defect scattering, thermal diffuse scattering, and Compton scattering from the solid. Scattering from defects can be minimized by using perfect single crystals (e.g. Si). In order to minimize bulk liquid scattering as well as the parasitic background contributions from the solid, the beam height of the incident x-ray beam must be limited to the projected height of the interface which is typically 10µm depending on the thickness of the sample and the wavelength used. In order to meet this requirement we have installed tungsten collimators in the incoming beam producing an effective beamsize of 50µm with a vertical divergence of 50µrad at the sample position. The beam intensity was maximized at E=70keV using a recently installed SiGe gradient crystal as monochromator.

For the experiments the sample tower of the BW5 experimental station (consisting of a linear translation, a rotational degree of freedom, and a double-tilt) has been equipped with an UHV chamber on top of a...
precision vertical translation stage (z-stage). The mobile UHV chamber is designed for simultaneous preparation of the liquid and the solid surface before the two surfaces are contacted. Since structure factor measurements at thin solid-liquid interfaces are intensity limited even at modern synchrotron radiation sources, it is favorable to use a high Z liquid in order to maximize the scattering signals from the liquid structure factor. First experiments at the interface Pb(liq.)-Si(100) with a photon energy of E=70keV have demonstrated the capabilities of this new technique. Fig.3 shows the bulk liquid structure factor measured at a drop of Pb in an UHV chamber. After contacting solid and liquid, the liquid structure factor at the interface is modified by the presence of the periodic substrate potential of the solid. Fig.4 shows the raw data of a measurement of the liquid structure factor together with some background scattering at an arbitrary azimuth $\Phi$. The measurement shows that for an accurate determination of the liquid structure factor the background at large q-values has to be minimized further by reducing the beam size at the sample position to match exactly the projected interface height. Fig.5 shows a z-scan of the sample through the incident beam while keeping the detector at two different q-values fixed (arrows in Fig.3).

![Figure 3: Bulk liquid structure factor of Pb measured at E=70keV.](image1)

![Figure 4: Liquid structure factor at the solid-liquid interface measured at E=70keV.](image2)

![Figure 5: Linear translation of the interface through the incident beam. The scattering vector Q is fixed at the two positions marked in Figure 3.](image3)
Two–dimensional CCD detector for single crystal diffractometry at beamlines F1 and D3

W. Morgenroth\textsuperscript{1}, and H.–G. Krane\textsuperscript{2}

\textsuperscript{1}Mineralogisch–Petrographisches Institut, Universit"at Hamburg, Grindelallee 48, 20146 Hamburg
\textsuperscript{2}Mineralogisch–Petrologisches Institut, Universit"at Bonn, Poppelsdorfer Schloss, 53115 Bonn

Beamlines F1 and D3 (Teilprojekte of BMBF–Verbund 47) bought a SMART CCD system \cite{1} manufactured in 1996. The CCD (Photometrics Ltd.) is directly coupled to a fiberoptics taper with a 9 cm diameter input imaging area. It has a 60 micro pixel–to–pixel resolution, and a $1024 \times 1024$ pixel frame output ($512 \times 512$ pixel in binning mode). The detector has a short readout time of approximately 2 seconds per frame. The linear range is 18 bit. The GGCS (general goniometer control system) is modified to have full SMART control over both diffractometers at F1 and D3 which have Kappa and Euler geometry, respectively.

![Figure 1: CCD detector mounted at Kappa diffractometer, beamline F1](image)

SMART is the single crystal frame data acquisition program for collection and imaging. It is a graphical user interface for unit cell determination, least squares, Bravais lattice determination, and data collection of hemisphere for triclinic or other strategies for higher symmetry data. SAINT, the data reduction software, processes data frames to create data sets of 3D integrated intensities. The frame buffer (WindowsNT) is connected via ethernet to a SGI for data storage, online data evaluation and integration. In order to get a high number of reflections per frame, the crystal to detector distance has to be small, i.e. preferably 3.0 to 5.0 cm, and the photon energy should be high ($20 – 30$ keV). The short distance favours beamline F1 for combination with the CCD system over beamline D3. We tested the CCD system on Na–Prusside and compared the intensity data and the structure refinements with results from a scintillation counter data set to get information on the CCD system data quality. The scintillation counter data set has a smaller $\sigma(I)/I$ compared to the CCD system.

In order to increase the data quality we changed our data collection strategy and use longer exposure times in higher 2 theta regions. Additionally, we can use a modified SAINT version, which is improved in the reflection profile modelling especially for weak reflections. The CCD system gives access to x-ray structure analyses for structures formerly unavailable (due to limited beamtime) and even for electron density studies \cite{2}. The specimen with the largest cell volume studied up to now is a new heteropolyanion \(Na_2K_4(NMe_4)_3[Pd_3(TeW_9O_{39})_2]\cdot 11 H_2O\), $a = 13.233(2)$ Å, $b = 19.350(3)$ Å, $c = 21.535(1)$ Å, $\alpha = 70.854(9)^\circ$, $\beta = 86.951(16)^\circ$, $\gamma = 88.819(13)^\circ$, $V = 5201.69$ Å\(^3\) in space group P\(\overline{1}\), $Z = 2$ \cite{3}. For this experiment 76000 unique reflections were collected in 2 days. With a scintillation counter the maximal number of reflections measurable is 2000 per day. Using...
the CCD system, low temperature data down to 110 K can be collected using the Oxford cryostream cooler. A second type of usage is the collection of data for the analysis of diffuse scattering. The FWHM of reflection widths for Bragg reflection and diffuse maxima can be analysed using the SMART system [4]. The collection of scans for orientation matrix determination is fast (15 min approx.), time and temperature dependent experiments with samples exhibiting phase transitions can be performed easily.

Finally, experimental work with respect to incommensurately modulated structures was started and has to be finished in following years [5]. The aim is to extend the data reduction software to higher dimensional description of reciprocal space and to use it for aperiodic structures. In contrast to a scintillation counter the CCD system has the disadvantage of no straightforward collimation or energy discriminating devices. In order to reduce background scattering a ‘vacuum chamber’ was constructed and tested [6]. This device was build for beamline D3, can be adopted for beamline F1, and reduces the background scattering in a low 2θ region. It can be used without vacuum (reduction factor approx. 2.5) or with vacuum (reduction factor 4, 10^-4 bar). It has the disadvantage of additional goniometer limits (only φ-scans for 2θ = ω = 0°).

References

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High-Energy Microtomography (\(\mu\)CT) using Attenuation- and Phase-Contrast at BW5

F. Beckmann, U. Bonse\(^1\), T. Biermann\(^1\), T. Lippmann

\(^1\) Institute of Physics, University of Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany

In recent years X-ray tomography became an important tool for the non-destructive 3D-investigation of samples in the fields of e.g. medicine, biology and material science. Using synchrotron radiation the method could be improved to obtain structural information at a spatial resolution of a few microns [1,2].

Microtomography using attenuation- and phase-contrast at photon energies up to 30keV is well tested at BW2 and applied to small samples consisting of normal and weakly absorbing elements [3,4]. In order to extend this method to a wider range of very interesting samples, i.e.

- samples consisting out of high-absorbing elements (attenuation contrast)
- samples consisting out of absorbing elements but with greater diameter (attenuation contrast)
- samples consisting out of weakly-absorbing elements but with greater diameter (phase contrast)
- samples consisting out of weakly-absorbing and absorbing elements (phase contrast)

higher photon energies are needed.

Therefore the apparatus used at BW2 was installed at BW5 to use photon energies in the range of 60keV to 100keV. The principal experimental setup used for microtomography is shown in Fig. 1. The incident white beam is monochromatized by an imperfect 111-Si-Laue crystal (FWHM 5\(^{\circ}\)) and limited in its size by the use of two collimators to 6 x 6 mm\(^2\).

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Principal experimental setup for X-ray microtomography at BW5.}
\end{figure}
Attenuation-contrast microtomography

A more detailed view of the 2-dim. X-ray camera and the sample manipulator stage is given in Fig. 2. The monochromatic beam projects a sample onto a fluorescent screen, which converts X-rays to visible light. The magnified image is then digitalized by a CCD-camera. To protect the CCD-chip from the incident X-rays a lead glass is added between the fluorescent screen and the lens. By rotating the sample a set of 2-dim. projections are measured. By the method of filtered back-projection the 3-dim. representation of the sample can be reconstructed. For attenuation-contrast microtomography the attenuation coefficient at a special position \((x,y,z)\), called voxel, of the sample is given.

Fig. 3 shows a reconstructed slice and a 3-dim. view of a steel sample, which was fractured by tension. In order to penetrate the specimen the scan was performed at 70keV photon energy. 180 projections were taken with an angular increment of 1°. In the reconstructed slice on the left several defects are shown. Using the software VGStudio of the Volume Graphics GmbH, Heidelberg Germany, a stack of 198 slices is visualized. The volume rendering on the right shows the fracture surface.

Figure 3: Reconstructed slice (left) and a 3-dim. volume rendering (right) of a steel sample in collaboration with the Department of Technical Mechanics, University of Bochum.
Phase-contrast microtomography

For phase-contrast microtomography the apparatus shown in Fig. 2 was modified by introducing an X-ray interferometer (Fig. 3). The monochromatized beam is incident on the skew-symmetric LLL interferometer which contains the specimen in its upper interfering beam. A rotating phase shifter located immediately behind the beam splitter crystal serves to scan the overall phase shift of the interferometer. By taking several interference pattern at different rotor positions a single phase projection can be calculated. The tomographic reconstruction of a set of phase projections at different sample rotations yields the 3-dim. data stack of the sample. Each voxel then represents the phase shift that is direct proportional to the electron density of the sample.

In Fig 5 first results are given. On the left phase projections of a mouse kidney embedded in PMMA at different sample rotations are presented. The slice shown on the right is reconstructed from 90 projections with an angular increment of 2°. The surrounding liquid (water), the embedding material (PMMA) and the structure of the mouse kidney is clearly visible.
References

News from the Max-Planck Wiggler Beamline BW6

P. Bösecke, H.-D. Bartunik

Max-Planck-Arbeitsgruppen für Strukturelle Molekularbiologie
c/o DESY, Notkestraße 85, D-22603 HAMBURG, Germany

Since the beginning of 1998, BW6 is dedicated to protein crystallography (monochromatic, MAD, Laue). The beamline is primarily used by groups from the Max-Planck Society and the Gesellschaft für Biotechnologische Forschung GBF in Braunschweig. It is also accessible for groups from other research institutes and from industrial companies.

Information on the design and performance of BW6 is available on the web site http://www.mpasmb-hamburg.mpg.de/bw6. There, proposal and declaration forms for beam time application can also be found.

Figure 1: Image plate detector (left) and CCD detector (right) on the BW6 detector table during a sample change. The image plate detector is in its park position. The color TV monitor is connected to a microscope for observing the sample.
Improvements on BW6 during 1998

During the last year the following improvements have been made on BW6. They refer to the extension of the useful X-ray range for MAD work to wavelengths up to 3.5 Å, to the possibility of nanosecond time-resolved Laue diffraction, the installation of a CCD-detector system and the development of LabView control software with the option for automatic realignment of the beamline.

Vacuum Windows

Except for the vacuum window immediately before the detector table all beryllium windows have been replaced by thin graphite windows. The thickness of the remaining beryllium window was reduced from 1 mm to 0.18 mm. As a result, the upper limit of the usable wavelength range is shifted to about 3.5 Å. Close to the sample a He-filled beam path (collimator tube) is in development to reduce absorption in air. This will allow a powerful extension of the application range of resonant X-ray scattering for MAD-phasing of protein structures. Experiments at the L-absorption edges of cadmium, iodine, tellur and xenon and at the M-absorption edges of uranium will be possible.

Figure 2 shows a calculated spectral transmission curve including the transmissions of all vacuum windows and the reflectivities of all mirrors.

![Figure 2: Calculated bandpath including the reflectivities of two gold mirrors with 4 mrad angle of incidence and the transmission of all installed vacuum windows. The red curve shows the new bandpass (180 μm Be, 30 μm C, 5 μm Al), the blue curve shows the old band path (2mm Be, 20 μm C, 5 μm Al). An effective thickness of 10 μm has been assumed for each graphite windows. The transmission of 1 m air is shown for information in green color.](image)

X-ray Chopper

An X-ray chopper has been developed and tested. It allows to extract a single polychromatic (white) X-ray puls during single and double bunch operation of DORIS. The chopper is based on a new principle: By using
a rotating X-ray mirror the required high time resolution can already be obtained with much lower rotation
speeds than with a conventional chopper. Part of the development is a device for the synchronisation of
lasers for optical excitation of reactions in protein crystals. By varying the time interval between the laser
pulse and the X-ray pulse the structure can be probed with Laue diffraction at different times after the
excitation. Figure 3 shows the experimental time window of the chopper at a rotation speed of 140 Hz and
the extraction of a single bunch during double bunch mode operation of DORIS. For this measurement the
chopper was operated asynchronically to the X-ray pulses in multi-bunch mode. The width of the curve is
400 ns measured at 5% of the maximum. This is sufficient to separate subsequent bunches in single and
double-bunch-mode. Thus, time resolved protein crystallography in the nanosecond range is possible despite
the relatively short bunch-to-bunch distances at DORIS.

Figure 3: Extraction of a single polychromatic X-ray pulse with the chopper which is rotating at 140 Hz
during double bunch operation of DORIS-III (orange: incoming bunches measured at lower rotation speed,
green: experimentally determined time window, black: extracted single bunch). On the top of the figure the
DORIS bunch clock is shown. (Thesis work of Dirk Kosciesza)

New Detector Systems
A MarCCD detector with 135 mm active diameter (2048x2048 pixels) is in operation since the beginning of
1998. It is used in alternation with a Mar345 image plate detector with a diameter of 345 mm of the active
area. Both detector systems are mounted on a common table and can be rapidly exchanged under computer
control. The minimum distance between the sample and the CCD detector is 35 mm. The upper limit in the
cell dimensions is approximately 250 Å; for larger cell dimensions the image plate scanner is used. Both
detectors have comparable efficiencies. The short read out times of the CCD detector have substantially
enhanced the speed of data acquisition. It is an important aspect that it is possible with this detector to take
data with a very small rotation range, e.g. with 0.1°, per image. This permitted in many cases to record full
data sets, despite high crystal mosaicity.

Figure 1 shows the detector table with the two detectors

Data Acquisition
The data acquisition programs of both detectors are running on a PC under the Redhat Linux operation
system. A data frame with 2048x2048 pixels requires 8 MB of storage space. With an average speed of 1
image per minute about 480 MB data per hour are taken, resulting in more than 11 GB data per day. With
the new CCD-detector some applications created more more than 50 GB of data per day. Currently, we are
therefore improving the data acquisition system with respect to computer speed, hard disk capacity and fast
backup possibilities on DDS3-, MO- and DLT7000-drives. In addition, a fast local(152,159),(864,186) network between the front end computer (Pentium-PC) and a DEC-server is under construction. Then, the real bottle neck will be the data reduction. Currently, new powerful UNIX workstations are being installed for this purpose. The immediate crystallographic data analysis up to the inspection of electron density maps is very important for interactive analysis, especially for MAD-applications.

Beamline Control With LabView (XYZ)

A beamline control program with a graphical user interface has been developed at BW6 and is now in operation. It replaces the MS-DOS application software that was running until recently. XYZ is based on LabView and is running on a PC with the operating system NT4.0. It controls VME electronics via a PCI-MXI-VME interface and NI-VISA software from National Instruments. CAMAC electronics is controlled via an 8-bit Kinetic Systems PC-CAMAC interface. We developed Windows NT and LabView drivers for a number of cards.

The control program XYZ has the following features:

- graphical user interface
- several motors are password protected for operation by expert users
- relative and absolute movements of motors
- parallel movements of several motors
- definition of pseudo motors, e.g. for wavelength, slit width and detector table inclination
- pseudo motors can be used in the same way as real motors
- use of physical and mechanical motor values to separate mechanical calibration (dial values) from functional calibration (user values)
- calibration of absolute motor position with reference switches (currently using limit switches)
- integration of position encoders
- soft limits
- writing of a log file of all motor movements and errors
- use of counters and timers
- intensity scans (subsequent movement of a motor and counting with a scaler)

The new beamline control program was developed with the support of Francis Golding.

Automatic Optimization of Intensity

An application has been developed that maximizes the intensities which are measured by two ionization chambers in the collimator. It optimizes the alignment of the monochromator, the toroidal mirror and the detector table. If required, any other motor can be added. The program runs cyclicly during the entire data collection. It is based on the LabView program XYZ that is presented above. Due to this development, the user of BW6 can now concentrate on the experiment; it is possible to leave the beamline in unattended automatic mode, provided the experiment does not involve hazards. Details about unattended mode are available from the beamline scientists. Figure 5 shows the control window during optimization.
Figure 4: Control panel of the automatic alignment: motor positions are yellow and intensity values are red. The motor positions are optimized cyclicly.