Manual Beamline 6ID-D

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Introduction

Chapter 2

General description of the 6ID-D Beamline

This section gives a general description of the 6ID-D Side Station and its features. In Section 2.2 all motors used at the sidestation are described. In Section 2.5 some general safety precausions are listed.

2.1 Beam Conditions

The 6ID-D Side Station is a beamline which uses the white beam of an undulator A insertion device. The optics for both, the 6ID-B Main Station and 6ID-D Side Station are installed in the 6ID-A and 6ID-A extension hutches. First the monochromator of the 6ID-B Main Station, a Kohzu double crystal monochromator with silicon (111) crystals uses the low energy portion of the beam in the range of 3-30 keV. The monochromatic beam of the 6ID-B Main Station is 25 mm higher than the white beam. Directly after the Kohzu monochromator the first monochromator chamber of the 6ID-D Side Station is installed. A white beam mask is used to reduce the beam to a size of 2×4 mm^2. Next the low energy x-rays are cut off by different combinations of filters:

- 1mm C & 1mm Al: for energies above 30 keV
- 1mm C & 1mm Al & 1mm Cu: for energies above 60 keV

The sidestation uses a Bragg double monochromator in horizontal geometry. The monochromatic beam has a distance of 600 mm from the white beam. As monochromator crystal annealed silicon crystals are used. Three different cuts has been chosen to cover an energy range from 30 keV to 130 keV:

- Si 111 annealed: 28 – 54 keV
- Si 311 annealed: 53 – 103 keV
- Si 331 annealed: 69 – 136 keV

Both beamlines, the 6ID-B Main Station and the 6ID-D Side Station, can operate simultaniously, experiments at the 6ID-B Main Station are carried out at the 6ID-B and 6ID-C hutches, experiments at the 6ID-D Side Station in the 6ID-D hutch. Both beamlines have their own monochromatic beamshutters. If both beamlines are operated at the same time the position of the undulator gap is critical. As is shown in figure 2.1 the intensity of the primary beam at the 6ID-D Side Station decays with wider openings of the undulator gap.

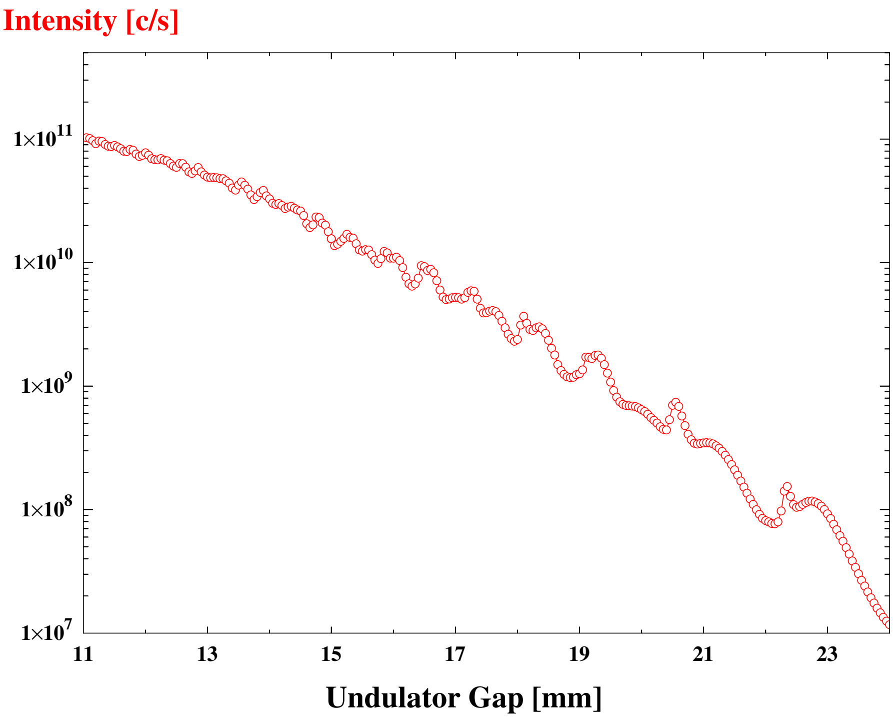

Figure 2.1: *Scan of the undulator gap. The integral intensity of the monochromatic beam at* 92 *keV is shown. At this high energies the undulator behaves like an wiggler and nearly no structure is seen for closed gap. If the gap is fairly wide open some structure is seen due to higher harmonics.*

Even though the distances between the first and second monochromator crystal are quite large the 6ID-D Side Station runs very stable as is shown in figure 2.2.

A drawing and pictures of the sidestation can be found on the webserver of the 6ID-D Side Station.

2.2 Motors

This section is intended to give an overview about which motors are available at the sidestation. In table 2.2 all motors are listed with a short description of there purpose. For troubleshooting in table 2.3 the actual motorparameters are listed. If one motor is not working as it is supposed to be compare its parameters to the one in this table.

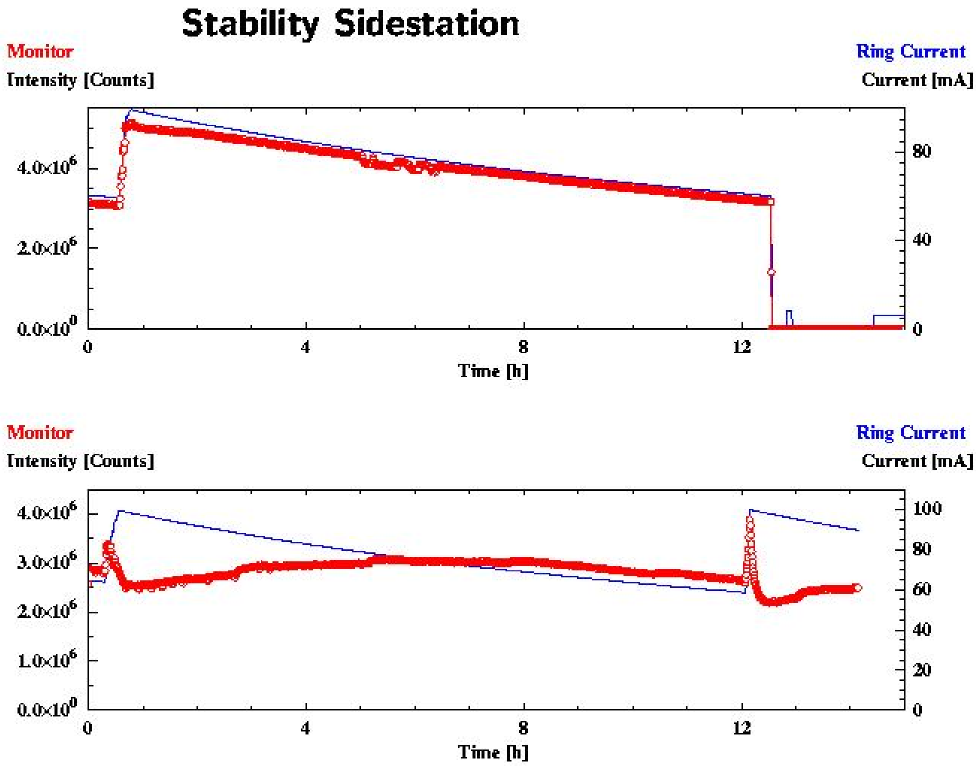

Figure 2.2: *Stability of the monochromatic beam at the 6ID-D Side Station. The intensity of time compared to the ring current is shown. Top nearly perfect stability is shown but also in the bottom plot the beamline is quite stable. Regularily performed adjustments (every one to two hours) of the first monochromator (motor momu) or a monochromator stabilizer could easily solv the problem.*

The motor racks with number 0 and 1 are mounted in the 6ID-A extension. All motor drivers for the optics of the 6ID-D Side Station are mounted in those two racks. Both monochromator crystals including the crystal changers are fully motorised so no access to the 6ID-A or 6ID-A extension hutch should be necessary during operation of the beamline.

The motor drivers of the racks 2 to 6 are mounted inside the 6ID-D hutch. Directly behind the beam entrance is a motorized table (motors xm and ym) with a vertical and horizontal translation. On this table slitsystems 1 and 2 (motors sl1t, sl1b, sl1l, sl1r, sl2t, sl2b, sl2l and sl2r), collimators and a filter bank are mounted to define the incoming beam. For a description of the filter bank see section 2.3.1.

On the fully motorised ψ diffractometer sample environments can be mounted either in an eulerian cradle or on a double tilt. In the setup with a eulerian cradle horizontal and vertical ϑ motors are available (om_v and om_h) and for the ϕ and χ rotation (chi and phi). In the setup with the double tilt the same motors as with the eulerian cradle are available but the movement of ϕ and χ is restricted to

± 10 degree. In addition a z translation is mounted below the double tilt and a x and y translation above (motors zs, xs and ys). In addition the whole diffractometer can be moved horizontally and vertically (motors xd and yd). Those motors are very slow and driven by SPD-3M stepping motor drivers. These motor drivers create a lot of electronic noise which is disturbing the detector signal so they are normally switched of once aligned.

On the diffractometer three slit systems are mounted (motors sl3t, sl3b, sl3l, sl3r, sl4t, sl4b, sl4l, sl4r, sl5t, sl5b, sl5l and sl5r). Slit sytstem 3 is mounted in front of the analyser, slit system 4 behind the analyser and slit system 5 in front of the detector.

This ψ diffractometer was exspecially adapted to the needs of a high energy beamline. The distance between sample and analyser can be as large as 900 mm and between analyser and detector between 300 mm and 600 mm, depending on the setup. This was done by using translations instead of a rotation to simulate the detector arm. This way even heavy detectors, analyser and filter equipment can be mounted. The analyser is also fully motorised and offers 2ϑ, ϑ, χ and ϕ movements (motors tta, oma, chia and phis). The filters are described in section 2.3.1. To simulate the 2ϑ movement of the vertical detectorarm a vertical and horizontal translation (motors tt_v and tt_h)is used on which the analyser rotations are mounted. The horizontal rotation is done in the conventional way (motor tt_h). To give users the possibility to operate this diffractometer as easy as a conventional diffractometer virtual motors (tth and th) have been implemented which simulate the ϑ and 2ϑ movements, see table 2.1. In case of horizontal geometry those virtual motors are identical to the real motors though tth is driving tt_h plus motor sl3_rot and th is driving om_h. In case of vertical geometry th is driving om_v. But the virtual motor tth is driving the motors tt_h, tt_v, tta, oma and sl3_rot. All the movements have to be calculated with respect to the 2ϑ value and the used or not used analyser crystal. This is done automatically by the **spec** macro hp_motor_6idd.mac. In section 4.11.7 the setup of these macros is described.

No	name	units	description
1	tth	degree	Virtual 2ϑ motor difractometer
2	th	degree	virtual ϑ motor diffractometer
3	dummy		dummy motor, nothing is moved

Table 2.1: *List of the available virtual motors. These motors are simulated by* **spec** *programs and are not available under epics.*

2.3 Special equipment

In this section some of the special equipement which was build for the 6ID-D Side Station is described. Due to the fact that some things were still in work when this manual was written not everything in here might work as described or might not be available.

2.3.1 Filter banks

There are 2 filter banks with 15 filters each available to reduce the intensities either in front of the sample or in front of the detector. Both filter banks can be loaded with iron or aluminum filters with a thickness of 3 mm each. There are two of the iron and one aluminum filter banks available which can be exchanged very easily within a few minutes. Both filterbanks are controlled by compressed air regulators which are controlled by a 0 to 10 V signal from the digital analog converter (DAC). The DAC can be operated through the macro hp_dac.mac described in section 4.11.9. The filters are operated by the macro hp_dac.mac described in section 4.11.10. The macros also provide an automatic absolut calibration for the filters.

2.3.2 Detector systems

There are four different detector systems available at the sidestation. Photodiodes are mainly used as monitor systems. They are normally connected to current ampliefiers. The current amplifiers delivers a signal in the range from 0 to 10 volt with is then converted by a volt to frequency converter (VFC) into a frequency with the regular counters can handle.

As a second system two Bicron NaI detectors including amplifiers, single channel analysers and high voltage supplies are available. These detectors are equipped with 10 mm thick crystals in contrast to the standart 1 mm crystal to be able to absorb most of the high energy photons. Warning! This detector can not withstand high countrates and will get damaged if for example hit by the direct not attanuated beam. Make sure that not to much intensity is getting into the detector.

As a third system a Canberra Germanium Detector is available. This system is working together with a digital signal processor (DSP) and a high voltage power supply, both are completely computer controlled through a Canberra AIM. To operated these electronics special MEDM windows are available. The detector can be accessed through **spec** with the help of the macro package hp_mca.mac which is described in section 4.11.8.

As a fourth system an image plate system is available. This is described in detail in chapter 6.

2.4 Sample environments

For the sidestation several sample environments will be available in the near future including a closed cycle with aluminium windows, an Orange liquid helium flow cryostat with aluminium windows, an Orange liquid helium flow cryostat with superconducting coils with magnetic fields up to 5 T and beryllium windows and a furnace.

2.5 Saftey

No	spec	epics	units	C	S	home	description
1	monu	m1_om	degree	0	0		ϑ first monochromator crystal
2	m1_chi	m1_chi	degree	0	1		χ first monochromator crystal
3	m1_phi	m1_phi	degree	0	2		ϕ first monochromator crystal
4	m1_xtal	m1_xtal	mm	0	3		crystal changer first monochromator
5	m1_y	m1_y	mm	0	4		vertical movement first monochromator chamber
6	m1_x	m1_x	mm	0	5		horizontal movement first monochromator chamber
7	filter	filter	mm	0	6	HomR	filter changer for the white beam
9	mond	m2_om	degree	1	0		ϑ second monochromator crystal
10	m2_chi	m2_chi	degree	1	1		χ second monochromator crystal
11	m2_phi	m2_phi	degree	1	2		ϕ second monochromator crystal
12	m2_xtal	m2_xtal	mm	1	3		crystal changer second monochromator
13	montrav	m1_z	mm	1	4	HomF	translation of second monochromator chamber
17	xd	xd	mm	2	0		horizontal movement of the diffractometer
18	yd	yd	mm	2	1		vertical movement of the diffractometer
19	om_v	om_v	degree	2	2	HomF	vertical ϑ diffractometer
20	chi	chi	degree	2	3		χ diffractometer
21	phi	phi	degree	2	4	HomF	ϕ diffractometer
22	om_h	om_h	degree	2	5	HomF	horizontal ϑ diffractometer
23	xs	xs	mm	2	6		horizontal translation below double tilt
24	zs	zs	mm	2	7		translation in beam direction below double tilt
25	ys	ys	mm	3	0		vertical translation below double tilt
26	tt_h	tt_h	degree	3	1	HomF	horizontal 2ϑ diffractometer
27	tt_y	tt_y	mm	3	2		vertical movement 2ϑ diffractometer
28	tt_z	tt_z	mm	3	3		horizontal movement 2ϑ diffractometer
29	oma	oma	degree	3	4	HomF	ϑ analyser
30	chia	chia	degree	3	5	HomF	χ analyser
31	phia	phia	degree	3	6	HomF	ϕ analyser
32	tta	tta	degree	3	7	HomF	2ϑ analyser
33	sl1t	sl1_t	mm	4	0		first slit system in the hutch
34	sl1b	sl1_b	mm	4	1		first slit system in the hutch
35	sl1l	sl1_l	mm	4	2		first slit system in the hutch
36	sl1r	sl1_r	mm	4	3		first slit system in the hutch
37	sl2t	sl2_t	mm	4	4		slit system in front of the sample
38	sl2b	sl2_b	mm	4	5		slit system in front of the sample
39	sl2l	sl2_l	mm	4	6		slit system in front of the sample
40	sl2r	sl2_r	mm	4	7		slit system in front of the sample
41	xm	xm	mm	5	0		horizontal movement of yellow table
42	ym	ym	mm	5	1		vertical movement of yellow table
44	sl3_rot	sl3_rot	degree	5	3		rotates the slitsystem 3
45	sl3t	sl3_t	mm	5	4		slit system in front of the analyser
46	sl3b	sl3_b	mm	5	5		slit system in front of the analyser
47	sl3l	sl3_l	mm	5	6		slit system in front of the analyser
48	sl3r	sl3_r	mm	5	7		slit system in front of the analyser
49	sl4t	sl4_t	mm	6	0		slit system behind the analyser
50	sl4b	sl4_b	mm	6	1		slit system behind the analyser
51	sl4l	sl4_l	mm	6	2		slit system behind the analyser
52	sl4r	sl4_r	mm	6	3		slit system behind the analyser
53	sl5t	sl5_t	mm	6	4		slit system in front of the detector
54	sl5b	sl5_b	mm	6	5		slit system in front of the detector
55	sl5l	sl5_l	mm	6	6		slit system in front of the detector
56	sl5r	sl5_r	mm	6	7		slit system in front of the detector

Table 2.2: *Table of all motors implemented at the 6ID-D Side Station. First column contains motor number, second the* **spec** *motor name, third the epics motor name, fourth the units, fifth and sixth the crate and slot where the driver is placed, seventh the direction in which the home position has to be accessed if implemented and there is a description of the function of the motor in the eighth column.*

No	DESC	EGU	C	DIR	VELO	VBAS	ACCL	BDST	BVEL	BACC	MRES	PREC	DHLM	DLLM	SREV	S	SBAK	SBAS	UREV
1	m1_om	degrees	0	Pos	1	0.1	0.2	0.01	1	0.2	5e-05	5	7.5	0	2000	10	10	1	0.1
2	m1_chi	degrees	0	Pos	4	0.4	0.2	0.1	4	0.2	0.0025	5	3	-5.0125	400	4	4	0.4	1
3	m1_phi	degrees	0	Pos	4	0.4	0.2	0.1	4	0.2	0.0025	5	2	-2	400	4	4	0.4	1
4	m1_xtal	mm	0	Pos	2	1	0.2	0	2	0.2	0.005	5	199.35	0	400	1	1	0.5	2
5	m1_y	mm	0	Pos	0.15625	0.0046875	0.4	0	0.15625	0.4	3.90625e-05	5	8.3	2.3	400	10	10	0.3	0.015625
6	m1_x	mm	0	Pos	1.2	0.5	0.5	0	1.2	0.5	0.005	5	5.17	-5.105	400	0.6	0.6	0.25	2
7	filter	mm	0	Pos	5	0.5	0.4	0	2.5	0.4	0.000625	5	80	-7	400	20	10	2	0.25
8	motor 8	degrees	0	Pos	1	0.1	0.2	0	0.5	0.2	0.00025	5	100	-100	200	20	10	2	0.05
9	m2_om	degrees	1	Pos	1	0.1	0.2	0.01	1	0.2	5e-05	5	8.9961	-0.0039	2000	10	10	1	0.1
10	m2_chi	degrees	1	Pos	4	0.4	0.2	0.1	4	0.2	0.0025	5	4	-4	400	4	4	0.4	1
11	m2_phi	degrees	1	Pos	4	0.4	0.2	0.1	4	0.2	0.0025	5	4	-4	400	4	4	0.4	1
12	m2_xtal	mm	1	Pos	2	1	0.2	0	2	0.2	0.005	5	200	4.81188e-06	400	1	1	0.5	2
13	m2_z	mm	1	Pos	25	0.1	0.7	0	25	0.7	0.003125	5	36.67	-3947	400	20	20	0.08	1.25
14	motor 14	degrees	1	Pos	1	0.1	0.2	0	1	0.2	0.00025	5	100	-100	200	20	20	2	0.05
15	motor 15	degrees	1	Pos	1	0.1	0.2	0	1	0.2	0.00025	5	100	-100	200	20	20	2	0.05
16	motor 16	mm	1	Neg	10	1	0.3	0	5	0.4	0.00625	5	90	-100	200	8	4	0.8	1.25
17	xd	mm	2	Pos	0.04	0.002	0.3	0	0.02	0.3	5e-05	5	65.8117	-49.2469	400	2	1	0.1	0.02
18	yd	mm	2	Pos	0.032	0.00064	0.03	0	0.0064	0.03	1.6e-05	5	66.7275	-100	400	5	1	0.1	0.0064
19	om_v	degrees	2	Pos	0.5	0.05	0.5	0	0.5	0.5	0.0001	5	60	-60	1000	5	5	0.5	0.1
20	chi	degrees	2	Pos	1.4	0.02	0.4	0	1.4	0.4	0.0002	5	360	-360	1000	7	7	0.1	0.2
21	phi	degrees	2	Pos	2	0.02	0.4	0	2	0.4	0.0002	5	100	-100	1000	10	10	0.1	0.2
22	om_h	degrees	2	Pos	0.5	0.05	0.5	0	0.5	0.5	0.0001	5	60	-20	1000	5	5	0.5	0.1
23	xs	mm	2	Pos	1	0.1	0.2	0	1	0.2	0.000125	5	100	-100	400	20	20	2	0.05
24	zs	mm	2	Pos	1	0.1	0.2	0	1	0.2	0.000125	5	100	-100	400	20	20	2	0.05
25	ys	mm	3	Pos	1	0.1	0.2	0	1	0.2	0.00025	5	100	-100	200	20	20	2	0.05
26	tt_h	degrees	3	Pos	1	0.1	0.3	0	1	0.3	0.00025	5	95	-16	400	10	10	1	0.1
27	tt_y	mm	3	Pos	4	0.4	0.4	0	4	0.4	0.00125	5	950	-24.06	400	8	8	0.8	0.5
28	tt_z	mm	3	Pos	5	0.5	0.4	0	5	0.4	0.00125	5	950	-30	400	10	10	1	0.5
29	oma	degrees	3	Pos	1	0.01	0.4	0.01	1	0.4	0.0001	5	100	-10	1000	10	10	0.1	0.1
30	chia	degrees	3	Pos	1	0.1	0.3	0.1	1	0.3	0.0025	5	12	-12	400	1	1	0.1	1
31	phia	degrees	3	Pos	1	0.1	0.3	0.1	1	0.3	0.0025	5	13	-13	400	1	1	0.1	1
32	tta	degrees	3	Pos	1	0.1	0.3	0.1	1	0.3	0.00025	5	120	-110	400	10	10	1	0.1
33	sl1_t	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	10	-1	400	5	5	1	0.5
34	sl1_b	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	10	-1	400	5	5	1	0.5
35	sl1_l	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	10	-1	400	5	5	1	0.5
36	sl1_r	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	10	-1	400	5	5	1	0.5
37	sl2_t	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	10	-1	400	5	5	1	0.5
38	sl2_b	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	1.20125	-9.79875	400	5	5	1	0.5
39	sl2_l	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	10	-1	400	5	5	1	0.5
40	sl2_r	mm	4	Pos	2.5	0.5	0.2	0.1	2.5	0.2	0.00125	5	1.1875	-9.8125	400	5	5	1	0.5
41	xm	mm	5	Pos	2	0.00469	0.4	0.5	2	0.4	0.005	5	41.26	-40	400	1	1	0.002345	2
42	ym	mm	5	Pos	0.15625	0.0046875	0.4	0.5	0.15625	0.4	3.90625e-05	5	18	-18	400	10	10	0.3	0.015625
43	motor 43	degrees	5	Pos	1	0.1	0.2	0	1	0.2	0.00025	5	100	-100	200	20	20	2	0.05
44	motor 44	degrees	5	Pos	1	0.1	0.2	0	1	0.2	0.00025	5	100	-100	200	20	20	2	0.05
45	sl3_t	mm	5	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10.1	0	200	20	20	2	0.25
46	sl3_b	mm	5	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10.1	0	200	20	20	2	0.25
47	sl3_l	mm	5	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10.1	0	200	20	20	2	0.25
48	sl3_r	mm	5	Pos	2.5	0.5	0.2	0	2.5	0.2	0.00125	5	10.1	0	400	5	5	1	0.5
49	sl4_t	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10	-10	200	20	20	2	0.25
50	sl4_b	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10	-10	200	20	20	2	0.25
51	sl4_l	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10	-10	200	20	20	2	0.25
52	sl4_r	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10	-10	200	20	20	2	0.25
53	sl5_t	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10	0	200	20	20	2	0.25
54	sl5_b	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	10	0	200	20	20	2	0.25
55	sl5_l	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	8.8	-4.2	200	20	20	2	0.25
56	sl5_r	mm	6	Pos	5	0.5	0.2	0	5	0.2	0.00125	5	3.5	-3.5	200	20	20	2	0.25

Table 2.3: *Configuration of all important motor parameters (20th of April 2001). This configuration was done by Norbert Bayer. This table was automatically created by the macro hp_motor_parameter.mac.*

Chapter 3

Getting spec running for a beamtime

To have a nicely working spec makes beamtimes much more convenient. In this chapter it is described what is necessary to customize **spec** for your needs (section 3.1) and the most important configuration steps at the beginning of a beamtime (section 3.2).

3.1 Preparing the spec macros

Normally all major spec macros which provides you with features like opening the beamshutter with a command line or calculating the absorption of the filters should be installed on the 6ID-D Side Station and 6ID-B Main Station. Mainly on the 6ID-B Main Station not all commands described in chapter 4 are installed. This can be easily done by downloding those macro packages from this internet-server, see http://idefix.mu.aps.anl.gov/hupfeld/spec_macros/ and automatically calling them from the file “spec.mac”, which is automatically loaded if found in the same directory **spec** is started in. Also in this file all definitions should be made if additional data should be saved during scans.

3.1.1 6ID-D Side Station

All necessary macros are preloaded at the side station. A spec.mac file is not required. If you want to load additional macros or change the data written to harddisk during a scan use spec.mac as an example.

3.1.2 6ID-B Main Station

Not all macros are necessarily preloaded, exspecially hp_fio.mac or hp_lakeshore340.mac might not be preloaded. Use spec.mac as an example to load those packages. In this example of spec.mac complete path names to a directory where those packages are available on the computer su1a.mu.aps.anl.gov are included or the packages can be downloaded from this webserver (http://idefix.mu.aps.anl.gov/hupfeld/spec_macros/).

3.2 Setting up spec

To get spec running in a state where it is convenient to use for a whole beamtime roughly ten minutes of time is needed. This section will show all necessary steps in the correct order to get a running environment. This procedure has to be done only at the beginning of a new beamtime. Only in rare cases like a fatal crash of spec or the beamline computer it might be necessary to repeat this procedure. This is the recommended procedure for both the 6ID-D Side Station and the 6ID-B Main Station.

3.2.1 Doing a fresh start

First do a fresh start with **spec**. To do so close **spec** with the command **quit** if it is still running. Now change the directory you have created in section 3.1 and start it again with the command **spec -f**. This erases any changes prior users might have made and the standart macros are reloaded in their original version as should be shown on the screen. Now exit **spec** again and start it the regular way with the command **spec**. You should avoid any fresh starts during your beamtime because you will lose all changes and configurations you made.

3.2.2 Executing the startup script

Now execute the command **startup** in spec. Here you are doing all the basic configurations. For most of the questions the default configuration is fine or the question is selfexplanatory and depends for example on your sample so just hit enter if you want the default or do not know what to do. There are only two really important questions: "Data file (/dev/null)?" Here you definitely should enter a data file name. It is recommended that you put the data files into a separate directory which is a subdirectory of the directory you are currently working in and giving the ening ".spc" to the filename. So for example you could answer: data/sample1.spc

The second important question were you should chose something else then the default is "128) Use high resolution plotting device (NO)?" Please answer yes if you want to see graphics during your scans, which is recommended.

The following questions are about your sample and the UB-matrix you want to work with, all those parameters can be changed easily during the experiment so if you want you can stay with the defaults and do the changes later. If you made mistakes answering the questions just start again with the command **startup**.

3.2.3 Getting the automatic creation of fio files to run

The automatic creation of fio files is not a standart **spec** feature. Nevertheless it is recommended to use it because it created data files for each scan which are easy to read and can copy those data files to another computer which gived additional security in case of a computer crash. If you want to know how to run a data analysis of these fio files see chapter 5. See section 4.11.1 for an explanation of the **spec** macros related to fio files and hp_fio.mac for the code.

First a name and a number for the fio files has to be defined. To do so execute the command **fio_new_filename**. First you are asked to enter a new filename: “Data file (0)?” In brackets the old filename is given, “(0)” means that this program was not in use since the last fresh start. Enter for example **data/sample1_** which will store the fio files in subdirectory data and the filename will be sample1_xxx.fio where xxx is replaced by the scan number. In the next question you are asked for the last used scan number: “Last scan number (0)?” which is normally zero. In some cases it might be advisable to start with a different number, for example after a crash and you want to continue your measurements or to match the scan numbers used in the data files written in the **spec** format. It is strongly recommended to use the same scan numbers in the **spec** and the fio data format even though they are completely independent.

Second you can automatically copy your fio data files to another computer. This is recommended as a safety precausion because this gives you an automatic immidiate backup of all of your data. To do so execute the command **fio_new_copy**. You are asked for computer where the data should be copied: “user@computer: (user@idefix.mu.aps.anl.gov:)?”, the default in brackets. If you are working at the 6ID-D Side Station it is recommended to use “idduser@idefix.mu.aps.anl.gov:” or “idduser@mar.mu.aps.anl.gov:” (the colon is important, do not forget it!). If you are working at the 6ID-B Main Station it is recommended to use “user@idefix.mu.aps.anl.gov:” or “idbuser@mar.mu.aps.anl.gov:”. Next you are asked for a directory where the files should be stored:”directory (trashcan/)?” Once again, the default is in brackets. Please create you own directory at “idefix” or “mar” in one of the user accounts that your data files are not mixed up with files from other users. Warning! Data files might be removed at any time after the experiment from the beamline or data analysis computers so it is strongly recommended that you make a copy of your complete data set after the experiment on one of the computers at your home institution. Read section 6.1 for advice about how to copy your data.

It is possible to copy fio files to any other computer even in your home institution automatically. But it is necessary that a ssh daemon is running on this mashine and you have to set it up that the beamline computer can access it through the public-private key structure of ssh without having to enter a password or passphrase.

To check how the creation of the fio files is configured use the command **fio_show_settings**. There you also get advice how to stop the automatic creation and copying of fio files. If you do not want to use fio files any more you just have to execute the command **FIO_NAME=""** (please be sure to use capital letters). No deinstallation of the hp_fio.mac macros is necessary.

If for any reason the commands **fio_new_filename**, **fio_new_copy** and **fio_show_settings** are not available then the hp_fio.mac was not installed by default. This is very likely for the 6ID-B Main Station the case. See section 3.1.2 how to do this.

3.2.4 Checking the creation of proper data files

It is recommended that you check very carefully before starting with taking data if the data is written into either fio or spec data files. To do so start a quick scan and check if you can find it in the spec file, that you can find a fio file which belongs to this scan on the beamline control computer and you also find this scan on the mashine where it is supposed to be copied to.

You might encounter problems exspecially with the automatic copying if you are working at the 6ID-B Main Station. This is due to the fact, that the beamline control computer of the side station is using ssh2 which in some versions is incompatible to the most commonly used openssh or ssh1 standart. There is no solution to this problem until a compatible version has been installed. You have to copy the files manually from time to time. It looks like if the files can be accessed from outside mashines so that you can use Spectra to ask for a data file whenever you want to look at a specific file during your data analysis. See chapter 5 for explanation.

Chapter 4

spec

spec * is a x-ray diffraction software which is used at our beamline for the control of all devices, from the monochromator, slit systems up to the diffractometer. A general description of the capabilities of **spec** is give in the reference manual [Spe99]. See also the Internet page of Certified Scientific Software (CSS) http://www.certif.com/ for more information.

The aim of this chapter is to provide a simple manual for the use of the most important commands of **spec** and a description of the beamline specific features and macros. It is not intended to describe all commands implemented in spec. Advanced users should only read section 4.1 to learn about the non standart commands implemented exspecially for our beamline. Beginners should skip that section and start reading at section 4.2.

4.1 Site specific macros

atten value Reads the actual setting of the filters and displays the thickness and the transmission for the actual energy if no argument is supplied. At the 6ID-B Main Station with argument it moves the absorbers according to the value $(0-255)$, each bit represents one filter. At the 6ID-D Side Station the command **atten bank value** might have two arguments. If one argument is supplied $(0-15)$ the specified number of filters is moved into the beam. At the 6ID-D Side Station there might be two filter banks installed. If two arguments are supplied the first argument is the filterbank which is to be used (1 or 2)

ugmv,umgvr move up to 10 motors at the same time, see section 4.3

theta0 two theta correction, see section 4.9

read_ubm reads a UB-matrice from rafin, see section 4.9

* spec is a trademark of Certified Scientific Software

ana_elast moves analyser theta and two theta, see section 4.7

absorption calls a fortran program which calculates the transmission for different elements and energies

shutter command opens or closes the main shutter, command are the words open or close. For the shutter of the idb- and idd-station the command **idbshutter command** and **idbshutter command** exists

new_fio_filename and **new_fio_copy** implements the automatic creation of fio (Spectra) files during all scans. Package hp_fio.mac has to be loaded. **new_fio_filename** defines necessary variables and implements the creation of fio files. **new_fio_copy** defines a variable necessary for automatic copying of fio files to another computer. Package ssh has to be installed on both computers and the public key of the beamline computer has to be installed on the other computer. Look in the man pages of ssh. The macro **show_fio_settings** can be used to show the status of the fio package.

4.1.1 To move and scan PVs

The following commands are used to move or scan PVs, that are epics variables, e.g. the gap, that behave like motors.

pvwa lists all PVs and their position

pvmv moves a PV

pvascan absolute scan of a PV

pvdscan relative scan of a PV (also **pvlup**)

pvconfig configure (add, delete, ...) PVs

4.2 Handling macros

qdofile(”filename”) load macros defined in filename so that they are known to the program

prdef macroname show code of macro macroname

lsdef lists the names and sizes of macros

lscmd lists build-in keywords and functions

newmac reloads the startup macros, normally done when entering **spec**

4.3 Motors

umv motor pos move motor to absolut position

umvr motor value move motor relativ to actual position

wa show positions of all motors (**wu** shows only mnemonic and user position)

wm mot1 mot2 mot3 ... show positions of the specified motors

lm mot1 mot2 mot3 ... show limits of the specified motors, without options the limits of all motors are shown.

ugmv mot1 pos1 mot2 pos2 ... move group of motors to absolute positions

ugmvr mot1 val1 mot2 val2 ... move group of motors relative to absolute positions

set motor position sets the actual motor position to a new value

set_dial motor position sets the actual dial motor position to a new value

set_lm motor low_limit high_limit set new soft limits for a motor

zero motor sets the dial value to the mechanical zero for motors which are equipped with a home position feature

tw mot1 mot2 ... delta1 delta2 ... sample_time moves one ore more motors in small steps each time you hit the return key. The parameter sample_time is optional, if given after each move a count will be performed and displayed

4.4 General stuff

startup Should be performed at the beginning of an experiment to set up data files and so on

newfile changes to a new file where the data is written to

whats ??? gives information about an expression

gpset variable1 variable2 variable2 gets the same value than variable1 and the change is documented in the data file

sleep value spec waits until the specified time in seconds has passed. If you use the command **do_sleep** instead spec will show a counter running backwards

setmono set parameters for monochromator

4.5 Counting

ct time counts for time seconds

uct time counting is updated during count, try **uctn** if you have more than six counters

counters changes the counter displayed during the scans

_show_cntr shows current configuration of the counters

count is the macro called by all scans and ct commands to do the counting

chk_beam tests if beam is there, but normally the macro is not defined. Look into standard.mac to change this. If it is defined properly it waits until the beam is back if the intensity in the monitor (defined by global variable **MON**) is below the value defined in the global variable **chk_thresh**

Please note that a positive value of **time** represents counting for the defined time and a negative value represents counting against a monitor, which has to be defined by the **counters** command.

The global variables **DET** and **MON** contain the channel displayed during the scan and the monitor channel. They might be changed just by typing **DET = ion1** then ion chamber 1 will be displayed during the scans.

4.6 Scans

Here a list of possible scans with a short explanation is shown. For details about the different scan types use spec command **help**.

ascan motor start_position end_position points sample_time normal scan, positions are given in absolut values, scan contains one more point than given in points, last parameter is the sample time

a2scan motor1 start1 stop1 motor2 start2 stop2 points sample_time two motor scan, also **a3scan**, **a4scan** and **a5scan** exist

dscan motor start_position end_position points sample_time (or **lup**) relative scan, same like **ascan** but the values of start_position and end_position are added to the actual position. Also **d2scan**, **d3scan**, **d4scan** and **d5scan** exists

th2th tth_start_rel tth_finish_rel points sample_time theta-two-theta scan

hklscan start_h stop_h start_k stop_k start_l stop_l points sample_time Q-scan. In addition also **hscan**, **kscan** and **lscan** exists, easier to use if you are only doing scans in one Q-direction. Also more fancy Q-scans are available like **hkcircle**, **hlcircle**, **klcircle**, **hkradial**, **hkradial** and **hkradial**.

mesh motor1 start1 stop1 interval1 motor2 start2 stop2 interval2 sample_time nested motor scan which is able to scan a two dimensional area defined by the two motors. Data is written to a single scan in the data file so make sure you are able to read the data with your data analysis software. The same exists for Q-scans, see **hklmesh**

aziscan azi_start azi_finish intervals sample_time scan azimuthal angle

Escan start_E stop_E points sample_time Energy scan

In addition also **tscan**, **dtscan**, **abscan** and **abmesh** scans exist but are not described here.

Please note that a positive value of **sample_time** in all scan types represents counting for the defined time and a negative value represents counting against a monitor, which has to be defined by the **counters** command.

After performing the scan the data of the counter displayed during the scan can be analyzed by the following commands (Note that to display a value a print command has to be added, e.g. **p pl_MIN** or the value has to be given to a variable, e.g. **i = pl_MIN**. Also a motor can be driven to the value **umv tth CEN**):

pl_MIN	smallest measured value (y)
pl_MAX	biggest measured value (y)
pl_xMIN	position (x) of minimum (y)
pl_xMAX	position (x) of maximum (y)
pl_SUM	sum of all measured values (y)
pl_SUMSQ	sum squared of all measured values (y^2)
pl_FWHM	full width half maximum (y)
pl_CFWHM	center of FWHM (y)
pl_COM	center of mass (y)
pl_MINX	minimum (x)
pl_MAXX	maximum (x)
pl_LHMX	upper half-maximum of (x)
pl_UHMX	lower half-maximum of (x)

For convenience **CEN** is identical to **pl_CFWHM**.

4.7 Energy

Here commands related to the monochromator are given. **Warning!** Energies in spec are given in keV and not in eV! Make shure to type **moveE 7.930**, do not forget the dot if you want to go to the gadolinium L_{II}-edge. Do not mix it up with the HASYLAB standart. The 6ID-D Side Station is using a special custom designed monochromator. In addition to the commands mentioned in this section the commands special for the sidestation are described in section 4.11.6.

getE displays the actual energy

moveE energy move monochromator to energy.

setE energy this command recalibrates the monochromator motors. Never use it unless you are really knowing what you are doing

ana_elast value drives the theta and two theta of the analyser (tha, ttha) to the correct positions for the actual energy. For this purpose to the variable **ANALYSER_d_spacing** has to be assigned the correct value. If this is done the analyser will also be moved automatically whenever the energy of the monochromator is changed (also in an Escan (section 4.6)). To omit this assign a value ≤ 0 to **ANALYSER_d_spacing**. If an energy is submitted as an arguement to **ana_elast** the analyser will not be moved but the positions will be calculated and shown. This is for testing purpose

setanalyser calculates lattices constants for different analysers. This is a command only available at the 6ID-D Side Station. Should be self explanatory.

spec is internally working with the wavelength lambda, which is accessible through the global variable **LAMBDA**. With the command **calcE** which is automatically invoked by **moveE**, **getE** and **setE** a new value for **LAMBDA** can be calculated. The Energy in keV can easily be calculated with the global variable **hc_over_e** performing **hc_over_e/LAMBDA** as is done by **getE**.

4.8 Temperature control macros

There are some predefined temperature control macros:

te value reads temperature or sets setpoint if value is supplied

teramp ramps a temperature

These macros are only working if the macros **settemp** and **measuretemp** are defined. For an example to define these macros see the **spec** manual or call your system administrator.

4.9 UB-matrix

List of usefull commands related to the UB-matrix:

4.9.1 Commands from

ca h k l calculate positions for h k l

ubr h k l move to position h k l

wh display h, k, l, tth, th, chi, phi, etc.

pa display geometry parameter

showUB Displays the actual used UB-matrix. Please note that it differs by a factor of 2π from the results of the program rafin, also the matrix was transponated.

enterUB enables you to enter a UB-matrix directly.

setlat sets the lattice parameters of the sample. Is is also possible to set directly the reciprocal lattice parameters with **setrlat**

or0 set actual position to be first orientation reflection

or1 set actual position to be second orientation reflection

setor0 and **setor1** same like the commands **or0** and **or1** but not the actual position is used, you have to enter the position of the reflections manually

or_swap exchange first and second orientation relection set with the commands **or0** and **or1**

savegeo prints all information necessary for UB-matrix or monochromator setup on the screen. The user is responsible for printing this or writing it into the logbook!

save executes **savegeo** and **saveusr** and saves it to hard disk. **saveusr** is normally empty and could for example contain user defined global variables

cuts displays the angles which th, chi and phi will not cross but instead reach the position from the other direction. **cuts name value** will change one of them, **cuts value value value value** will change all four

setmode sets the mode the UB-matrix is working in. Value is stored in variable **g_mode**. For explanation execute command **setmode** or look into the **spec** manual [Spe99]

freeze value Freezes depending on the mode (see **setmode**) one or more angles to the actual value or if parameter value is supplied to the supplied value. This is exspecially usefull if you always want to go to your reflections is one or more angles fixed regardless where the actual position of this angles is. The command is rewoked with the command **unfreeze**. The command **pr_freeze** displays the actual frozen values

setsector value choses a symmetry transformation out of 8 possible transformations, value 0 means no transformation. See the **spec** manual for an detailed explanation [Spe99]

sectors H K L displays all motor positions for all possible sectors

setaz set azimutal reference

startgeo asks for all necessary information, executing the commands **setmode**, **setsector**, **setlat** and **setaz**

cz H0 K0 L0 H1 K1 L1 calculate zone: prints the values of chi and phi needed to put two vectors in the scattering plan

mz H0 K0 L0 H1 K1 L1 move zone: calculates the necessary chi and phi, moves there and then goes into the fixed zone mode (**g_mode = 2**)

sz H0 K0 L0 H1 K1 L1 set zone: calculates the necessary chi and phi and then goes into the fixed zone mode (**g_mode = 2**), freezing chi and phi on these values

calcG calculates the UB-matrix. This routine is normally called by all commands which change the configuration of the UB-matrix, for example **or0** and **or1**

reflex H K L stores the actual position as reflex named H K L in a file. Before the first reflection can be stored command **reflex_beg** has to be executed. After all reflections are stored execute **reflex_end**. Follow the instructions on the screen if you want obtain a new UB-matrix from a fit of these reflections

calcL after a custom made UB-matrix was entered or fitted with the **reflex** commands, **calcL** calculates the lattice parameters for the real and reciprokal lattice from the UB-matrix

The following commands are custom made commands, defined in the file hp_ubm.mac, see 4.11.11.

richt small programm that calculates reflex positions fast and efficient and is in principle self-explanatory, at least if you understand german

theta0 this command reads the information about the two reflections from which the UB-matrice was derived and calculates a correction for two theta and the lattice constant. It works only for cubic systems or if both reflections used pointing in directions with the same lattice constant

ubm_read filename reads a UB-matrix from filename. If filename is not given it will be read from ubfrom.raf. Afterwards UB-matrix will be transposed and multiplicated with a factor 2π to make it workable with **spec**.

For a definition of the UB-matrix see [Bus67].

Small trick if you only plan to do measurements in one direction: Measure two reflections, for example (0 0 2) and (0 0 4) and do a correction with the program **theta0**. Afterwards with the commands **or0** and **or1** use the same reflection (e.g. (0 0 4)) for the UB-matrix, but name it (0 0 4) for **or0** and (0 4 0) for **or1**. Of course you get an error message. Now set one of the variables g_u12 or g_u13, they represent chi and phi of the second reflection, to a value which differs by 90 degree from the original one. You now have created a virtual (0 4 0) reflection. To calculate a new UB-matrix finally execute the command **calcG**. You now have a UB-matrix which should work perfect in the (0 0 4) direction but contains no information about other directions.

4.10 Tips for programmers

Usefull macros that should be loaded at each **spec** session wether or not you are starting fresh can be saved in the file *spec.mac* in the current directory where **spec** is executed or in the file *site.mac* in the specd directory, usually /usr/local/lib/spec.d. In addition site macros which only should be loaded while starting with option fresh should be saved in *site_f.mac*.

Very important for programmers is also the possibility to execute loops, this is done by the command **for**. A short example for doing a mesh-scan manually follows:

```
for (i=20; i<=21; i+=0.1) {
        umv th i
        lup tth -1 1 20 1
        }
```

Also a **while** command using the C-syntax exists.

Very important: When defining macros put the complete macro in a {} surrounding if you want to avoid that local defined variables become global known.

_check0 motor checks if a motor name is valid

move_em is a macro that starts all motor movements with the build in function **move_all**. Before the movement starts the macro **user_premove** is executed and afterwards **user_postmove**. Both are normally emty.

show_cnts reads the scalers and shows the contents but did not count by itself

4.11 Explanation of the different custom made macros

In this section a collection of macros, sorted by the filenames in which they are defined is explained. They are not of general interest for every user but might be usefull for specific tasks. At the 6ID-D Side Station most of these macros are preloaded by the macro site_f.mac which is residing in the home directory of **spec** macros (normally in /usr/local/spec/lib/) at the beamline computer and executed at every fresh start.

4.11.1 hp_fio.mac

This package contains macros which are usefull for people who are familiar with the HASYLAB, DESY program spectra and are using it for their data analysis. The package redefines user entry points supported by the standart.mac package delivered with spec to write fio-files. In addition the following commands have been defined to do the setup of the package:

fio_show_settings shows if the writing of fio files is in use

fio_new_filename this command is used to start creation of fio files or to change the name of the created fio files

fio_new_copy if fio files are created and the beamline computer is able to use ssh (not the case for ID-B) and has an authorized key on another system this command can be used to set up an automatic copying of the fio files to the second computer. Might be usefull as backup or for data analysis

See also section 3.2.3 for an explanation of these commands.

4.11.2 GPIB macros

Normally GPIB and serial input and output is directly supported by **spec**. Because of the problem with the generic EPICS serial and GPIB support it is necessary to have special macros available which allow users a conveniant and consistant way to address external devices. The macros in this section provide the users with the following two commands:

hp_gpib_get address reads a value from a serial or GPIB device. Address is the GPIB address of the device if it is a positive integer, the absolut value of address is the serial address of the device if address is a negative integer. Because **spec** does not support user functions (at least not very easy), the return value will be found in the variable GPIB_val

hp_gpib_put address value writes value to the serial or GPIB device address (see above)

Because of spec problems with the proper handling of **value** which can be a string or a variable it is strongly recommended to use the command in the following way: **dummy = "test1234";hp_gpib_put address dummy** Usage of for example **hp_gpib_put 24 "SETP? 1"** which is a typical command for the lakeshore model 340 will lead to strange error messages. **dummy = "SETP? 1";hp_gpib_put 24 dummy** is the workaround, so only use variables as argument for **hp_gpib_put**.

If only the **hp_gpib_get** and **hp_gpib_put** commands are used macros can be easily interchanged between beamlines. For example hp_SI_controller.mac (section 4.11.3) and hp_lakeshore340.mac (section 4.11.4) only use these two commands to communicate with the devices independent if they are connected to the serial port or the GPIB. A beamline specific macro package than connects these two commands to the actual used serial port or GPIB. Two examples are given, section 4.11.2 for sector 11, BESSRC-CAT and section 4.11.2 for sector 6, μ-CAT

hp_gpib_11id.mac

At BESSRC-CAT a gpib card is used which is supported by **spec**. Thus hp_gpib_11id.mac is very short and the commands **hp_gpib_get** and **hp_gpib_put** are only projected to the **spec** commands. Only a terminating character is added if necessary.

hp_gpib.mac

At the μ-CAT 6ID-B Main Station and 6ID-D Side Station EPICS generic serial and GPIB records are used to communicate with for example temperature controllers. This complicates the communication with devices and made the development of hp_gpib.mac necessary. These macro package supports both the generic serial record and the generic GPIB record. It allows the usage of several GPIB devices at the same time even though only one generic GPIB record is available and handels all necessary changes which have to be made to the generic GPIB record automatically. It has to be configured properly which is normally done by the system administrator. For configuration read the source code in the file hp_gpib.mac.

4.11.3 hp_SI_controller.mac

This is a package for the use of a Scientific Instruments temperature controller. It requires that hp_gpib.mac is loaded first. It is not recommended to use the Scientific Instrument temperature controller in experiments, it is outdated hardware, for example the temperature setpoint can only be changed in 0.1 K steps. This package redefines the macros **measuretemp** and **_settemp** so that the temperature commands supplied by standart.mac (see section 4.8) are working.

4.11.4 hp_lakeshore340.mac

The hp_lakeshore340.mac package is for the use with a lakeshore model 340 temperature controller. It works together with package hp_gpib.mac (see 4.11.2), this package has to be loaded first. It has three main funtions: Change the setpoint and measure the temperatures during the scan. The measurements are done during the scalers are busy with counting, look into the source code for details. Second, write and read sensor calibration curves to and from the lakeshore and third, allow the configuration of importand parameters and allow to save or read them from hard disk.

lakeshore340_help Displays a short help of all commands and also shows the values of global variables used to configure the lakeshore macros.

lakeshore340_config_settemp configures the global variables for the **settemp** macro

lakeshore340_read_curve curve_number filename Reads a curve and displays it. If optional filename is given it will be written to harddisk

lakeshore340_write_curve reads a curve from disk and send it to the lakeshore

lakeshore340_settings option execute program without parameter option, it will show all possible values of mode. Allows to change, save, restore of lakeshore parameters

lakeshore340_set_pid changes PID parameters and heater range

lakeshore340_set_mode changes temperature control mode

lakeshore340_set_control configures control sensor

lakeshore340_set_zone configures one zone of PID parameters

lakeshore340_set_ramp configures ramp parameter

lakeshore340_set_settle configures settle parameters (lakeshore signals with status bit if temperature is stable)

For the **lakeshore340_set_pid** and the **lakeshore340_set_ramp** command parameters can be set up on the command line, just enter the command followed by the appropriate number of parameters (4 and 2).

This short description does not replace the manual of the lakeshore 340 model. Read the manual und use the **hp_gpib_put** and **hp_gpib_get** commands to write your own macros.

4.11.5 hp_move.mac

The hp_move.mac package provides the commands **gmv**, **gmvr**, **ugmv**, **ugmvr**, which are able to drive one to ten motors at the same time. This package might be used to replace the old move commands of standart.mac. For a description of these commands see 4.3.

4.11.6 hp_mono_6idd.mac

The macro hp_mono_6idd.mac provides special commands for operating the 6ID-D Side Station monochromator. These special commands are needed for two reasons: First the 6ID-D Side Station monochromator consists of three monochromator crystal pairs and these macros enable the user to easily exchange them. Second the second monochromator moves over a large distance. If the energy is changed by several MeV a realignemend is necessary.

setmono value This macro replaces the setmono macro distributed with **spec**. The original macro can be found under **_setmono**. With the **setmono** command a monochromator crystal pair can be choosen and spec automatically makes all changes necessary to change the monochromator crystals. If value is the number of a valid monochromator crystal pair the change will be done immidiately, otherwise an interactive menue will be displayed

mono_accept_position energy The 6ID-D Side Station monochromator covers a very large energy interval. The monochromator is working very stable but if big changes in the energy are made the alignement of the monochromator changes a little bit. Once the monochromator has been aligned for a certain energy **mono_accept_position** can be used to calibrate the monochromator to the correct energy. Warning! Do not use the standart **spec** command **setE** for this purpose, it will work for the moment, but the energy calibration of the monochromator will be lost in the long term.

mono_calc_position energy calculates the theoretical positions for the motors monu, mond and montrav for a given energy.

mono_calc_energy_range calculates the energy range which is covered by the actually used monochromator.

mono_show_settings n shows all parameters for the monochromator with number n, if no number is supplied it shows the parameters for the actually used monochromator.

mono_show_all shows all parameters for all available monochromators.

mono_align_crystals This macro aligns the beam on the second monochromator crystal. To do so the second monochromator is moved to several different positions and at each position a scan with the ϑ of the first monochromator crystal is done. The range where these scans are done depends on the energy and the chosen monochromator crystal pair. This macro does not do any data analysis. The user is responsible to analyse the data and to chose a suitable position for the monochromator pairs.

mono_save_values filename all relevant information about all three monochromators is stored in a file named filename on the harddisk. To reset all variables to these values execute this file with the command **qdofile**, for an explanation see section 4.2. These information is also stored on harddisk, whenever for example the command **mono_accept_position** is executed. The files are stored in the subdirectory monochromator in the SPECD directory. This is normally the directory where for example the standart macros of **spec** are placed. To see where this is just type **p SPECD**.

_mono_determine_crystal This macro determines which crystal is actually in use by looking at the position of motor m1_xtal, the crystal changer of the first monochromator and than assigns the number of the crystal to the global variable **mon_num**.

4.11.7 hp_motor_6idd.mac

The commands defined in the file hp_motor_6idd.mac are used to control the special Huber diffractometer if the 6ID-D Side Station. The 2ϑ rotation for the vertical scattering mode of this diffractometer consists of two translations and one rotation. All motors of the 6ID-D Side Station are described in section 2.2. In this macro the movement of the virtual motors described in table 2.1 is implemented. All motor movements are normally done automatically, the following commands are intended for the setup of the diffractometer.

diffractometer_mode_change value Changes the mode in which the virtual motors operate. Mode 0 means no coupling between virtual and real motors, all movements of virtual motors will not affect any real motor. Mode 1 means the diffractometer is in vertical mode and mode 2 means the diffractometer is in horizontal mode. If virtual motors are used in this mode the corresponding real motors will move. See section 2.2 for a detailed description which motors are coupled. If no value is given the command will show the options and ask for a value.

ana_elast see section 4.7

setanalyser see section 4.7

To be able to simulate the vertical 2ϑ rotation three variables have to be set. This is done in the first lines of the file hp_motor_6idd.mac, for the actual values see table 4.1. The variable dist_sample_analyser defines the distance between the sample mounted in the center of rotation of the diffractometer and the analyser. During the simulated 2ϑ rotation this distance will stay constant. The variables zero_tt_y and zero_tt_z define the position of the motors tt_y and tt_z for $2\vartheta = 0$. For tt_y this is the difference between the zero of the encoders and the beam hight, when the beam is going through the center of rotation of the diffractometer. Because in the moment the encoder for motor tt_z is not working the zero position is determined by using a plumb to put the analyser directly above the sample position. Therefore, zero_tt_z and dist_sample_analyser have the same value.

Variable name	value
dist_sample_analyser	924.31
zero_tt_y	5.26
zero_tt_z	924.31

Table 4.1: *Actual values for the variables used for the setup of the virtual 2ϑ movement in vertical scattering geometry*

4.11.8 hp_mca.mac

The Canberra Detector system used at the 6ID-D Side Station is operated through a Canberra computer interface called AIM 556. This AIM controls a digital signal processor (DSP) with integrated support of a multi channel analyser (MCA) and a high voltage (HV) power supply for the detector. There are several MEDM screens available to control the HV power supply and the DSP. In addition a graphical display of the MCA is provided. The setup of the HV power supply and the DSP should be done by experienced staff members. Normally not two many changes should be necessary. Two remarks to operation:

- The DSP can be used in coincidence or anticoincidence mode. It is only counting if the regular counters are running or not running at the same time, respectively.
- it is possible to connect an analog single channel analyser (SCA) to the test output of the DSP, this way the DSP is used as an ordinary amplifier. This makes life a lot easier, because the regular counters can be used.

Warning! hp_mca.mac requires that hp_fio.mac was loaded before hp_mca.mac.

The MCA features are available in **spec**, they are provided by the macro package hp_mca.mac. This package does not use any specific commands of the DSP and therefore should work together with any MCA system supported by EPICS. This package only provides basic features. In the moment the data is only stored in the fio format of Spectra. During counting done with this macro package the display of the MEDM window is not updated. The reason is that updated consume to much time so that not all photons will be collected if the MCA is read out.

mca_count filename time The mca counts for the given time and the result is saved into a file with name filename. Both arguments are optional. If only one argument is given that must be time. If no or only one argument is given the filename is constructed from the variables **MCA_NAME** and **MCA_NUMBER**.

mca_new_filename Use this command to define a filename and a starting number. Whenever the **mca_count** command is used without the optional filename the name defined in here is used. If MCA files are written during scans they will have the name of the fio file with an additional number corresponding to the point in the scan where the MCA spectrum was taken. If no **FIO_NAME** is defined the **MCA_NAME** will be used and the user is responsible to keep track which file belongs to which point and scan.

mca_mode_change number The MCA macro knows three modes:

0 - MCA not in use

1 - MCA in use but only regions of interest (ROI) are read out

2 - MCA in use, at each scan point a MCA spectrum is written to disk

Argument number is optional, if omitted possible arguments are shown and the user is asked for his choice.

mca_energy_calibration With this command the user gets an easy interface to do an energy calibration. In principle nothing more is done then defining four variables, MCA_cal_ch1, MCA_cal_ch2, MCA_cal_ener1 and MCA_cal_ener2. Two channel numbers and the corresponding to energies are needed. For the 6ID-D Side Station a Co_{57} source is a good choice, it has two lines at 122 keV and 136.5 keV.

MCA data files will be automatically copied to the same place like the fio files, see section 4.11.1 for explanation how to copy files.

4.11.9 hp_DAC_vmic4116.mac

The macros in this file control the VMIC 4116 digital analog converter (DAC). This device is a 16 bit DAC which is able to provide voltages in the range from -10 V to $+10$ V.

dac_volt channel value Applies a voltage to one of the eight channels. Channel has to be a value between 0 and 7, value is the voltage between -10 and $+10$

dac_bit channel value Applies a voltage to one of the eight channels. Channel has to be between 0 and 7, value is a bit value between 0 (corresponds to -10 V and 65535 (corresponds to $+10$ V)

dac_init This command initialises the DAC. This command is automatically called by **dac_volt** or **dac_bit** if necessary. It should only be necessary if the VME crate was switched off. Nevertheless this command can be called at any time without doing any harm.

4.11.10 hp_filter_6idd.mac

hp_filter.mac controls the filter. It also calculates the absorption. All values are automatically stored in each scan. It is also possible to calibrate the filters at certain energies and have those calibrated values written into the data files. See section 4.1 for commands for explanation of the **atten** command which controls the filters. In addition there are some more commands in this file which might be usefull:

marshutter word Opens or closes a small shutter built by Peter Hiller which might be very helpfull together with the image plate system. Word has to be replaced by open or close.

absorption Calculates absorption values

filter_calibration This command does an automatic calibration of the filter bank which is actually in use by changing the intensity with detuning the monochromator and moving the filters out of the beam one by one at the same time. This command might not work correctly and is very primitive. It should be replaced as soon as possible with a programm which uses both filterbanks instead of detuning the monochromator.

filter_show_calibration bank Shows if the filter bank with number bank has been calibrated and if this is the case shows the calibration

filter_save_calibration filename Saves the actual calibration of both filter banks in a file named filename. This file can later be executed with the **qdofile** command to regain the stored values

4.11.11 hp_ubm.mac

hp_ubm.mac contains macros which allow you to do some calculations related to the ub-matrix and other usefull stuff. See section 4.9 for details, all commands of this macro are listed in the section with the custom made commands. Originally this macro package was intended to work together with the rafin program which refines UB matrices from a given list of reflections and provide other usefull things related to UB matrices. Unfortunately it was never finished. The only things which are usable right now is the **theta0** command based on an old fortran program from Thomas Brückel which helps to set up a UB matrix from two reflections for cubic systems and the **hp_read_ubm** command which is able to read output from rafin into **spec**. **richt** is a small programm to calculate the positions of reflections written by Oliver Hermann Seeck (unfortunately in German).

4.11.12 hp_mar.mac

The macro hp_mar.mac is a preliminary macro to control the Mar Image Plate Scanner with spec written on November 27th, 2001 during a beamtime at the 6ID-D Side Station. It is not fully tested but it was working during that beamtime and it is only providing very limited support of the features the Mar Image Plate Scanner offers. Feel free to improve it.

Known bugs: Sometimes a command is given by spec and never reaches the Mar Image Plate Scanner. Commands are transfered by the program package ssh which is one ore two times a day not working reliable. Also keep in mind that this package is only working if there is a working and compatible version including public and private key infrastructure on the beamline and image plate control computers. Due to changes in the operating systems of the computers the used ssh and scp commands might have to be modified.

There is one important global variable: **MAR_ON**. If **MAR_ON** is greater then 0 The small shutter build by Peter Hiller will be opend and closed for each counting command.

mar_show_settings Shows the configuration of the Mar Image Plate scanner control variables.

mar_setup Configures the Mar Image scanner control variables.

mar_execute Sends a command to the Mar Image Plate Scanner.

mar_wait_for_imageplate Waits until a command is finished on the Mar Image Plate Scanner.

mar_read Reads and erases the Mar Image Plate Scanner and waits until it is finished and ready for the next exposure.

4.11.13 dw_shutter.mac

dw_shutter.mac written by Didier Wermeille contains the commands **shutter word**, **idbshutter word**, **idcshutter word** and **iddshutter word**. They are used to open the shutters. word has to be replaced by open or close to open or close the shutter, respectively.

4.11.14 dw_pv.mac

This macro package written by Jonathan Lang and Didier Wermeille provides commands to move and scan epics variables, the commands are described in section 4.1.1. On the 6ID-D Side Station a version is running which automatically executes the command **pvdefine** if necessary. On the 6ID-B Main Station if one of the PV macros asks you to execute the command **pvconfig** and you do not want to make changes to the configuration file it is sufficient to execute the command **pvdefine**.

4.11.15 dw_escan.mac

In this macro written by Didier Wermeille the **Escan** command provided within the **spec** package is redefined. During every energy scan the actual Q-position at each energy will be written to the data file. The macros in hp_fio.mac will automatically notice this change and the Q-positions are also written into the fio files.

Chapter 5

Data analysis with spectra

Spectra is a beamline control and data analysis program written by Thorsten Kracht from Hamburger Synchrotronstrahlungslabor at Deutsches Elektronensynchrotron. It is widely used at Institute for Scattering Methods for data analysis because it uses the fio standart for data files defined at Hamburger Synchrotronstrahlungslabor. Therefore, to keep the compatibility with data taken at Hamburger Synchrotronstrahlungslabor it was decided to implement Spectra as the standart data analysis program at the 6ID-D Side Station.

Spectra is installed on all unix mashines belonging to the sidestation. It is not recommended to use it directly on the beamline computer. For use together with data created at the 6ID-D Side Station there are the idduser accounts at idefix.mu.aps.anl.govand mar.mu.aps.anl.gov. For use together with data created at the 6ID-B Main Station there are the useraccounts user at idefix.mu.aps.anl.govand idbuser at mar.mu.aps.anl.gov.

Spectra is only running when a X-connection is available for graphics output. To start spectra enter the command **spectra** in any terminal window.

5.1 Getting spectra to run properly

When Spectra is invoked it automatically reads the file spectra_ini.gra from the actual directory. If this file is not present it tries to read the spectra_ini.gra file from the home directory of the user. In all of the above mentioned accounts a spectra_ini.gra file is present in the home directory. Normally no changes to the spectra_ini.gra file are necessary.

spectra_ini.gra calls a file named set_names.gra which has to be present in the directory from which Spectra was started. In this file it is defined which information of the scans is plotted and what the filenames to look for are.

To get spectra running this file has to be adopted to your setup of **spec**. The first block in this file

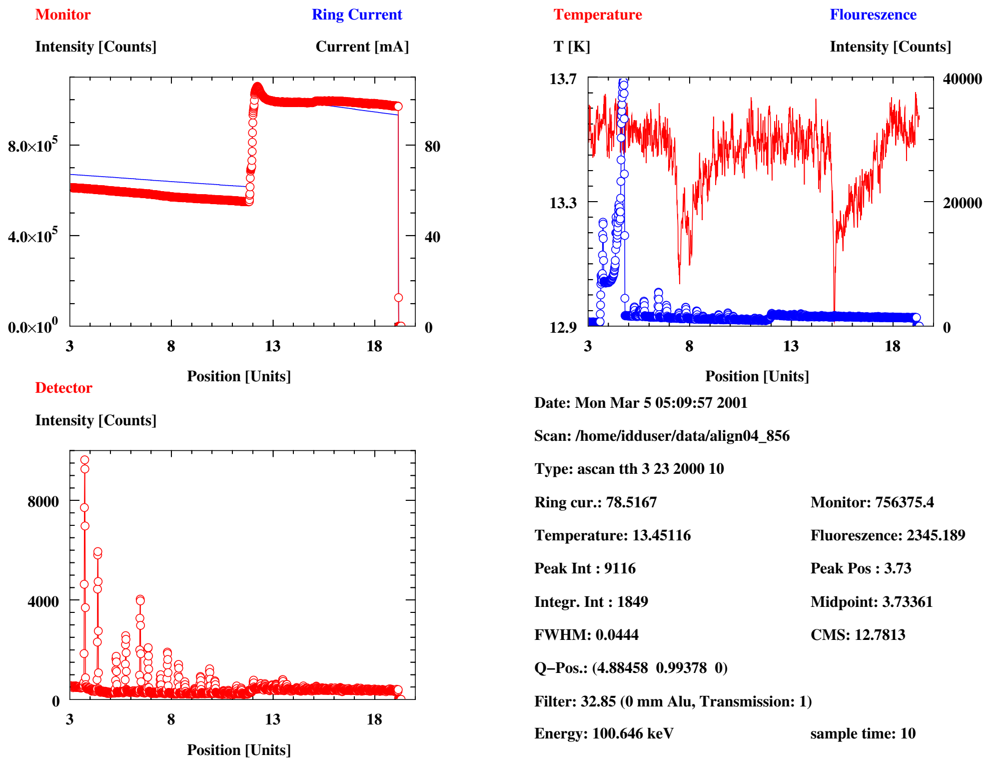

Figure 5.1: *Example for a typical spectra picture of a data set. Here scan align04_856.fio is shown, a* 2ϑ *scan of a Si powder sample measured at* 100 *keV. The detector signal is shown in the lower left corner, the monitor signal and the ring current in the upper left corner and the sample temperature and for example a fluorescence measurement on the right. In addition information about the scan in general, the peak in the detector window and averages of the other for data sets displayed are shown.*

contains definitions which enables the macro to access the data files created during the beamtime.

store_zone $= [[\sim .data]]$ Gives the directory where the fio files are copied from the beamline computer. Please use exactly this notation, $\sim$ marks the home directory of the user so in this example it links to /home/idduser/data/ if idduser is the username. Relative links are not permitted.

filename = **"align04_"** A filename is assigned. Thus files named align04_xxx.fio will be analysed where xxx is replaced by scan_number which is only initialised in set_names.gra and can hold any integer number.

get_zone = "specadm@muhex.mu.aps.anl.gov:/export/home/spec/hp/data/" If a fio file is not present in the directory given by store_zone Spectra tries to copy it from the directory given in get_zone. Here the format is user@computer:directory/, the usual format for the scp command.

In addition five more symbols have to be defined:

detector = det

monitor = mon

current = cur

countera = coa

temperature = DegK_sample

This way the user can chose wich information is displayed in which window. The symbols have to have the exact names given in this example, than the name of a column out of the **spec** data sets is assigned, for example det. If the symbol is not defined nothing will be displayed except a column with the same name exists in the **spec** data sets. Once these definitions are made at the beginning of a beamtime normally no changes are necessary any more.

5.2 Commands usefull for data analysis

Spectra is a very powerfull programm with lots of possibilities to treat data. But it takes some time to get used to its commands. This short manual is in no way intended to replace the Spectra manual which can be found on the Hamburger Synchrotronstrahlungslabor web pages. In this section four commands will be explained which allow even users without any experience to display and print their data to be able to check the progress of their measurements during the experiment.

single xxx displays the scan with number xxx as seen in figure 5.1. If no number is given the scan following the last scan displayed will be shown (single_plot_6idb.gra).

multi xxx multi searches the hard disk for the highest scan number and than waits for the next arriving scan. Once this scan arrives it is displayed and multi waits for the next scan. The program can be aborted by hitting the space key. It is only necessary to supply a number xxx if there are already several thousand scans on the hard disk and you do not want the program wasting time with finding the last number. If xxx is supplied the search starts with xxx (auto_plot_6idb.gra).

hplot the actual content of the graphic window of Spectra is send to the beamline printer (plotit.gra).

settings Shows the actual configuration which was done in set_names.gra as described in section 5.1. This command also shows the status of two more variables: yeslaser and nolaser. The choice of names has historical reasons. If the variable yeslaser is defined (just assign any number at the commandline, for example yeslaser=42) every scan displayed by single or multi will automatically be printed on the beamline printer. If nolaser is not defined (to revoke a definition type nolaser= at the command line), a postscript file will be created for each scan with the same name and in the same directory of the fio files with extension ".ps" (settings_spec.gra).

hilfe This gives a short help and shows some variables (hilfe_spec.gra).

after This command should not be called by users. This is the macro which displays the scans and it is called by **single** and **multi** (after_spec.gra).

All these commands are symbols which are defined in spectra_ini.gra. You can not make changes directly to these programs because on the computers for data analysis they are stored in the directory /home/hupfeld/common/. You have to copy these macros to a directory of your choice and modify them there. All you have to do afterwords is to change the symbol definitions in spectra_ini.gra so that they are now pointing to your directory. Please do not change the spectra_ini.gra file in the home directory. Copy it to your directory and make the changes there. If you start Spectra from your own directory with a spectra_ini.gra file present the one in the home directory will not be read. Same rule applies for the set_names.gra file.

Chapter 6

Using the image plate scanner mar345

This section still has to be written. For a short introduction to the spec software which is able to operate the mar image plate scanner automatically see section 4.11.12.

6.1 Taking your data home

Chapter 7

Alignement of the 6ID-D Side Station monochromator

In this chapter the general procedure to align the 6ID-D Side Station from scratch is described. In this chapter only procedures affecting equipment of the 6ID-D Side Station are described. Before any work is done on the side station it should be assured that the 6ID-B Main Station and its equipment, exspecially the white beam slits and the monochromator are aligned properly. Warning! All alignement procedures described in this chapter should only be executed by staff personal from Forschungszentrum Jülich or μ-CAT, which has been trained to do so. This chapter is not intended for beamline guests. Whenever this text refers to white beam mask or filters the respective equipment of the 6ID-D Side Station is meant and not of the 6ID-B Main Station.

In general the alignement of the 6ID-D Side Station should be performed in same order like it is described in this text. Nevertheless a complete realignement of the beamline might not be necessary in all cases.

Exspecially the alignement of the white beam mask (section 7.1) and the filters (section 7.2) is critical. Any misalignement of those two components can lead to a water leak inside the UHV-vacuum of the windowless main beamline which has to be avoided under any circumstances.

7.1 Alignement of the white beam mask

The first steps in the alignement process of the 6ID-D Side Station are done optically with the fluorescence sreen of the 6ID-B Main Station mounted directly in front of the white beam stop of the 6ID-B Main Station. To make sure that no beamline components are destroyed and the fluorescence sreen is not burned by the white beam the undulator gap has to be opened to at least 40 mm so that only a few Watt of power are produced. As a saftey precausion ask the flour coordinator to set the lower limit of the undulator gap to 40 mm. That way the undulator can not be closed by accident causing serious damage to the beamline.

Next put in the white beam stop in front of the white beam mask. Remove the spacers before putting in the screen controlled by the 6ID-B Main Station computer. The spacers normally prevent the fluorescence screen from being hit by the white beam. The camera looking at the fluorescence sreen has to be realigned because it normally looks at the monochromatic beam of the 6ID-B Main Station, which is 25 mm above the white beam.

Now try to get the white beam through the white beam mask. The filters and the monochromator should be at a position where they do not obstruct the beam (see tables 7.1 and 7.2).

To align the white beam mask the whole first monochromator chamber can be moved horizontally and vertically with the two motors m1_x and m1_y, respectively. The aperture of the entrance side of the white beam mask is 10×20 mm^2 (vertically $\times$ horizontally), the beam is reduced to a maximal size of 2×4 mm^2. The mask should be aligned optically with the help of the above mentioned fluorescence screen. Warning! On the downstream side of the first monochromator chamber is a stand for the beam pipe. This beampipe is directly attached to the first monochromator chamber, therefore the stand has to be disconnected from the beam pipe before the m1_x or m1_y motors are moved. To avoid unwanted movements of those motores the motor drivers are normally switched of. After alignement of the motors you should connect the stand to the beampipe and switch of the motor drivers again.

7.2 Alignement of the filters

Position	F5	F4	F3	F2	F1	Hole
Filter	empty	AlCu	AlCu	Al	Al	
Oct 2000	86.85	68.85	50.85	32.85	14.85	-4.0

Table 7.1: *Position of the water cooled filters in front of the monochromator (filter). There are 5 filter positions, 1 empty, 2 aluminium filter and 2 aluminium copper combinations, seperated by 1 mm. There is an additional hole, where the beam can pass through. The positions in the last line are from the survey done by Peter Hiller in October 2000.*

The first filter, a 1 mm carbon foil is directly attached to the white beam masked and permanently in the beam. In addition either a 1 mm aluminium filter or a combined 1 mm aluminium +1 mm copper filter can be moved into the white beam with a filter changer (filter). To align the filter horizontally the undulator gap should be open as described in 7.1. The horizontal alignement is done optically with the motor filter. The filter is not correctly aligned if any round shapes of the beam are observed on the fluorescence screen. The beam has a squared size after the white beam mask, assuming, that the beam profile is defined by the white beam mask. This is the case if the white beam slits in front of the Kohzo monochromator are wide open. Try to center the filter horizontally. If there is any cut off observed vertically the filters are not mounted at the correct hight with respect to the white beam mask. Warning! Do not proceed. Ask Peter Hiller or Thomas Brückel for advice.

Warning! Under no circumstances should the filter be exposed to the white beam with closed undulator gap if not all filter positions have been aligned correctly and one of the five filter positions is in the beam position. This might lead to serious damage to the beamline and a water leak inside the UHV vacuum. It is strongly recommended that the equipment protection system (EPS) (see chapter 8) is tested after each realignement of the filters.

Warning! Under no circumstances should the first monochromator crystal exposed to the white beam with closed undulator gap if there is no aluminium or aluminium-copper filter in the beam. This might lead to serious damage to the beamline and a water leak inside the UHV vacuum.

7.3 Alignement of the first monochromator crystal

Position	1	2	3
Crystal	(311)	(111)	(331)
October 2000	150.90	102.70	55.305
March 2001	150.65	102.55	55.6

Table 7.2: *Positions of the crystals of the first monochromator (m1_xtal). The maximum of* 3 *monochromator crystals is implemented. The positions in next last line are from the survey done by Peter Hiller in October 2000. The positions in the last line are from the alignement with the x-ray beam from march* 2001*. To move the first monochromator crystal out of the white beam move* 10 *mm in positive direction, for example if the* (331) *crystal is in the beam go to position* 65.6.

Once the white beam mask and the filters are aligned the ϑ-angle and the position of the first monochromator crystals can be aligned. Warning! This procedure has to be done with opened undulator gap. To do so the first monochromator crystal is driven into the beam using motor m1_xtal until roughly halfe of the white beam is cut off. Than motor monu is used until the crystal is parallel to the beam. The crystal is parallel to the beam when a rotation in positive as well as in negative direction leads to a larger cut off of the white beam seen on the fluorescence screen.

In the next step the horizontal position of the first monochromator crystal has to be aligned. To do this use motor m1_xtal to determine the position where the first monochromator cuts off the complete white beam and the position where the whole white beam can pass the crystal. The mean of these two positions gives you the position where the crystal is aligned in the center of the white beam.

This procedure has to be repeated for all three monochromator crystals. When this is finished the fluorescence sreen has to be pulled out of the beam and the spacers have to be put back into place so that the white beam cannot hit the fluorescence sreen any more. In addition the camera has to be realigned to look at the monochromatic beam of the 6ID-B Main Station, the position is 25 mm above the white beam.

The alignement procedures requiring an opened undulator gap are finished, the 6ID-D Side Station is now able to withstand the full heatload of the undulator. All the following steps should be executed for one of the three monochromator crystal pairs. Once one crystal pair is fully aligned the procedure should be repeated two times for the other two monochromator crystal pairs.

To proceed close the undulator gap to a value around 15 mm to 20 mm. The next task is to find the reflected beam from the first monochromator on the fluorescence screen behind the second monochromator. This fluorescence screen is operated through the small TV-system positioned close to the beamline computer. The fluorescence screen can be moved in controlled by an electro magnet. The camera is only operating while the corresponding switch on the TV-system is manually hold down. This is necessary, because the cameras cooling system is not sufficient in vacuum so the camera can only be operated for short time periods.

Move the second monochromator crystal to a position, where it is not in the beam (see table 7.3 and rotate it so that it is parallel to the beam, that means move motor monu to $2 \times \vartheta$. You should position the second monochromator chamber (motor montrav) somewhere in the middle of the railsystem, I usually used the value -2239.54. Use the command **mono_calc_position** to calculate the position of the motors monu, mond and montrav.

Now the reflected beam from the first monochromator has to be found. The fluorescence screen behind the second monochromator has to be put in and the camera switched on. Look for the beam a few degrees around the calculated ϑ angle of the first monochromator. If no beam is found, the chi angle of the first monochromator (motor m1_chi) has to be changed in 0.5 degree steps and the search has to be repeated. Once the beam from the first monochromator crystal has been found align with the motors monu and m1_chi that it is easily visible in the middle in the fluorescence screen.

The next step is to align the ϑ angle of the second monochromator crystal. Move motor m2_xtal until roughly half of the beam is cut of by the second monochromator crystal. This position is of by several millimeters from the positions given in table 7.3, because the beam from the first monochromator crystal is not in the correct position right now, this will be done later. Now align ϑ rotation of the second crystal in the same way as described in section 7.3 for the first monochromator crystal. But the aligned value now corresponds to two times your calculated ϑ value.

Now a precise alignement of the motor m1_chi has to be done. Move the beam up with this motor until you see a sharp edge in the beam profile which is still cut off by one half from the second monochromator. Move m1_chi until this sharp edge is in the middle of the beam. This sharp edge belongs to the crystal holder of the second monochromator crystal and gives you the upper and lower end of the 5 mm wide crystal. Now move the beam down and repeat the procedure. After both positions have been determined move the beam to the mean of the two positions, this is the final position for m1_chi.

Finally ϑ of the first monochromator crystal has to be aligned. For that reason align the second monochromator crystal (motor m2_xtal) that it cuts of exactly half of the beam. Now move the beam with motor monu a few hundrets of a degree that way that it is still fully visible on the fluorescence screen and align the second monochromator again in the center of the beam. Now you can calculate the relation between movements of m2_xtal and monu. Move m2_xtal to the last known position (see table 7.3) and calculate where you have to move monu and move monu to this position. The first monochromator crystal is now aligned, a fine tuning will be done lateron. On the fluorescence screen the direct beam from the first crystal might be seen on the edge of the sreen. This is normal and depends on the position of montrav. If montrav is close to zero (it is not recommended to do the alignement at this position) the direct beam should be fully visible at one side of the fluorescence screen.

7.4 Alignement of the second monochromator crystal

Position	1	2	3	4	5
Crystal	empty	test crystal	(311)	(111)	(331)
October 2000	194.68	164.68	134.68	104.68	74.68
March 2001			128.95	98.8	70.5

Table 7.3: *Positions of the crystals of the second monochromator (m2_xtal). A maximum of* 5 *monochromator crystals can be implemented.* 3 *crystals, matching the crystals of the first monochromator are implemented, one position is empty and one test crystal* ((111)) *is mounted. The positions in the next line are from the survey done by Peter Hiller in October* 2000*. The positions in the last line are from the alignement with the x-ray beam from march* 2001*.*

To find the reflected beam from the second monochromator crystal is straight forward because the fluorescence screen is very close to the crytsal and therefore it should only be necessary to scan motor mond. Once the beam is found the fluorescence screen can be taken out and the beam should be observable in the 6ID-D hutch. It might be necessary to optimize the undulator gap to get sufficient intensity from the diode.

If major work has been performed, for example the second monochromator crystals have been replaced it might be necessary to either scan m2_chi to adjust the height of the beam or to move m2_xtal to adjust the horizontal position of the beam. In the second case remember to adjust motor monu by the calculated dependence between monu and m2_xtal as described in section 7.3.

Once you have beam inside the hutch scan motor monu to make sure the maximum intensity is getting through. Now there is monochromatic beam inside the 6ID-D Side Station.

Now the fine tuning of the crystal positions has to be done. Make sure all slit systems in front of the first diode in the 6ID-D hutch are completely opend and all collimators are removed. Start macro **mono_align_crysals**. This command starts a macro which measures the beam position on the second crystal by changing ϑ of the second crystal and doing a rocking scan with the first crystal. That way the bragg angle for the first crystal is determined under which the bragg condition for both crystals is fullfilled and the beam hits the second crystal in the center. The data of the performed scans has to be analysed externally, for example with the programm Spectra.

The beamposition in the hutch can be aligned in a similar way. Position a slit system that defines the beamposition in front of the pin diode. Now run scans where the position of the second monochromator crytal (motor m2_xtal) is moved by a few millimeter, adjust the ϑ value of the first monochromator crystal accordingly and do a rocking curve with the second monochromator crystal. This will move the beam horizontally inside the hutch therefore it can be moved to the position it is supposed to be. After this alignement macro **mono_align_crysals** has to be repeated to make sure the beam is still centered on the second monochromator crystal.

This complete procedure has to be repeated for the other two monochromator crystal pairs.

Chapter 8

Equipment Protection System (EPS)

The equipment protection system (EPS) protects the components of the undulator beamline 6ID of damage by monitoring the state of all necessary components. Most of the components belong to the 6ID-B Main Station or both stations. In this chapter only a brief overview of the components of the side station which are protected by the EPS is given. The EPS itself should only be operated by staff personnal therefore this chapter is not intended to give an introduction.

I:7/0	0	Filter Position	Filter Position
I:7/1	1	Love Controller 1	Water cooling filter
I:7/2	2	Love Controller 2	Water cooling mask
I:7/3	3	Love Controller 3	Water cooling Monochromator crystal 1
I:7/4	4	Love Controller 4	Temperature downstream side of white beam mask
I:7/5	5	pressure gauge 1	pressure monochromator tank 1
I:7/6	6	pressure gauge 2	not used
I:7/7	7	pressure gauge 3	pressure monochromator tank 3

Table 8.1: *List of the inputs for the EPS. The first row shows the internal number of the inputs used by the EPS Computer. The input controller used for the 6ID-D Side Station equipment has* 32 *channels, the channels used are shown in the second row.*

In the moment there are seven inputs to the EPS from the sidestation as listed in table 8.1.

- The filter position is checked to prohibit the white beam hitting and melting pieces of the filter changer. Whenever the filters are moved (Warning! This is only permitted while the beamshutter is closed) the EPS will trigger an alarm and therefore has to be reset afterwords. This will be changed in future program versions. In case of an alarm the beamshutter will be closed.

- The water flow rates of the cooling of the white beam mask, filter and first monochromator crystal are monitored. In case of an alarm the beamshutter will be closed.

- The pressure of the first monochromator tank is monitored. In case of an alarm the valves around the first monochromator tank will be closed. This automatically triggers the closing of the beamshutter.

- The pressure of the second monochromator tanl is monitored. A vacuum leak in the second monochromator tank may cause problems with the movement of the second monochromator chamber because the flexible bellows connected to the second monochromator chamber might be damaged in that case. Therefore, the beamshutter is closed to alarm the operator.

B3:8/5	B3/133	fault_love_side_1
B3:8/6	B3/134	fault_love_side_2
B3:8/7	B3/135	fault_love_side_3
B3:8/8	B3/136	fault_love_side_4
B3:2/8	B3/040	IG5_A_Fault
B3:2/9	B3/041	Fault_Vac_side_2
B3:1/4	B3/020	Filter_Fault

Table 8.2: *Internally used binary registers by the EPS computer.*

The tables 8.2 and 8.3 are included for completeness for the case that changes to the EPS program have to be made by staff personal.

O:5.1/08	O:5/024	Fault_love_S1_live
O:5.1/09	O:5/025	Fault_love_S1_latch
O:5.1/10	O:5/026	Fault_love_S2_live
O:5.1/11	O:5/027	Fault_love_S2_latch
O:5.1/12	O:5/028	Fault_love_S3_live
O:5.1/13	O:5/029	Fault_love_S3_latch
O:5.7/10	O:5/122	Fault_filter_live
O:5.7/11	O:5/123	Fault_filter_latch
O:5.7/12	O:5/124	IG5_A_Fault_live
O:5.7/13	O:5/125	IG5_A_Fault_latch
O:5.7/14	O:5/126	Fault_vac_side2_live
O:5.7/15	O:5/127	Fault_vac_side2_latch

Table 8.3: *Internally used output registers by the EPS computer.*

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Bibliography

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