3rd sardana Workshop Feedback from scientists, DESY

3rd sardana Workshop

Dr. Sonia Francoual October 6th, 2015





Outline

- Resonant Scattering and Diffraction beamline P09
- Experimental control at P09
- Feedback from scientists at PETRA III



P09: Resonant scattering and diffraction beamline

heat load

46.5

DCM

Undulator

(optional)

Phase

P09 - OH

51.0 52.3 54.4

1 optics hutch P01 Monochromator: DCM Si-(111)/(311) P02 / P03 Energy range: 2.7 - 24 (50) keVP04 Flux at 10 keV: 2x10¹³ counts/sec P05 / P06 Focus size (moderate): 140 x 40 μm² (mirror) P07 $40 \times 4 \mu m^2$ (compound refractive lenses) (small): P08 / P09 Variable incident polarization: double phase plates, linear/circular P10 < 1 eV, <0.3 eV Energy resolution: P11 P12-14 2 experimental hutches P09 Optic hutch **P08 EH** P09 EH1 P09 EH2 P09 EH3 High HR mono Diffractometer Diffractometer



HAXPES

- EH3

93.0

84.6 86.5

CRLs

P09 - EH1

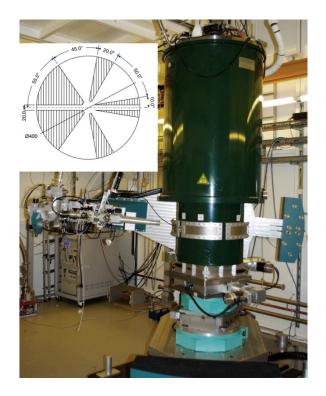
72.6 74.8 76.7

P09: Resonant scattering and diffraction beamline

EH1: High precision "4S+2D" 6circle diffractometer



 EH2: non-magnetic heavy-load 6-circle diffractometer in horizontal Psi geometry



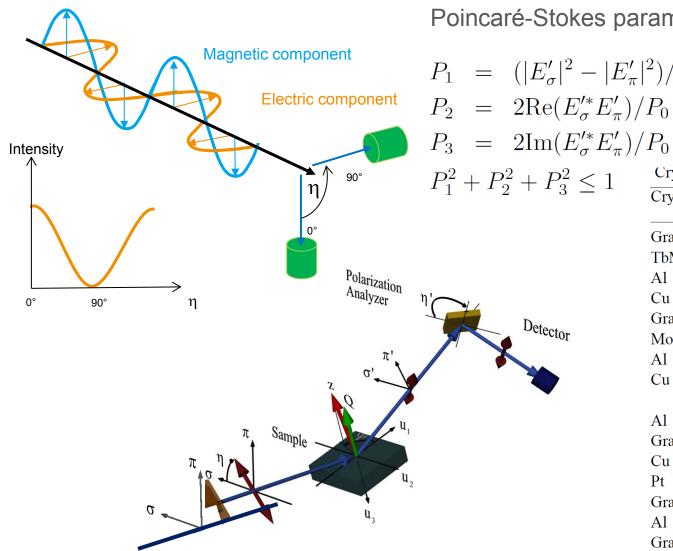


P09: Typical experiment

- Select an energy (monochromator = master device) and focus size; Energy determines mirror cut-off and settings, phase retarder crystals which to use, analyzer crystals which to use, angular access in reciprocal space, attenuation factor of attenuator foils, CRLs combination, ... (the slave devices)
- Mount the sample and orient it (2 Bragg peaks defining directions in reciprocal space)
- Search for magnetic / charge order / superlattice peaks in reciprocal space at temperatures of interest
- Probe behavior of those peaks upon applying temperature / magnetic field / pressure / electric field
- Probe behavior of those peaks upon varying azimuthal / angle of incident linear polarization / incident energy for the purpose of magnetic structure determination



P09: Polarization analysis



Poincaré-Stokes parameters:

$$P_{1} = (|E'_{\sigma}|^{2} - |E'_{\pi}|^{2})/P_{0} = (I_{\sigma'} - I_{\pi'})/I_{0}$$

$$P_{2} = 2\operatorname{Re}(E'_{\sigma}E'_{\pi})/P_{0} = (I_{+45^{\circ}} - I_{-45^{\circ}})/I_{0}$$

$$P_1^2 + P_2^2 + P_3^2 \le 1$$

 $P_1^2 + P_2^2 + P_3^2 \le 1$ Crystals available for polarization analysis from $\frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} = \frac{1}{2} = \frac{1}{2} + \frac{1}{2} = \frac{1}{2$

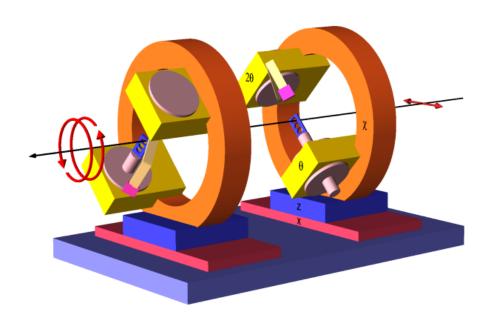
Crystai	(II K I)	u (A)	E (90) (Ke)
Graphite	(0 0 2)	3.358	2.61
TbMnO ₃	$(0\ 2\ 0)$	2.928	2.99
Al	$(1\ 1\ 1)$	2.338	3.75
Cu	$(1\ 1\ 1)$	2.084	4.21
Graphite	$(0\ 0\ 4)$	1.679	5.22
Mo	$(2\ 0\ 0)$	1.574	5.57
Al	$(2\ 2\ 0)$	1.432	6.12
Cu	(2 2 0)	1.276	6.84
Al	(2 2 2)	1.169	7.50
Graphite	$(0\ 0\ 6)$	1.119	7.83
Cu	$(2\ 2\ 2)$	1.042	8.41
Pt	$(4\ 0\ 0)$	0.981	8.94
Graphite	$(0\ 0\ 8)$	0.839	10.44
Al	$(3\ 3\ 3)$	0.779	11.25
Graphite	$(0\ 0\ 10)$	0.671	13.05

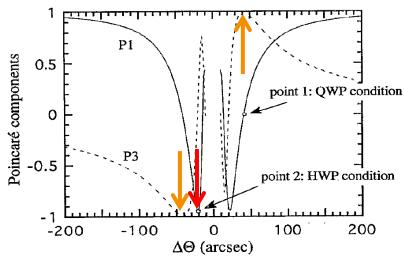


P09: variable incident polarization

Circular polarization in energy range between 2.7 – 14 keV using

 \rightarrow thin Si-plates (5 - 10 μ m): 2.7 - 3.2 keV \rightarrow diamond plates (100 - 900 μ m): 3.2 - 14 keV



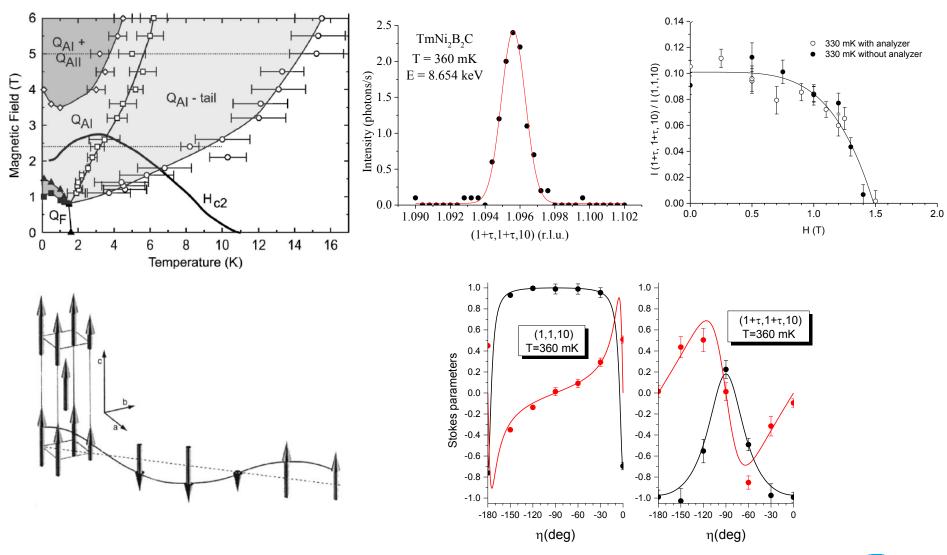


$$\Delta \Phi = -\frac{\pi}{2} \frac{r_e^2 \lambda^3 \operatorname{Re} \left[F_h F_h^{-} \right] \sin(2\theta) t}{\left[\pi V \right]^2 \Delta \Theta} \sim \frac{t}{\Delta \Theta}$$

Variable linear polarization between 3.2 – 12 keV



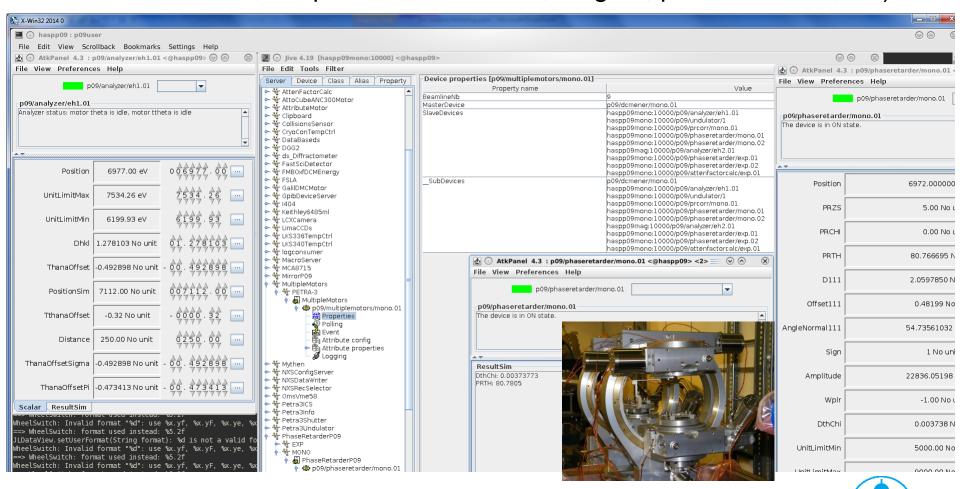
P09: example of outputs





P09: Experimental Control: Tango

> Tango servers for all devices (motors, counters, mirrors, monochromator, temperature controllers, magnet, phase retarder,)



P09: Experimental Control: several Tango database

> Two hutches: same motor names in the different hutches: two six-circles diffractometer (theta, del, gamma, mu, chi, phi, diff_height, diff_pitch, diff_x): a problem for spock, two motors can not have same name in the pool => split Tango database (3 beamline computers, 3 Tango database, 3 separate spock sessions)

> Specify the hostname for every device in the online.xml file (allows it to have devices from one hutch used in the spock session of another

hutch)

haspp09 : optics hutch + EH1

haspp09mag : EH2

haspp09dif : simulations

```
<name>s5dx</name>
<type>type tango</type>
<module>motor tango</module>
<device>p09/vmexecutor/dif.02</device>
<control>tango</control>
<hostname>haspp09dif:10000</postname>
</device>
<name>qbpml_position_x</name>
<type>counter</type>
<module>tangoattributectctrl</module>
<device>p09/i404/mono.01</device>
<control>tango</control>
<hostname>haspp09mono:10000</hostname>
</device>
<name>mag c01</name>
<type>counter</type>
<module>sis3820</module>
<device>p09/counter/mag.01</device>
<control>tango</control>
<hostname>haspp09mag:10000</hostname>
```

P09: Experimental Control: online.xml file

- Define all devices (motors, virtual motors, diffractometer controller, counters,) in the online.xml file
- Example : motors / virtual motors / diffractometer controller :

```
<!-- motors -->
<device>
 <name>del</name>
 <type>stepping motor</type>
 <module>oms58</module>
 <device>p09/motor/dif.13</device>
 <control>tango</control>
 <hostname>haspp09dif:10000</hostname>
</device>
<!-- virtual motor -->
<device>
 <name>ptth</name>
 <type>type tango</type>
 <module>motor tango</module>
 <device>p09/vmexecutor/dif.08</device>
 <control>tango</control>
 <hostname>haspp09dif:10000</hostname>
</device>
<!-- diffractometer controller -->
<device>
 <name>e6cctrl</name>
  <hkl>mu = motor/diffracmu mag/1, omega = 4, chi = 5, phi = 6, delta = 13, gamma = 14, crystal = /home/p09user/
crystals/defaultcrystal.txt, energydevice=haspp09mono:10000/p09/multiplemotors/mono.01</hkl>
  <module>PETRA3 P09 EH2</module>
  <type>diffractometercontroller</type>
  <device>haspp09dif:10000/p09/motor/dif.04</device>
  <control>tango</control>
  <hostname>haspp09mag:10000</hostname>
```

Stop / restart Sardana when changes in the online.xml file or new library to be taken into account: SardanaAlO.py –x



P09: Experimental Control: online.xml file

Define all Tango attributes that we want to have in the headers of the scans or as outputs of the scans as virtual counters in the online.xml file

```
<!-- example of virtual counters, motor positions -->
<device>
 <name>del position</name>
 <type>counter</type>
 <module>tangoattributectctrl</module>
 <device>p09/motor/dif.13</device>
 <control>tango</control>
 <hostname>haspp09dif:10000</hostname>
</device>
<!-- example of virtual counters, diffractometer position in reciprocal space -->
<device>
 <name>h position</name>
 <type>counter</type>
 <module>tangoattributectctrl</module>
 <device>pm/e6cctrl/1</device>
 <control>tango</control>
 <hostname>haspp09mag:10000</hostname>
</device>
<!-- example of virtual counter, 14T magnet -->
<device>
 <name>magnet14tf tempheatexchanger
 <type>counter</type>
 <module>tangoattributectctrl</module>
 <device>p09/magnet/exp.01</device>
 <control>tango</control>
 <hostname>haspp09mag:10000</hostname>
</device>
<!-- example of virtual counter, virtual executor -->
<device>
 <name>sumvfcs counts</name>
 <type>counter</type>
 <module>counter tango</module>
 <device>p09/vcexecutor/exp.02</device>
 <control>tango</control>
 <hostname>haspp09mono:10000</hostname>
</device>
```



P09: Experimental Control: online.xml file

- Define all measurement groups in the online.xml file
- Define which variables to be plotted by the SardanaMonitor (ExpConf mostly used to change headers (new variable))

```
<device>
 <name>mg magpilatus</name>
 <mgs>timers = exp t01, mag t01, counters=mag c01 -d, pilatus roi1 -d, pilatus roi2 -d, pilatus roi3 -d,
pilatus imaxx -d, pilatus imaxy -d, mag vfc01 -d, exp vfc01 -nd, petra beamcurrent -nd, abseh2 position -nd,
abseh2 attenfactor -nd, roiltimesattenfactoreh2 -d, roi2timesattenfactoreh2 -d, h position -nd, k position -nd,
l position -nd, del position -nd, th position -nd, ga position -nd, mu position -nd, chi position -nd,
phi position -nd</mgs>
 <type>measurement group</type>
 <module>None</module>
 <device>None</device>
 <control>tango</control>
 <hostname>haspp09mag:10000</hostname>
</device>
<device>
 <name>mq xmcd</name>
 <mgs>timers = exp t01, mag t01, counters=exp vfc01, exp vfc02, exp vfc03, sumvfcs counts, petra beamcurrent,
dac voltage, pr1th position, pr1chi position, pr2th position, pr2chi position, tga channel, tga frequency,
tga amplitude, xmcd mirrordelay1, xmcd mirrordelay2, xmcd i0plus1, xmcd i0plus2, xmcd i0minus1, xmcd i0minus2,
xmcd iOplus, xmcd itplus, xmcd iplus, xmcd iOminus, xmcd Itminus, xmcd Iminus, xmcd intensity, xmcdxas counts,
xmcddiff counts </mas>
 <type>measurement group</type>
 <module>None</module>
 <device>None</device>
 <control>tango</control>
 <hostname>haspp09mag:10000</hostname>
</device>
<device>
 <name>mg he3</name>
 <mgs>timers = exp t01, mag t01, counters=mag c01 -d, mag vfc01 -nd, mag vfc02 -nd, exp vfc01 -d, exp vfc02 -nd,
<mark>sumvfc</mark>s counts -nd, petra beamcurrent -nd, abseh2 position -nd, abseh2 attenfactor -nd, h position -nd,
k position -nd, l position -nd, magnet14tf persistentfieldt -nd, magnet14tf correctedprobe -d,
magnet14tf tempprobe -d, magnet14tf mainsorb -nd, magnet14tf minisorb -nd, magnet14tf tempheatexchanger -nd</mgs>
<type>measurement group</type>
```



```
o09/door/haspp09mag.01 [4]: setmg
[0] mg he3
[1] mg magapd
[2] mg magpilatus
   mg nurvfcs
[4] mg xmcd
Your choice [0]? 1
Active measurement group: mg magapd
p09/door/haspp09mag.01 [5]: anasetup
6.97199843767 1.77831652013
List of polarization analyzers available at P09:
 (1) Al100
  (2) Al110
  (3) All11
 (4) Al203100
  (5) Au 111
  (6) Cu 100
  (7) Cu110
  (8) Culll
  (9) Dy001
  (10) Ge100
  (11) Ge110
  (12) Gelll
  (13) LiF100
  (14) LiF110
  (15) Mg0110
 (16) Mg0111
  (17) Mo100
  (18) Pd110
 (19) Pt100
  (20) Pt110
  (21) PG001
 (22) Sil00
  (23) Sill0
 (24) Silll
 (25) TbMn03020
 (100) Analyser is not listed
Which polarization analyzer are you using ? 7
Cu (2,2,0): [6.241,7.605] keV
The calculated centered position for pth is: 44.08.
43.5 44.0819196321
Did you center the analyzer (y/n) ? n
```

- Spock : interface between user support and Tango servers for setting up experiment
- Online commands only (no click in jive, minimize number of opened windows / ATK panels) → Sardana Macros & interactive mode (iMacro)

```
p09/door/haspp09mag.01 [13]: mirror drive 2.65 1
Configuration 1 (Focus in EH1 (2.65 mrad, 11.5 keV)& EH2 (2.13 mrad,
Mirror offset: 10.95
Mlx: 39.101
M2x: 39.25
Mly: -3.64
M2y: -3.34715
Mlpitch: 1.7675
M2pitch: 1.7225
EH1, diaz:
                   10.94715
EH1, table height: 10.94715
EH2, table height: 10.94715
EH2, graz: 10.94715
EH2, diff height: 10.94715
Beamline components will be moved now to the above positions
and reset the attribute DiffHeightFlat from 10.94715 to 10.94715
Do you really want to proceed (y/n) [n]?
p09/door/haspp09mag.01 [14]: eslave
Possibilities: no slave device (0)
                undulator
                prcorr
                PR2
                analyzer EH2
                               (64)
                              (128)
                attenfactor
New setting [34]?
```

- Spock : scripting of macros by beamline staff and fs-ec group (Teresa)
- Different levels of scripting: communication to Tango servers (set_temp, mirror_drive) read/write only to more complicated computing (anasetup, virtual executors and motors,...)

```
925 class peak(Macro):
926
927
            move to center of scan
928
929
930
        param def = [
931
932
933
934
        def run( self):
935
            self.mvsa("peak".0)
936
937 class set335 xmcd(Macro):
938
939
             set335 xmcd
940
941
942
        param def = [
943
            ['setpoint', Type.String, "", 'Setpoint']
944
945
946
       interactive=True
947
948
        def run( self,setpoint):
949
            if setpoint != -999:
950
                self.lk335 = PyTango.DeviceProxy("haspp09mag:10000/p09/qpib/mag.14")
951
                setp="SETP 1 "+setpoint
952
                self.output("setpoint = %s K" % setpoint)
953
                self.lk335.GPIBWrite(setp)
954
955
            else:
956
                self.output( "Usage: set335 xmcd setpoint")
```



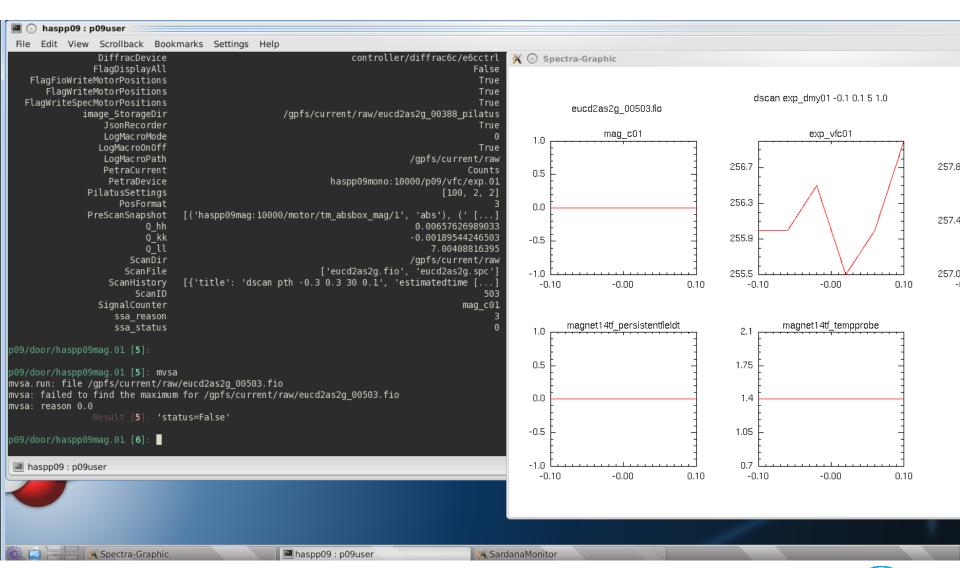
- Spock : scripting of macros by beamline staff and ec group (Teresa)
- Different levels of scripting : communication to Tango servers (set_temp, mirror_drive) read/write only to more complicated calculations (anasetup)

```
spacegroupnumber=float(SPLIT[11])
 009/door/haspp09mag.01 [5]: anasetup
                                                                                   special=SPLIT[12]
6.97199843767 1.77831652013
                                                                                   IN TABLE.close()
                                                                 89
List of polarization analyzers available at P09:
                                                                                   #Define here a function that calculates and returns the lattice spacing for t
 (1) Al100
                                                                                   def calcdhkl(h, k, l):
 (2) All10
                                                                                          if symmetry == "cub":
 (3) All11
                                                                 93
                                                                                                  dhkl2inv = (h*h+k*k+l*l)/(a*a)
 (4) Al203100
                                                                                          elif symmetry == "tet":
 (6) Cu 100
                                                                                                 dhkl2inv = (h*h+k*k)/(a*a)+(l*l)/(c*c)
 (7) Cu110
                                                                                          elif symmetry == "ort":
 (8) Culll
                                                                                                 dhkl2inv = (h*h)/(a*a)+(k*k)/(b*b)+(l*l)/(c*c)
 (9) Dy001
                                                                                          elif symmetry == "rho":
 (10) Ge100
                                                                                                 n = ((h*h+k*k+l*l)*pow(math.sin(alpha),2.0)+2.0*(h*k+k*l+h*l)*(
 (11) Ge110
                                                                100
                                                                                                 d = a*a*(1.0-3.0*pow(math.cos(alpha),2.0)+2.0*pow(math.cos(alpha))
 (12) Gelll
                                                                101
                                                                                                 dhkl2inv = n/d
 (13) LiF100
                                                                102
                                                                                          elif symmetry == "hex":
 (14) LiF110
                                                                103
                                                                                                  dhkl2inv = (4.0/3.0)*(h*h+h*k+k*k)/(a*a)+(l*l)/(c*c)
 (15) Mg0110
                                                                104
                                                                                          elif symmetry == "monoclinic":
 (16) Mq0111
                                                                                                  dhkl2inv = ((h*h)/(a*a)+(k*k*pow(math.sin(beta),2.0))/(b*b)+(l*a)
 (17) Mo100
                                                                    in(beta), 2.0)
 (18) Pd110
                                                                106
                                                                                          elif symmetry == "triclinic":
 (19) Pt100
                                                                                                  V=a*b*c*math.sqrt((1.0-pow(math.cos(alpha),2.0)-pow(math.cos(be
                                                                107
 (20) Pt110
                                                                    )*math(cos(beta))*math.cos(gamma)))
 (21) PG001
                                                                108
 (22) Sil00
                                                                                                 n1=pow(h*b*c*math.sin(alpha),2)+pow(k*a*c*math.sin(beta),2)+pow
                                                                109
 (23) Sill0
                                                                                                 n2=2*h*k*a*b*c*c*(math.cos(alpha)*math.cos(beta)-math.cos(gamma
 (24) Silll
                                                                110
                                                                                                 n3=2*k*l*a*a*b*c*(math.cos(beta)*math.cos(gamma)-math.cos(alpha
 (25) TbMn03020
                                                                111
                                                                                                 n4=2*h*l*a*b*b*c*(math.cos(alpha)*math.cos(gamma)-math.cos(beta
 (100) Analyser is not listed
                                                                112
                                                                                                  dhkl2inv=(n1+n2+n3+n4)/(pow(V,2.0))
                                                                113
                                                                                          else:
Which polarization analyzer are you using ? 7
                                                                114
                                                                                                  self.error("Lattice system not specified for this analyzer. Che
                                                                    exiting")
Cu (2,2,0): [6.241,7.605] keV
                                                                115
                                                                                                  return
The calculated centered position for pth is: 44.08.
                                                                116
                                                                                          dhkl = 1.0 / math.sqrt(dhkl2inv)
43.5 44.0819196321
                                                               117
                                                                                          return dhkl
                                                               118
                                                                                   dhkl=calcdhkl(hh,kk,ll)
Did you center the analyzer (y/n) ? n
                                                               110
```

- > Spock : interface between users and their experiment
- > Spec-like macros : (or0, or1, br, wh, set_temp, drive_field,...),
- Users have usually only a few of those commands to learn to manage their experiments
- > Typical scans: scans of diffractometer angles (dscan del -0.3 0.3 30 0.5, lscan 0.4 0.6 100 5) and energy (escan 6952 7952 100 1 fixq)
- > Scan analysis primordial! After scan, send scanned device to position of maximum intensity in the scan, or center of mass, or position of dip,:
 - command mvsa in spock
 - Environment variable : SignalCounter



P09: Experimental Control: spock (scan analysis)





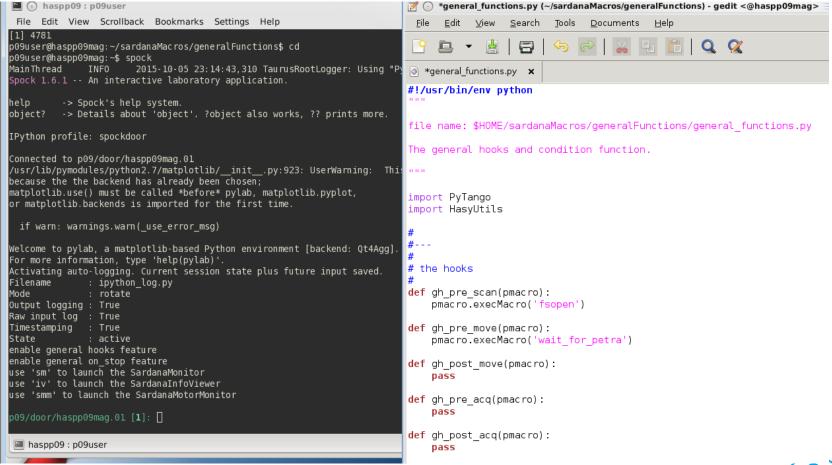
Typical macros imply loops: pol-scan, T-dep, ... (templates adapted by users to their needs)

```
class tdep(iMacro):
     def run(self):
          self.dscan("zs",-1.5,1.5,20,3)
          self.dscan("sperp", -1.2,1.2,20,3)
          for tt in np.arange(2.5,8.1,0.5):
             self.execMacro("set temp vti",tt)
             self.execMacro("wait",300)
             self.execMacro("gosigma")
             self.execMacro("ubr",0.00070 , 0.00030 , 4.50250 )
             self.dscan("th", -0.5,0.5,50,3)
             self.dscan("ga", -0.4,0.4,40,3)
             self.ascan("e6cctrl l",4.45,4.55,60,3)
             self.execMacro("ubr",0.00070 , 0.00030 , 4.50250 )
             self.execMacro("gopi")
             self.ascan("e6cctrl l",4.45,4.55,60,3)
             self.execMacro("ubr",0.00070 , 0.00030 , 4.50250)
          self.execMacro("gosigma")
          self.dscan("zs",-1.5,1.5,20,3)
          self.dscan("sperp", -1.2,1.2,20,3)
          self.execMacro("set temp vti",2)
class polanalysis(iMacro):
     def run(self):
         for mypeta in range(30, -121, -15):
                self.umv("peta",mypeta)
                self.dscan("pth", -0.3, 0.3, 30, 0.5)
                self.cen()
                self.dscan("ptth",-1,1,20,0.5)
                self.cen()
                self.dscan("pth", -0.3, 0.3, 30, 0.5)
                self.cen()
class moveinplates(iMacro):
     def run(self):
```



P09: Experimental Control: spock (general hooks)

In the case of beam loss, check for value of petra3 current at every point of the scan and wait that beam is back (wait_for_petra macro); needed for all scans → general hook functions + start_up file



Feedback from scientists at PETRA III: what we like

- spock: python-base programming language (friendly as compared to spec, perl or gra but for the indent)
- Measurement groups very easy to manage (w/ or w/o expconf)
- > Environment variables
- Scan analysis (desy)
- General hooks (desy)
- Diffractometer controllers (desy, p09)





Feedback from scientists at PETRA III: what we don't like

- Frequent restarts of macroserver
- Time outs (P08): "try" "except" otherwise macro interrupted and one full night of measurements lost; time-out occurs at one point of the scan, next point should be recorded (set error off);
- Scripting of macros unfriendly to users: self.execMacro?? Users want to type in their macros file what they type in the online command interface; command "runseq" insufficient: does not allow for loops for instance
- In the case of complicated unworking scripts, very difficult to work it out / debug during the experiment itself
- Scan viewer: miss a cursor
- Scan speed : can it be optimized ? Slower if too many variables read ? Counters read all at the same time or one after the other ?
- > 2D Detectors : fast data rate a problem (P10)



Feedback from scientists at PETRA III: room for improvement

- > Not all environment variables should be visible to the users
- Users macros should be in another folder than the sardanaMacro folder
- > Macros:
 - If one error is in the macro, all macros of a library are not loaded
 - If one error is in the macro (relmaclib does not work, you have to take addmaclib)
 - It is not possible to give a variable from one macro to the other within a library (only if one save them as environmental variable)
- Error messages not understandable:
 - Not understandable or sometimes even no messages and the macro is not loaded
 - CORBAtimeout one cannot see which device courses the trouble
 - "motion ended in FAULT" one cannot see which motor and all motors are in "normal" state afterwards
- Data Analysis and Visualization (SciPy ?)



Acknowledgements

- > Thanks to Teresa Nunez Pardo de Vera and Thorsten Kracht! Beamline staff at P09 very demanding, yet right solutions to tricky problems always looked for and implemented sometimes (often?) on a short time notice.
- > Experiment control at P09 : Dr. Joerg Strempfer
- > Pilatus ROIs at P09: Dr. Diana Haas
- Feedback from scientists: Diana Haas (P08), Uta Ruett (P07), Michael Sprung (P10), Ulrike Boesenberg & Jan Garevoet (P06)

Thank you for your attention!

