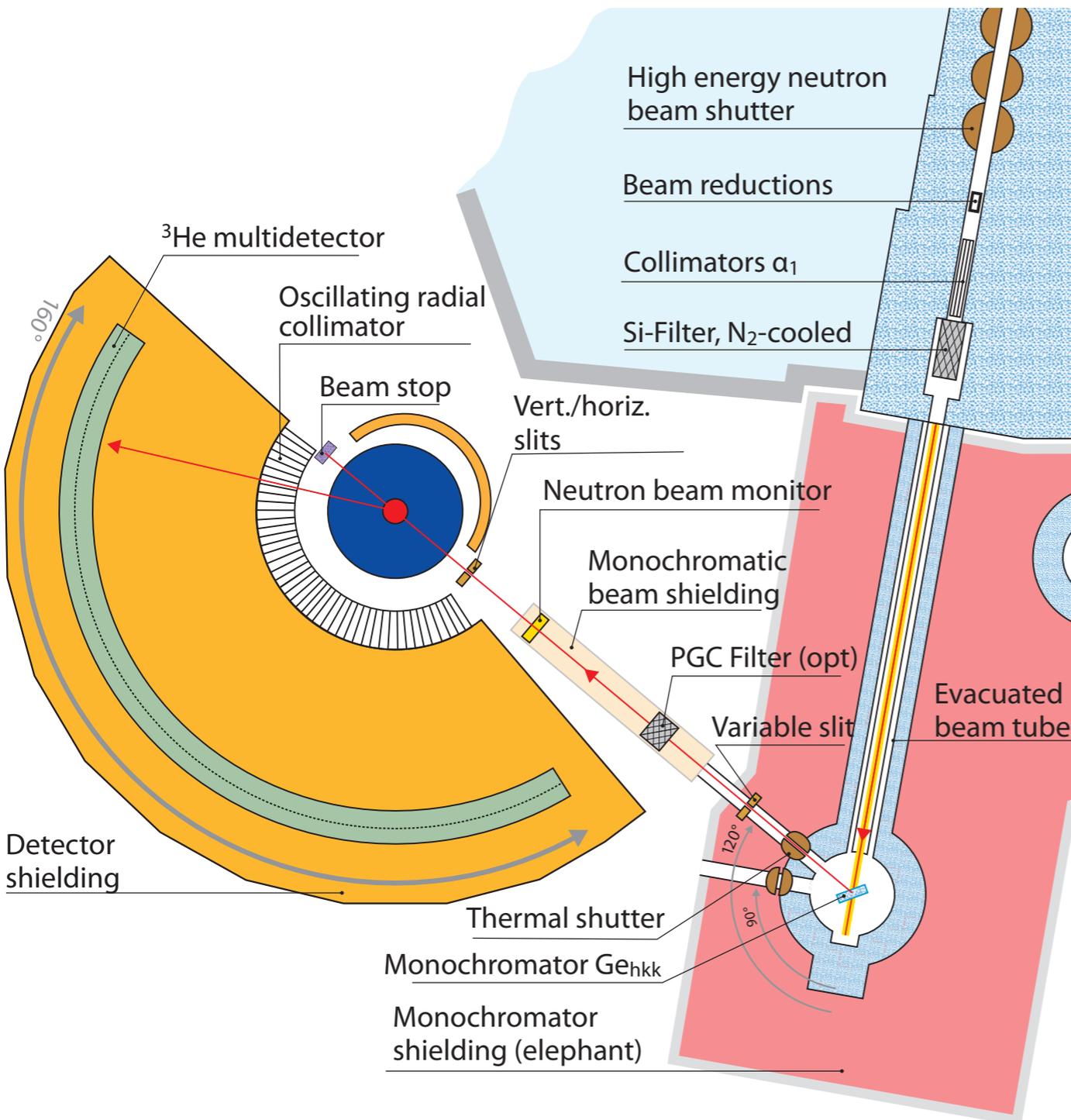


High Resolution Powder Diffractometer for Thermal Neutrons

Vladimir Pomjakushin and Denis Sheptyakov

Guidelines from Marc Janoschek

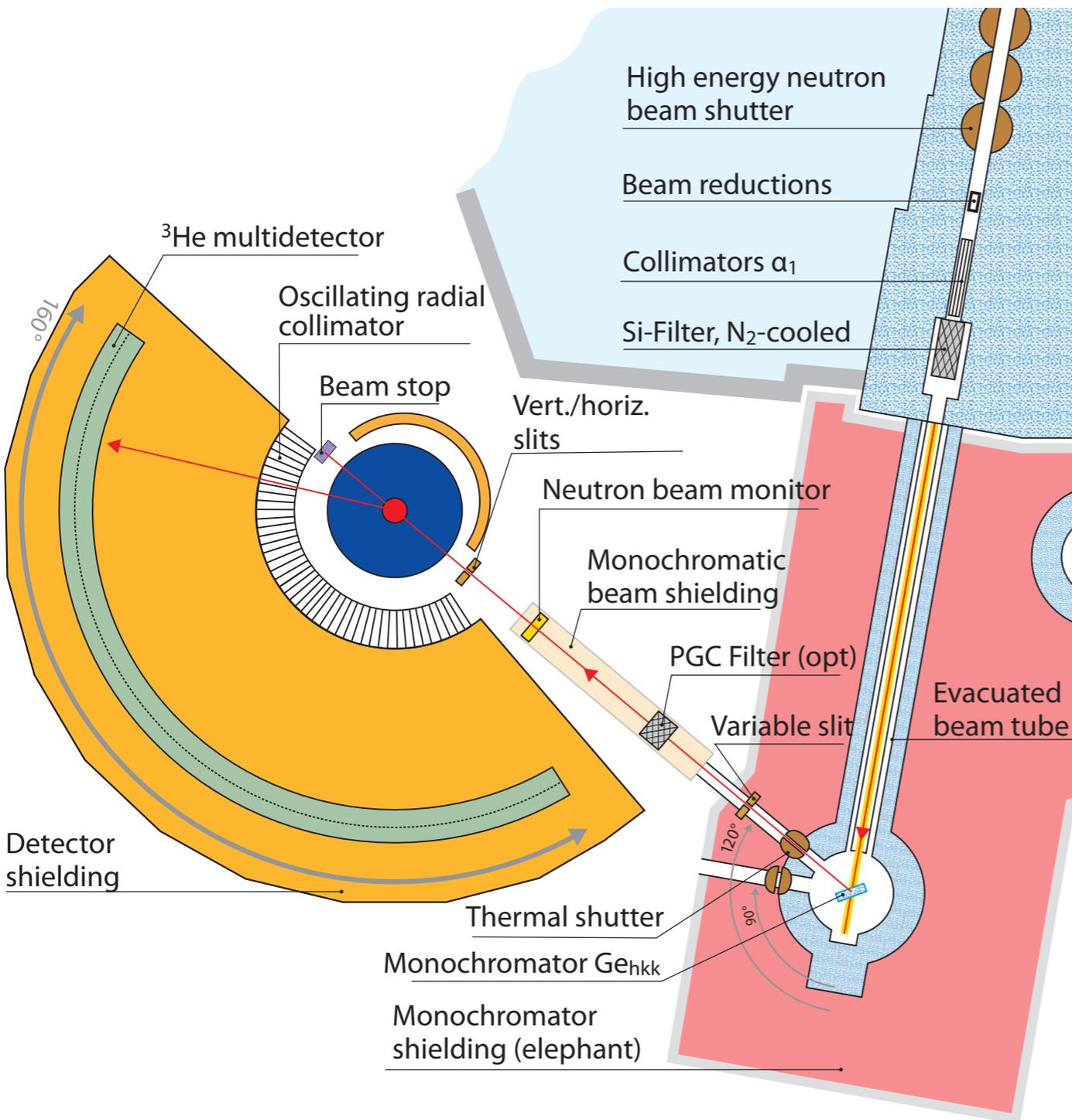


- Which parts of your instrument do have frequent technical problems?
- What parts of your instrument are outdated compared to other facilities?
- What is the percentage of user days you are not able to deliver due to ...?
- Which components result in additional work for you that could be avoided by upgrading aspects of the instrument.
- When you report on components that need to be exchanged/repaired due to technical difficulties, please also consider how this change could be additionally used to improve your instruments scientific capabilities.
- Are there quick wins to technically improve your instrument or extend its science case?
- Are there scientific questions for which your type of instrument is ideal but technical difficulties prevent such measurements?
- Please consider budget and procurement of items above.
- possible internal and external funding avenues. For example, which parts could be covered from internal LNS/LMU investment budget, which parts need additional funding.

High Resolution Powder Diffractometer for Thermal Neutrons

Vladimir Pomjakushin and Denis Sheptyakov

Guidelines from Marc Janoschek

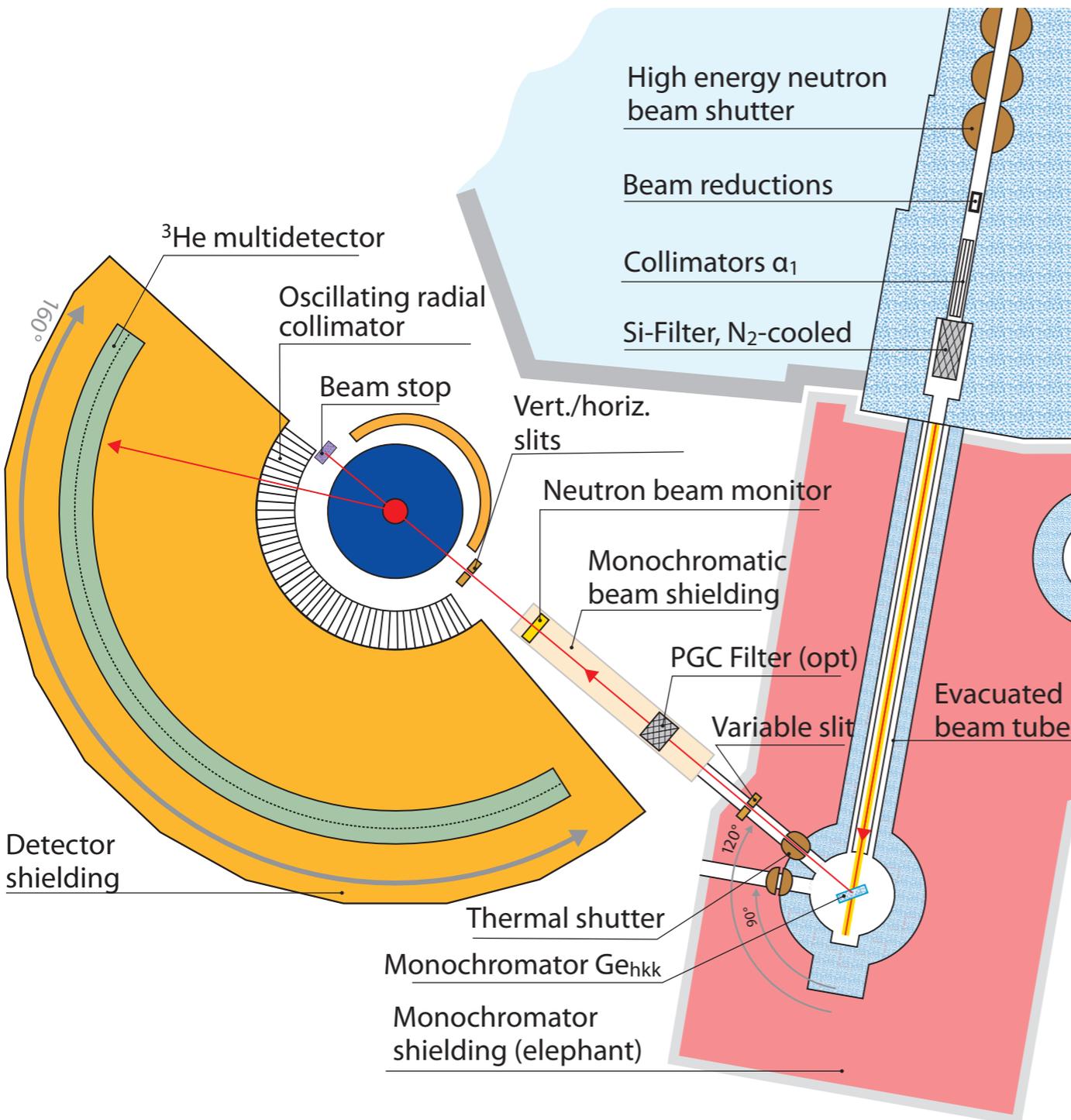


- Which parts of your instrument do have frequent technical problems?
- What parts of your instrument are outdated compared to other facilities?
- What is the percentage of user days you are not able to deliver due to ...?
- Which components result in additional work for you that could be avoided by upgrading aspects of the instrument.
- When you report on components that need to be exchanged/repaired due to technical difficulties, please also consider how this change could be additionally used to improve your instruments scientific capabilities.
- Are there quick wins to technically improve your instrument or extend its science case?
- Are there scientific questions for which your type of instrument is ideal but technical difficulties prevent such measurements?
- Please consider budget and procurement of items above.
- possible internal and external funding avenues. For example, which parts could be covered from internal LNS/LMU investment budget, which parts need additional funding.

High Resolution Powder Diffractometer for Thermal Neutrons

Vladimir Pomjakushin and Denis Sheptyakov

Guidelines from Marc Janoschek



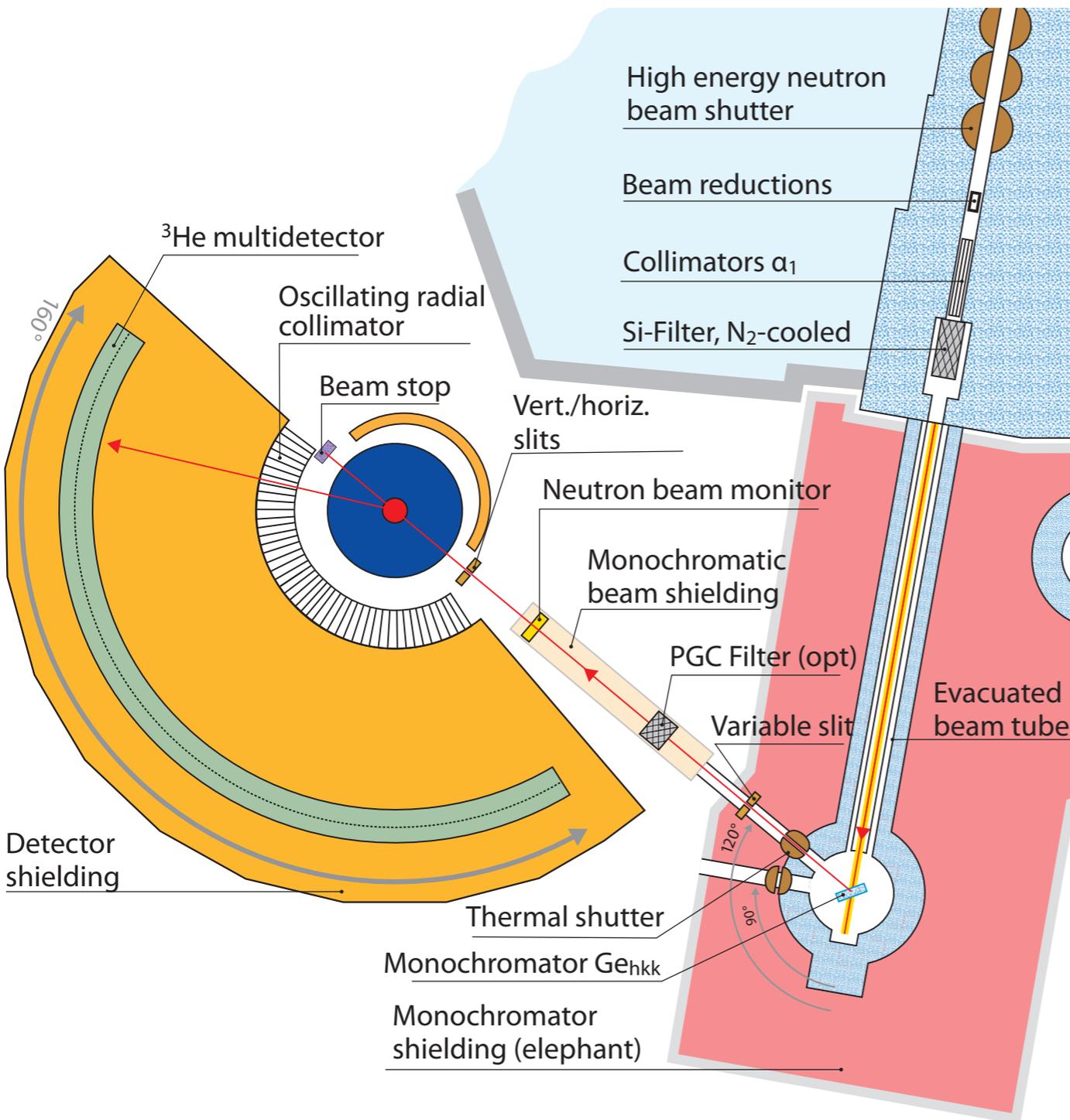
- Which parts of your instrument do have frequent technical problems?
- What parts of your instrument are outdated compared to other facilities?
- What is the percentage of user days you are not able to deliver due to ...?
- Which components result in additional work for you that could be avoided by upgrading aspects of the instrument.
- When you report on components that need to be exchanged/repared due to technical difficulties, please also consider how this change could be additionally used to improve your instruments scientific capabilities.
- Are there quick wins to technically improve your instrument or extend its science case?
- Are there scientific questions for which your type of instrument is ideal but technical difficulties prevent such measurements?

- Please consider budget and procurement of items above.
- possible internal and external funding avenues. For example, which parts could be covered from internal LNS/LMU investment budget, which parts need additional funding.

High Resolution Powder Diffractometer for Thermal Neutrons

Vladimir Pomjakushin and Denis Sheptyakov

Guidelines from Marc Janoschek



- Which parts of your instrument do have frequent technical problems?
- What parts of your instrument are outdated compared to other facilities?
- What is the percentage of user days you are not able to deliver due to ...?

- Which components result in additional work for you that could be avoided by upgrading aspects of the instrument.
- When you report on components that need to be exchanged/repaired due to technical difficulties, please also consider how this change could be additionally used to improve your instruments scientific capabilities.
- Are there quick wins to technically improve your instrument or extend its science case?
- Are there scientific questions for which your type of instrument is ideal but technical difficulties prevent such measurements?

- Please consider budget and procurement of items above.
- possible internal and external funding avenues. For example, which parts could be covered from internal LNS/LMU investment budget, which parts need additional funding.

HRPT schedule for one cycle 20-30 experiments

HRPT Schedule Sep – Dec 2022

DUO [SINQ Website](#)

Instrument: HRPT

[Change settings](#)

W	September	October	November	December
35	Th 1 Lampronti 2021 2893 (4d) ⁻¹	Sa 1 Král 2022 1012 (3d) (Pomjakushin) p20346 ORI4	Tu 1 Vayer 2022 1032 (2d)	Th 1 High Field Powder Diffraction Study of Magnetoelectric Coupling Phase of TbTaO4
	Fr 2 Internal developments Sheptyakov 2022 0314 (2d) ORI4	Su 2	We 2	Fr 2
	Sa 3	Mo 3 Determination of magnetic structure in Ce2Ni5C3	Th 3 Magnetic ordering of high-entropy garnet Dy3(ScGaInMgZr)2Ga3O12	Sa 3 Saxena 2022 0980 (5d) (Sheptyakov) p20342 MA6
	Su 4 Paunovic 2022 1165 (1d)	Tu 4 Kulbakov 2022 0757 (3d) (Pomjakushin) p20335 ORI4	Fr 4 Damay 2022 0909 (3d) (Sheptyakov) p20339 Variox/Dil	Su 4
36	Mo 5 Instrument and internal Pomjakushin 2022 1424 (3d) ORI4	We 5	Sa 5	Mo 5 Discerning the coke formation in the micropores of zeolite catalysts during methanol to-hydrocarbons reaction by... ⁻¹
	Tu 6	Th 6	Su 6	Tu 6 Paunovic 2022 1165 (2d) (Sheptyakov) p20352 Furnace FT
	We 7	Fr 7 Crystal and Magnetic Structure of CuSn(OD)6	Mo 7 ⁻¹	We 7 Structure determination of a substitution series of...
	Th 8 Magnetic structures of topological semimetals, LnSbTe (Ln = Nd, Dy, Tb, Ho)	Sa 8 Peets 2022 1210 (3d) (Pomjakushin) p20354 ORI4	Tu 8 Effect of cation disorder induced by substitution in the high-temperature multiferroics YBa(Cu,Co,Ni)FeO5	Th 8 Kronbo 2022 0930 (2d) (Sheptyakov) p20341
	Fr 9	Su 9	We 9 Aurelio 2022 1004 (4d) (Sheptyakov) p20345 Cryofurnace	Fr 9 Neutron scattering study on the magnetic and lattice structures of EuCo2Al9
	Sa 10 Plokhikh 2022 0904 (4d) (Pomjakushin) p20338 ORI4	Mo 10 Mannathanath Chakkingal 2022 1057 (2d) (Pomjakushin) p20348 ORI4	Th 10	Sa 10
	Su 11	Tu 11	Fr 11	Su 11 Mingfang 2022 1122 (3d) (Sheptyakov) p20351
37	Mo 12	We 12 Hydrogen induced magnetic... Cedervall 2022 0823 (2d) (Pomjakushin) p20337 ORI4	Sa 12 Study of the magnetic structures of the novel room temperature magnetocaloric compounds R6(Fe,Mn)Bi2 (R = Tb, Dy)	Mo 12 Internal developments Sheptyakov 2022 0314 (2d) ORI4
	Tu 13	Th 13	Su 13	Tu 13
	We 14	Fr 14 Instrument and internal Pomjakushin 2022 1424 (3d) ORI4	Mo 14 Aurelio 2022 0928 (4d) (Sheptyakov) p20340 Cryofurnace	We 14
	Th 15	Sa 15	Tu 15	Th 15 Instrument and internal Pomjakushin 2022 1424 (4d) (Sheptyakov, Pomjakushin) ORI4
	Fr 16	Su 16	We 16	Fr 16
	Sa 17 Negative thermal expansion of the spin-1/2 1D magnet Pauflerite	Mo 17	Th 17	Sa 17
	Su 18 Quintero Castro 2022 0971 (5d) (Sheptyakov) p20334 ORI4	Tu 18	Fr 18 Pomjakushin 2022 1424 (5d) (Sheptyakov, Pomjakushin) ORI4	Su 18 Instrument and internal Pomjakushin 2022 1424 (4d) (Sheptyakov, Pomjakushin) ORI4
38	Mo 19	We 19	Sa 19	Mo 19
	Tu 20	Th 20	Su 20	Tu 20 Instrument and internal Pomjakushin 2022 1424 (4d) (Sheptyakov, Pomjakushin) ORI4
	We 21 Crosnier-Lopez 2022 0815 (0d) ⁻¹	Fr 21 Two-dimensional antiferromagnetism in a fluoride FeTiF6 · 6H2O ⁻¹	Mo 21	We 21
	Th 22 Accurate b(coh) values of... Gehlhaar 2022 1470 (2d) (Sheptyakov) ORI4	Sa 22	Tu 22	Th 22
	Fr 23	Su 23 Dubrovskiy 2022 1068 (3d) (Sheptyakov) p20349 ORI4	We 23	Fr 23
	Sa 24 Internal developments Sheptyakov 2022 0314 (2d) ORI4	Mo 24	Th 24	Sa 24
	Su 25	Tu 25 Magnetic structures and... Sharma 2022 1070 (2d) (Sheptyakov) p20350 ORI4	Fr 25 Magnetic ground state of the Na2Co2TeO6 honeycomb	Su 25
39	Mo 26 Magnetic structure of non-centrosymmetric antiferromagnet Ce2PtAl7Ge4	We 26	Sa 26 Guo 2022 0989 (3d) (Pomjakushin) p20343 ORI4	Mo 26
	Tu 27 Shin 2022 1205 (3d) (Pomjakushin) p20353 ORI4	Th 27	Su 27	Tu 27
	We 28	Fr 28 Instrument and internal Pomjakushin 2022 1424 (4d) (Sheptyakov, Pomjakushin) ORI4	Mo 28 Magnetic field induced... Guo 2022 0990 (2d) (Pomjakushin) p20344 MA6	We 28
	Th 29	Sa 29	Tu 29	Th 29
	Fr 30 Král 2022 1012 (3d)	Su 30	We 30 Saxena 2022 0980 (5d)	Fr 30
		44		
		Vayer		

Publication Statistics about 20 publications /year

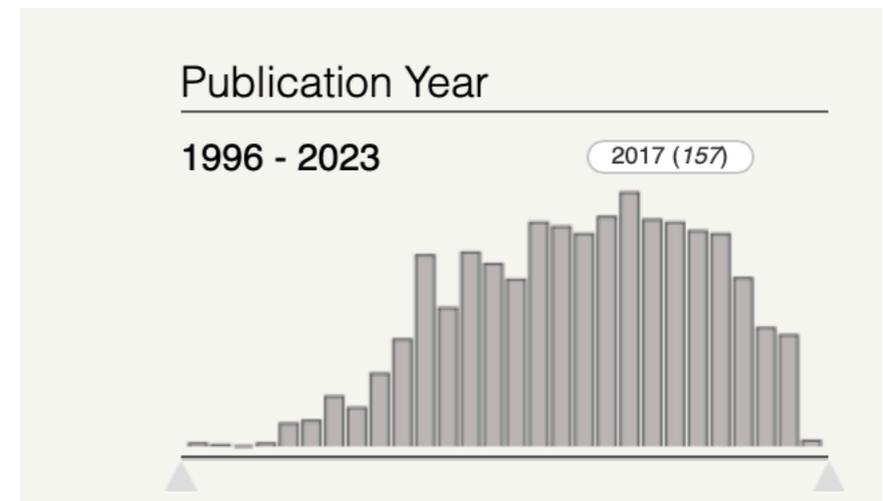
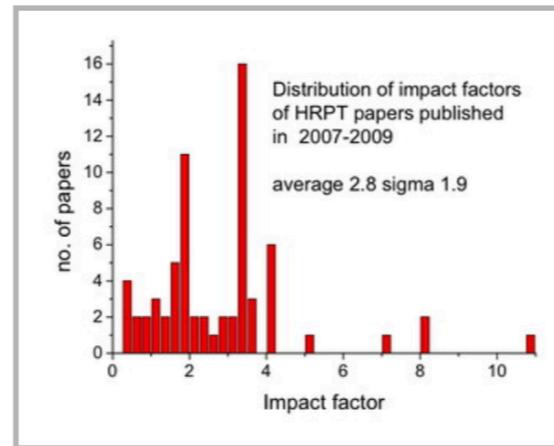
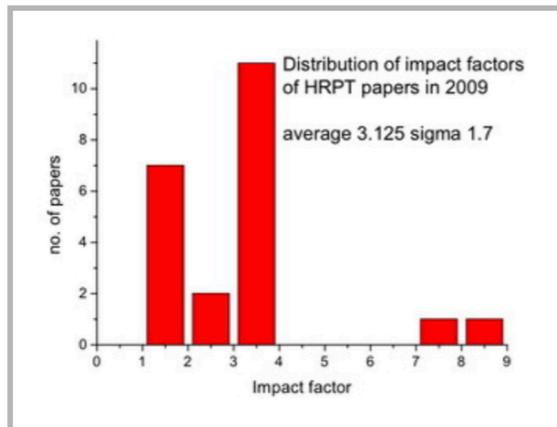
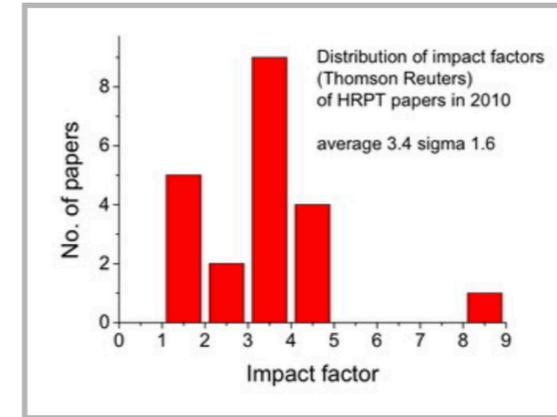
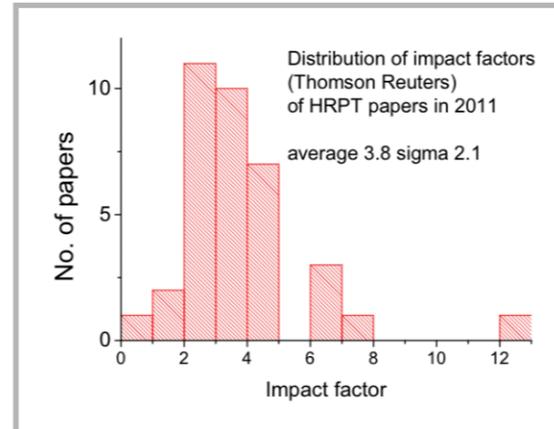
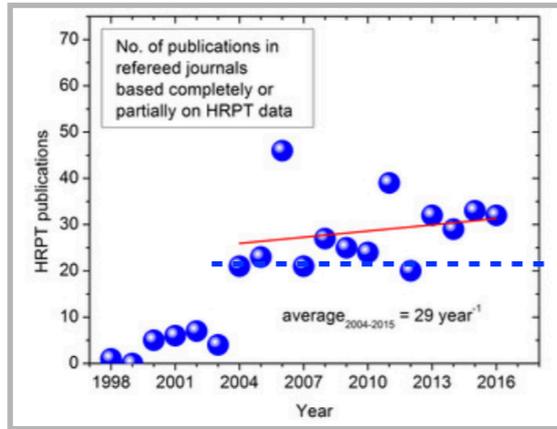
- Statistics of HRPT publications
- Examples of results
- References

Statistics of HRPT publications

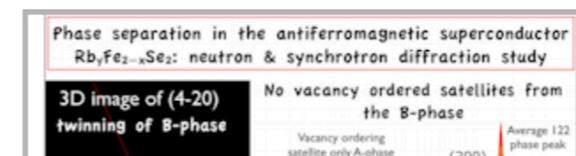
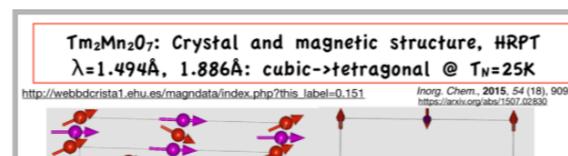
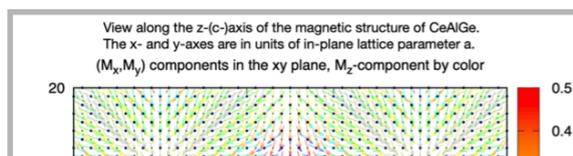
22, 18 publications in 2020, 2021

→ HRPT publications (automatically updated from DORA) ↗

TOTAL SINQ: 118, 83 publications in 2020, 2021

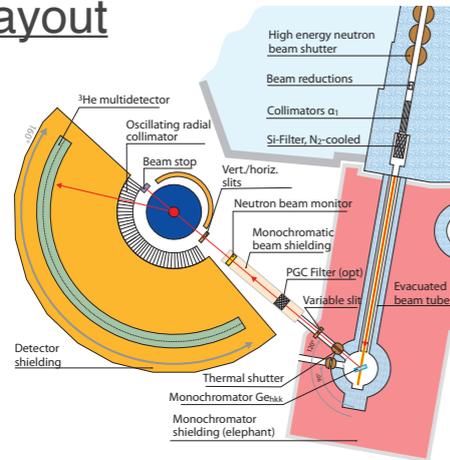


Examples of results



Technical Specifications

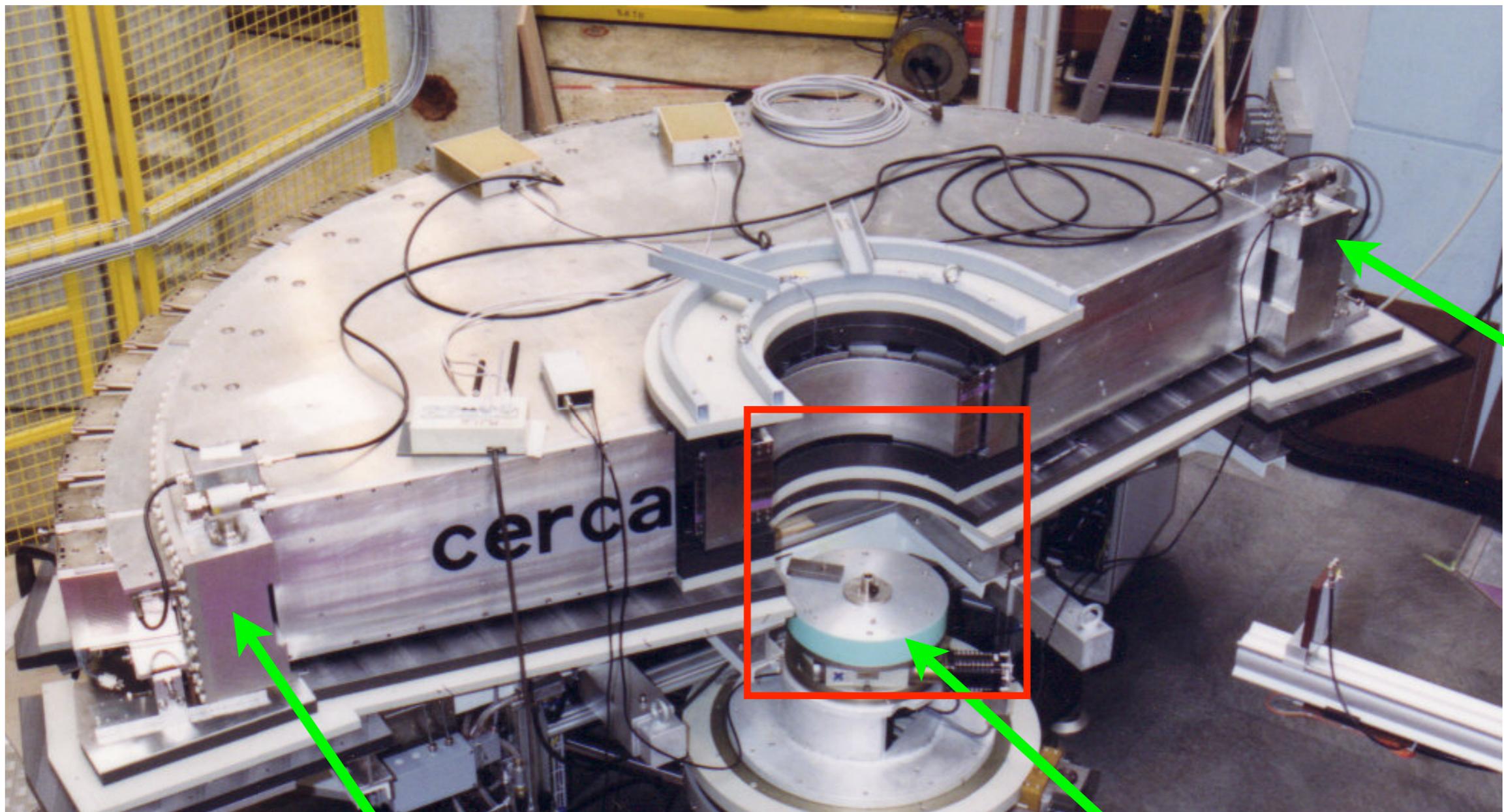
HRPT layout



<https://www.psi.ch/en/sinq/hrpt/specifications>

Neutrons:	thermal (0.84-2.954Å) beam 1RNS41 from a water scatterer close to the SINQ target.
Primary collimation:	Gd-O Soller collimators with primary white beam collimations $\alpha_1 = 6', 12', 24'$ (high resolution), - = approx. 40' (high intensity)
Liquid N ₂ cooled Si	20 cm length
Monochromator	Ge (hkk) of wafer type, 28 cm high, variable vertical focusing, total mosaic halfwidth 15'
Secondary collimation:	variable computer controlled slit system for monochromatic beam
Radial collimators:	Oscillating mylar-Gd-O collimators to eliminate Bragg peaks from sample environment such as from cryostat or sample holder.
PSD detector: (LCP1600 from Cerca, F-26104 Romans)	³ He (3.6 bar + 1.1 bar CF ₄), 25 x 64 = 1600 counters, step 0.1°, 15 cm high, radius 1.5 m, effective detection length 3.5 cm
HRPT gas mixture cleaning/adding system (more pictures)	cleaning of the gas mixture from (O ₂ , H ₂ O, etc) by a circulation of the gas mixture through the appropriate filters without pumping out the mixture.
Sample temperature:	50 mK - 1800 K
Magnetic field:	superconducting magnet MAO6, field H vertical to scattering plane, H up to 6 T.
Zero matrix pressure cells:	up to 8, 15 kbar for full scattering angle range. Example of pattern,
Sample changers:	Room temperature sample changer for eight (8) samples, low temperature sample changer for four (4) samples (more pictures), low temperature sample changer for five (5) samples with sample rotation

HRPT Detector and sample table



detector

detector

sample
table

HRPT short work list 2023-

HRPT 2017-18 to do list.

6.12.2017

1. • xyz sample table.
3. • Encoder on sample rotation for l+s, (2kFr)
Feasibility is OK from Alex B. *low-temperature sample changer*
- Some channels in the detector are dying

by 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023

Study: production of new analog cards/chann. for detector electronics. ? This is a long term project.

2. • motorised beam stop.

HRPT short work list 2023-

HRPT 2017-18 to do list.

6.12.2017

1. • xyz sample table.

3. • Encoder on sample rotation for l+5, (2kFr)
Feasibility is OK from Alex B. *low-temperature sample changer*

• Some channels in the detector are dying

by 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023

Study: production of new analog cards/chann. for detector electronics. ? This is a long term project.

2. • motorised beam stop.

HRPT short work list 2023-

HRPT 2017-18 to do list.

6.12.2017

1. • xyz sample table.
3. • Encoder on sample rotation for l+S, (2kFr)
Feasibility is OK from Alex B. *low-temperature sample changer*
- Some channels in the detector are dying

by 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023

Study: production of new analog cards/chann. for detector electronics. ? This is a long term project.

2. • motorised beam stop.

HRPT short work list 2023-

HRPT 2017-18 to do list.

6.12.2017

1. • xyz sample table.

3. • Encoder on sample rotation for l+S, (2kFr)
Feasibility is OK from Alex B. *low-temperature sample changer*

• Some channels in the detector are dying

by 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023

Study: production of new analog cards/chann.
for detector electronics. ? This is a long term project.

2. • motorised beam stop.

HRPT short work list 2023-

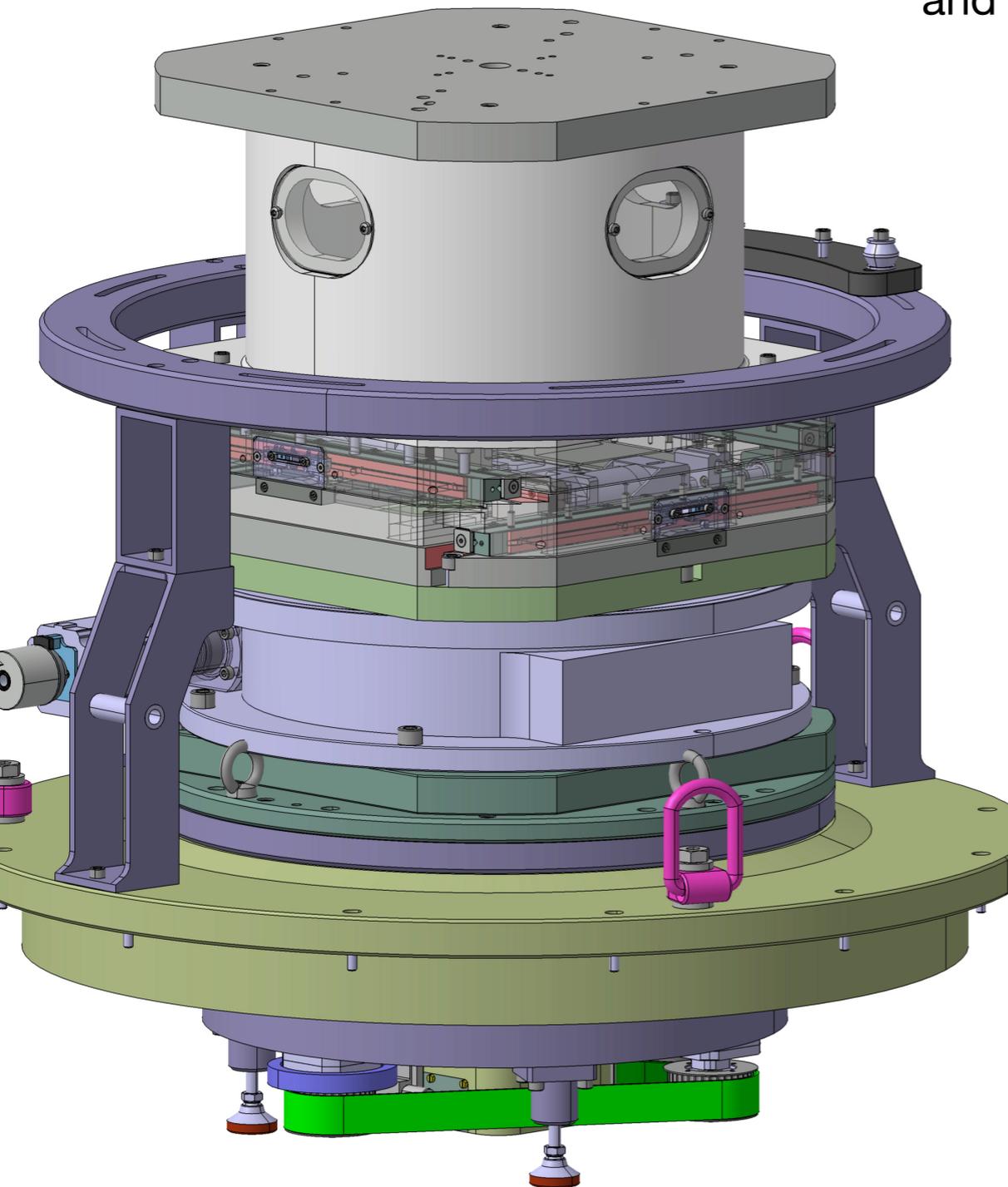
HRPT 2017-18 to do list.

6.12.2017

1. • xyz sample table.
3. • Encoder on sample rotation for l+s, (2kFr)
Feasibility is OK from Alex B. low-temperature sample changer
- Some channels in the detector are dying
by 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023
Study: production of new analog cards/chan. for detector electronics. ? This is a long term project.
2. • motorised beam stop.

“new” xyz sample table -hardware was ready and tested in 2017: Installation is still pending.

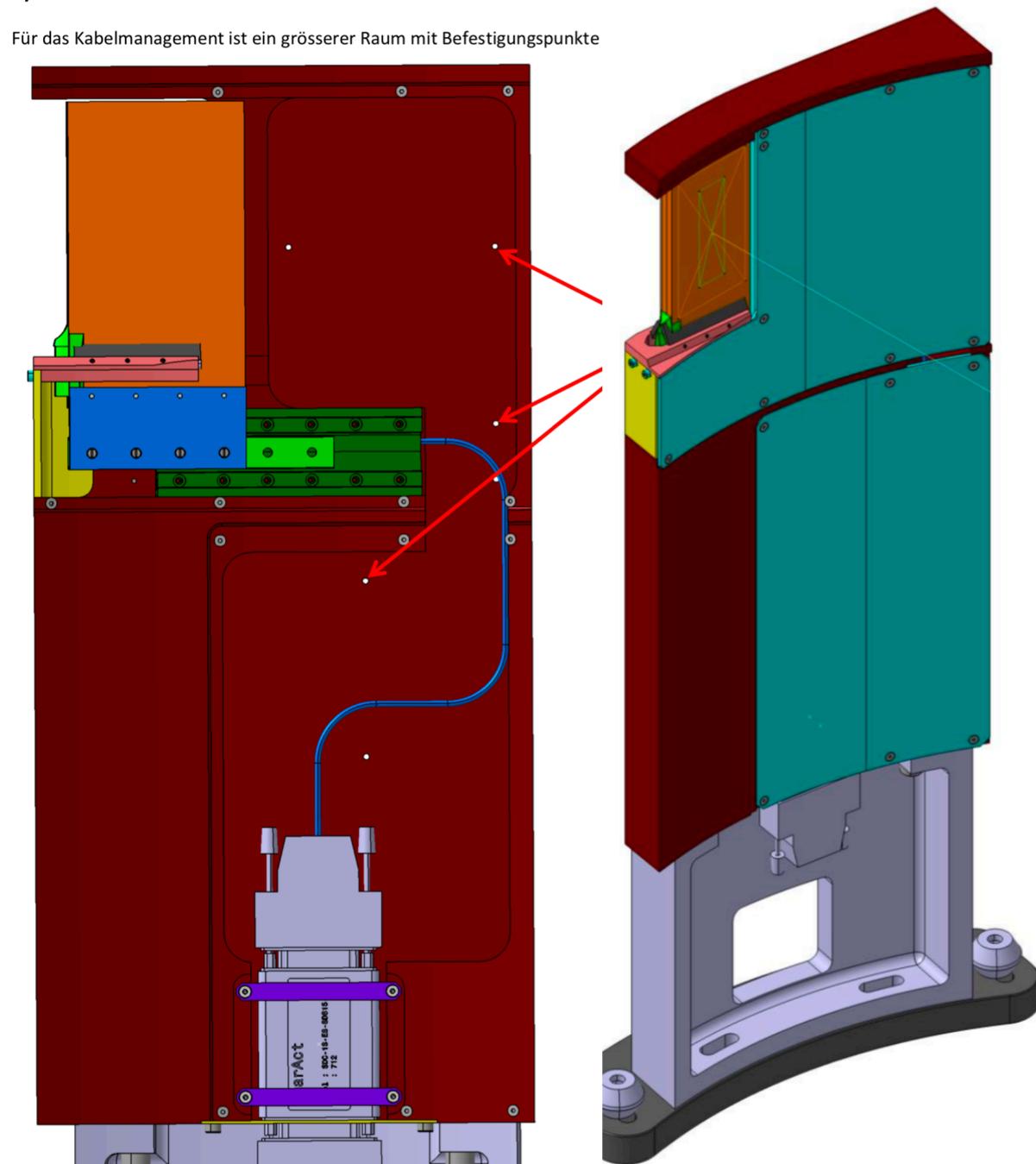
- The old sample table does not allow precise positioning along x,y-directions for some experiments, which is crucial to avoid aberration of diffraction patterns.
- Positioning along z-axis is needed for new low-T sample changer, and for some other special setups



motorised beam-stop - ready 2018: Installation is still pending.

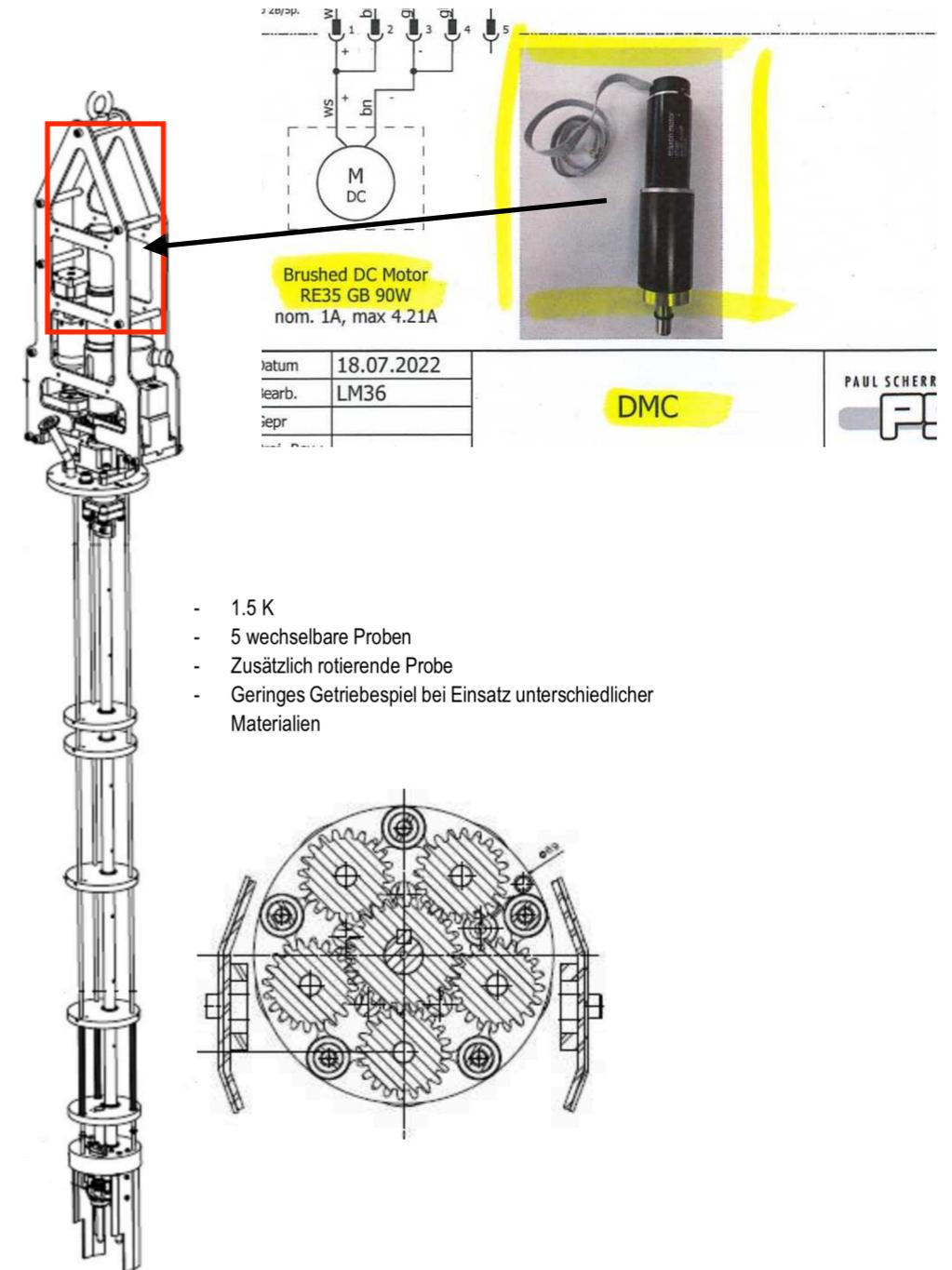
4) Kabelfreiheit

Für das Kabelmanagement ist ein grösserer Raum mit Befestigungspunkte



- fine position adjustment for SANS signals
- automatic measurements of muR absorption
- ...

encoder on sample rotation motor - design is done, Installation is still pending.



- 1.5 K
- 5 wechselbare Proben
- Zusätzlich rotierende Probe
- Geringes Getriebeispiel bei Einsatz unterschiedlicher Materialien

- measurements of single crystals in sample changer
- computer controlled rotation frequency

Summary of the planned HRPT maintenance/ development for 2023-...

New xyz-sample table. Hardware, including electronics on the table, was ready in 2017. Installation is still pending.

Motorised, computer controlled beam stop with adjustable position. Hardware, including electronics on the table, was ready in 2018. It is in the finished state, installation is still pending.

Absolute encoder for the sample rotation axis for the LT5 cryogenic sample changer. This extension of the LT5's functions has already been designed by Alex B. It requires either no or only extremely minor mechanical adjustments, but the installation of an additional encoder and corresponding commissioning of an additional axis.

The front-end analog electronics of the detector. Some modules are already misbehaving, but at the moment we can live with this problem by software tricks/recalibrations. Some preliminary study of the problem is foreseen in 2024. By 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023.

After the above list is done:

Power supply/UPS for the controls of resolvers (electronics cabinet at the elephant). - This is partially done. Otherwise, one day we risk losing the actual positions of very important motors that move our monochromator.

Controller of the refilling of the liquid nitrogen into the silicone filter. It fails from time to time.

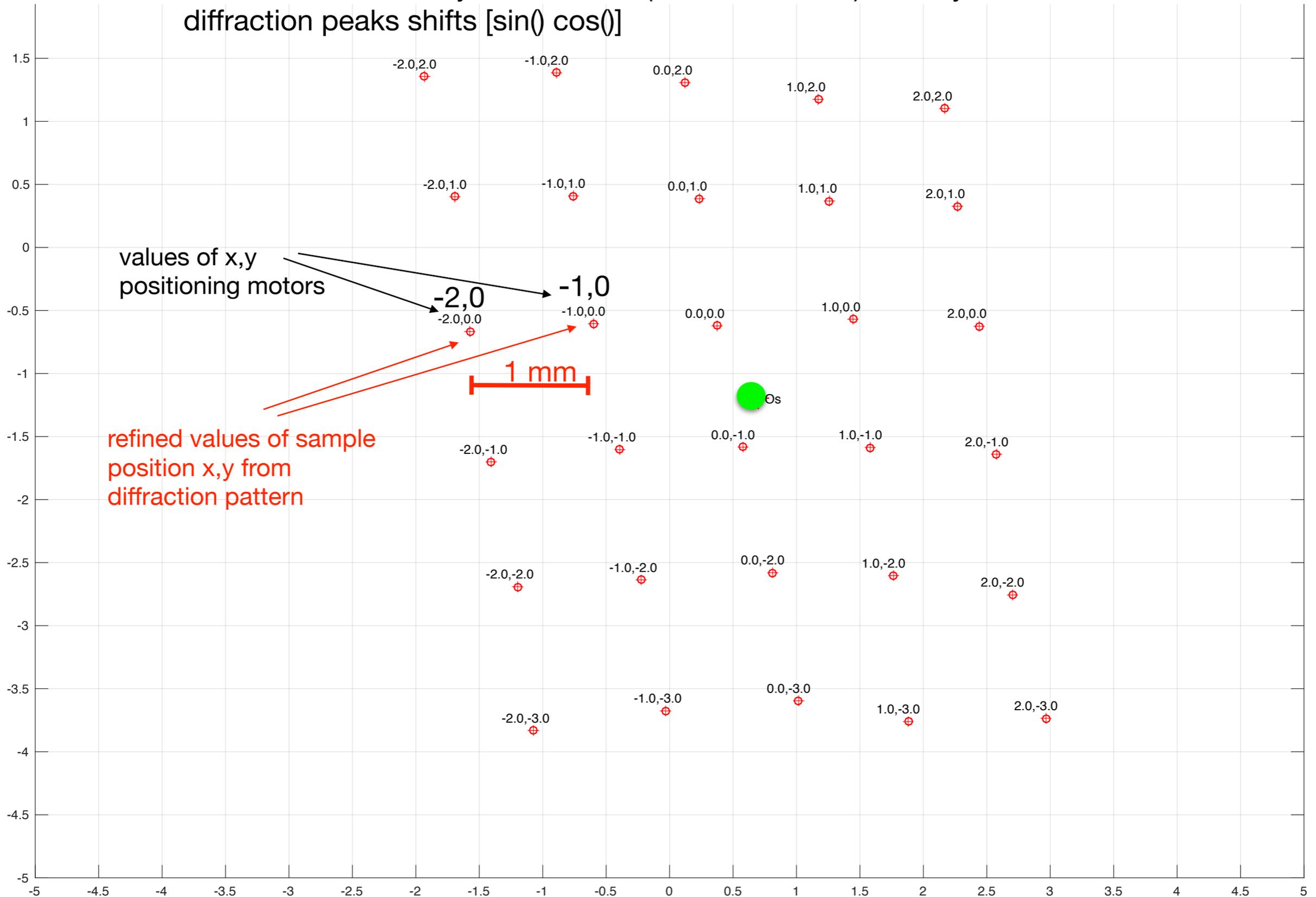
Check the electronics of the ^3He cleaning system pump. Repeat the cleaning, and maybe pressurising.

Further study of the decrease in the gas amplification ratio after cleaning and pressurising the gas mixture in the detector.

Thank you

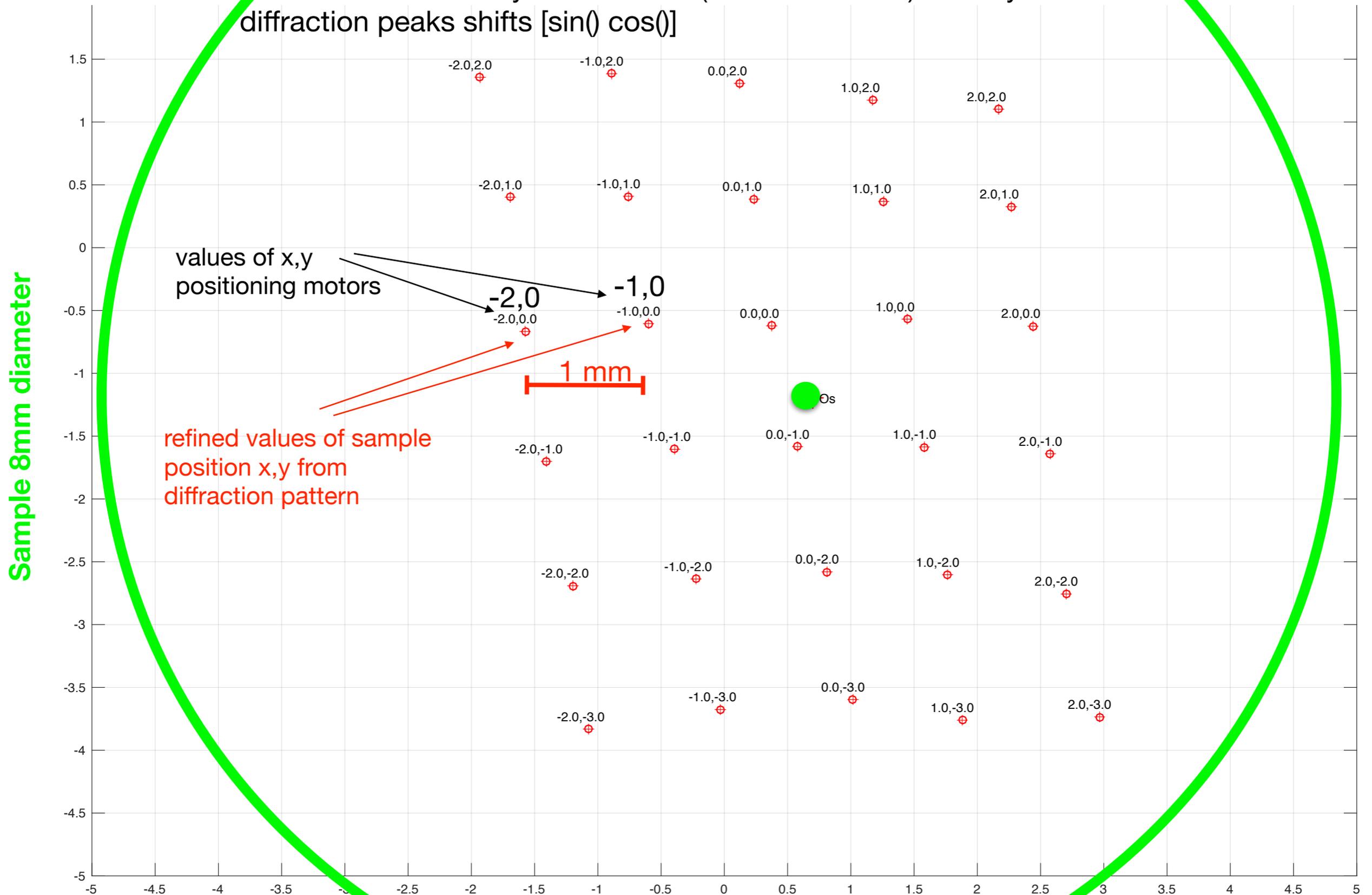
precise sample positioning with respect to calibration

We can determine by diffraction the (x,y) position of sample with the accuracy better than 0.1mm! by the detector (radius 1500mm) from systematic diffraction peaks shifts [sin() cos()]



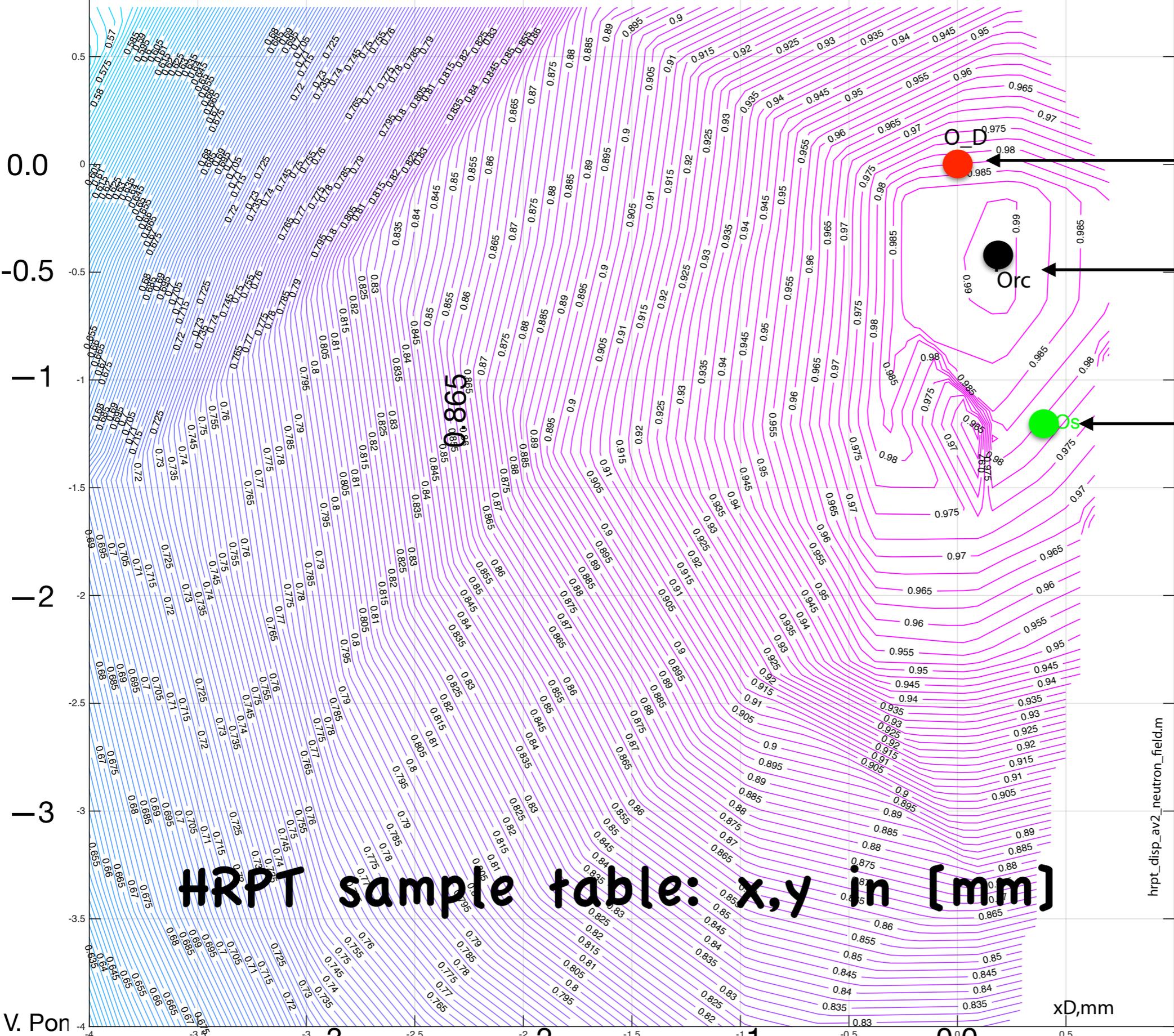
precise sample positioning with respect to calibration

We can determine by diffraction the (x,y) position of sample with the accuracy better than 0.1mm! by the detector (radius 1500mm) from systematic diffraction peaks shifts [sin() cos()]



yD, mm

Neutron intensity distribution with RC2. O_S is = Oxy, May'12



detector center

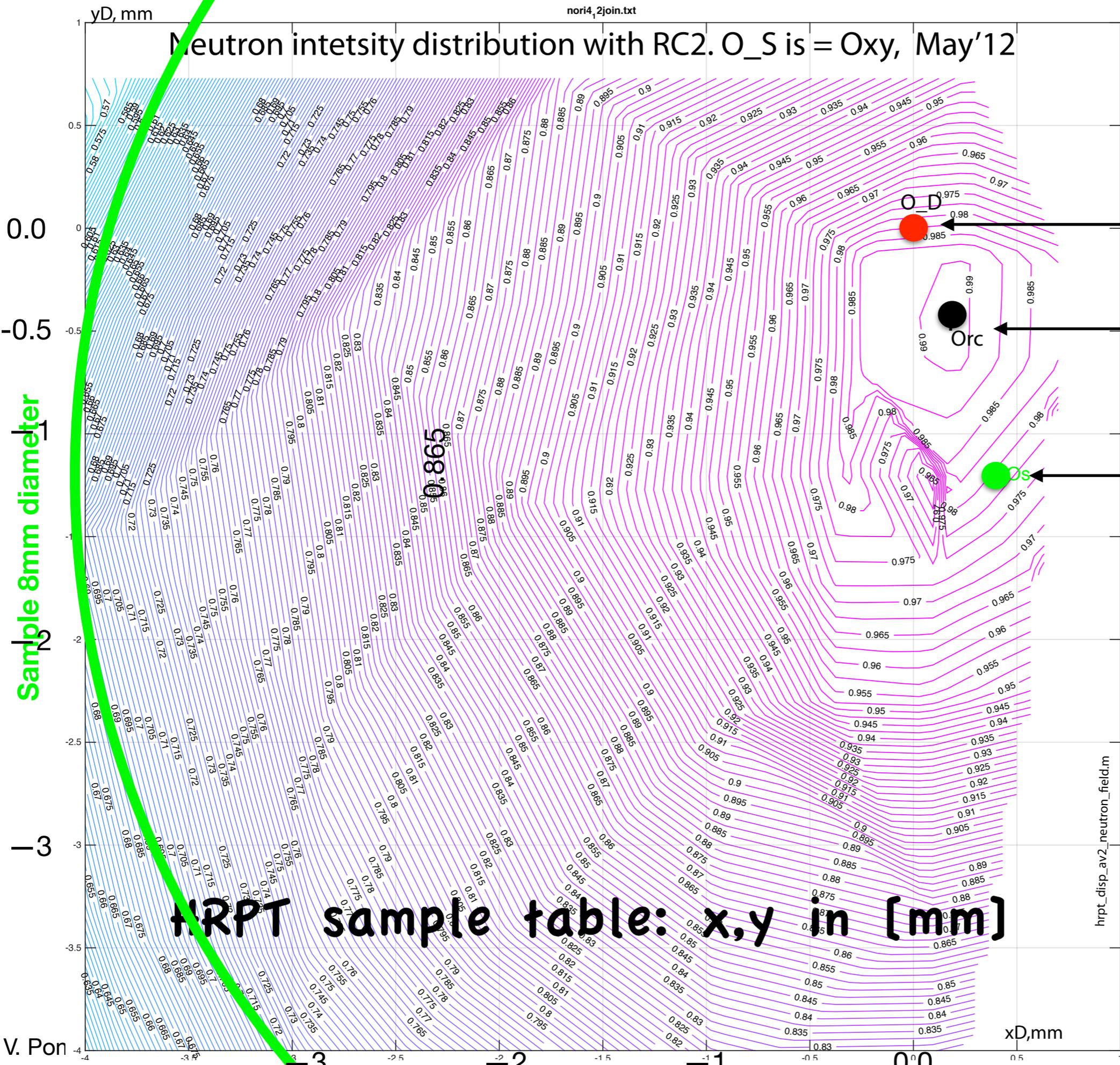
radial collimator center

sample table rotation center (calibration position)

HRPT sample table: x,y in [mm]

hrpt_disp_av2_neutron_field.m

Neutron intensity distribution with RC2. O_S is = Oxy, May'12



detector center

radial collimator center

sample table rotation center (calibration position)

Sample 8mm diameter

HRPT sample table: x,y in [mm]

hrpt_disp_av2_neutron_field.m

average Debay-Waller ADP(x,y) of Na₂Ca₃Al₂F₁₄ at 1.9Å

