

Rapid sample exchanger SPACE-II at SPring-8

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Outline

1. Introduction of SPring-8 MX
2. Brief history of sample changer SPACE
3. Development of SPACE-II and its performance
4. Future plan

MX Beamlines at SPring-8

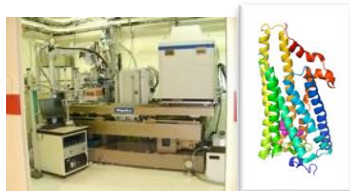
Various specification of MX-BLs allow for data collection from wide range of targets

Bending magnet beamlines

BL26B1/B2

Developed for structural genomic research in 2000s
Automation at SP8 MX started from here

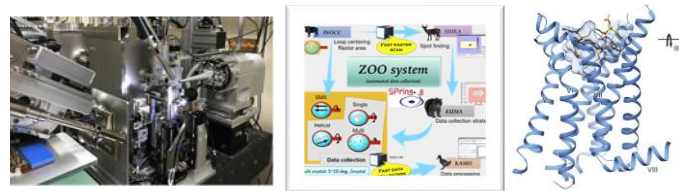
- Flux $\sim 10^{11}$ (phs/s)
- Data collection from well diffracting crystal



Undulator BL, BL45XU

High flux beam

- High flux 2×10^{13} ph/s @ $20 \times 20 \mu\text{m}$
- automated data collection ZOO system

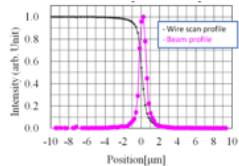


Common storage (1 PB)
Common cluster PCs

Undulator BL, BL32XU

Micro-beam minimum 1/μm

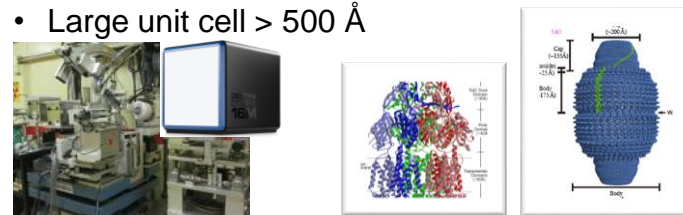
- micro-focus beam ($1 \mu\text{m}$; 6×10^{10} ph/s)
- micro-crystallography / challenging target



Undulator BL, BL44XU

Low divergence beam

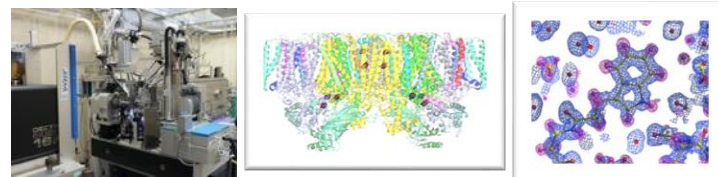
- Macromolecular complex
- Large unit cell $> 500 \text{ \AA}$



Undulator BL, BL41XU

High flux beam

- High flux (4×10^{13} ph/s @ $2 \times 20 \mu\text{m}$)
- Ultra high resolution ($\lambda \sim 0.5 \text{ \AA}$, ID 3rd H)

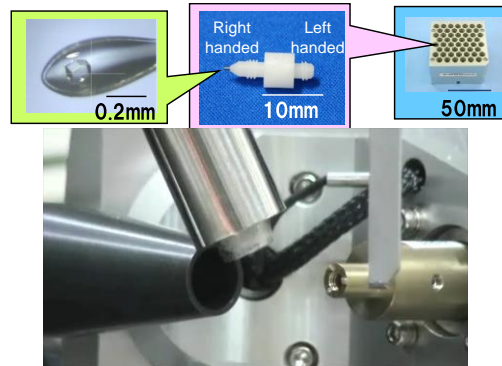


Operated three organizations, but use common data collection environment, data collection software, sample changer etc.

Sample changer SPACE

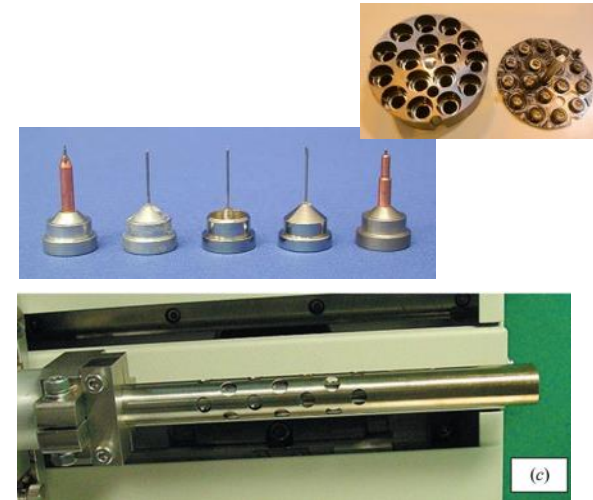
Sample changer SPACE (Spring-8 Precise Automatic Cryo-sample Exchanger)

Brief history of SPACE



Reproducibility of crystal position ($<10\mu\text{m}$)

Developed at BL26 for the structural genomics project (2002)
Use special sample pin with screw. (Ueno *et al.*, 2004)



Attachment for the generic pin
was developed (2009)
(Murakami *et al.*, 2012)



Enlarge storage (2010)
Uni-puck 2 \rightarrow 4
(Murakami *et al.*, 2012)



Enlarge storage (2014)
Uni-puck 4 \rightarrow 8



Speed up sample exchange (2017)

Development of SPACE-II

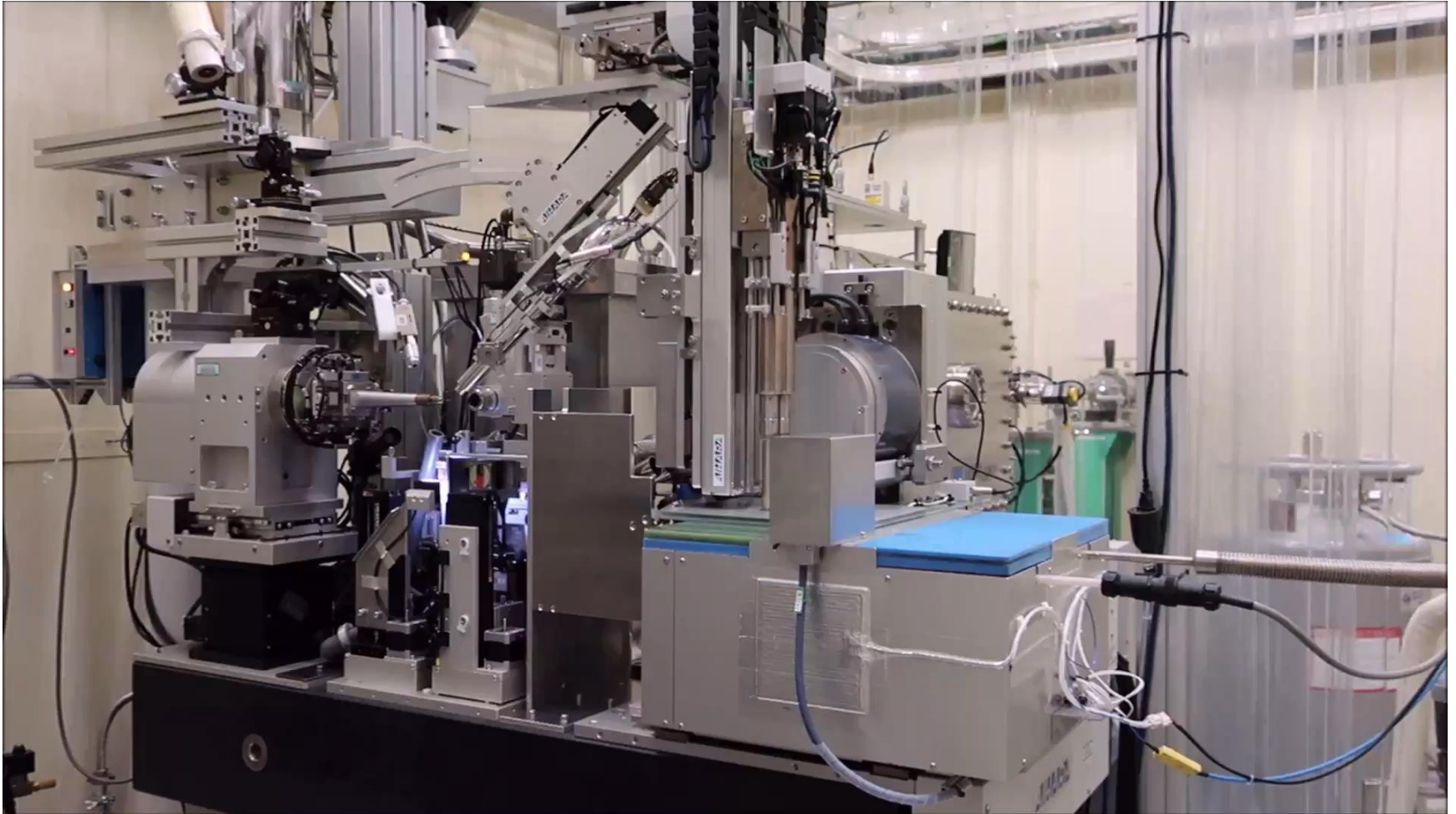
Motivation

Reduce time for sample exchange to the order of 10 s, because the sample exchange of 1 min by old SPACE was a large overhead in the era of pixel array detectors.

Our approach

1. Implemented twin arm to exchange samples in one cycle.
2. Use a high speed servo motor for the rapid movement instead of a stepping motor.
3. Use long mount arm to prevent interference between detector and SPACE to eliminate overhead due to withdrawal of detector/SPACE.

Sample exchange by SPACE-II



Overall architecture

Composed of a sample storage and mount arms

Rotation stage

- Change the orientation of the twin arm
- Speed 200 deg s^{-1}

Pneumatic translation stage

Switch position of the twin arms

Arm-1

Used for sample mount

Mount arm

Arm-2

Used for sample storage

Sample storage

Dryers

Uni-Pucks are installed after removing this lid

Small lid in open state

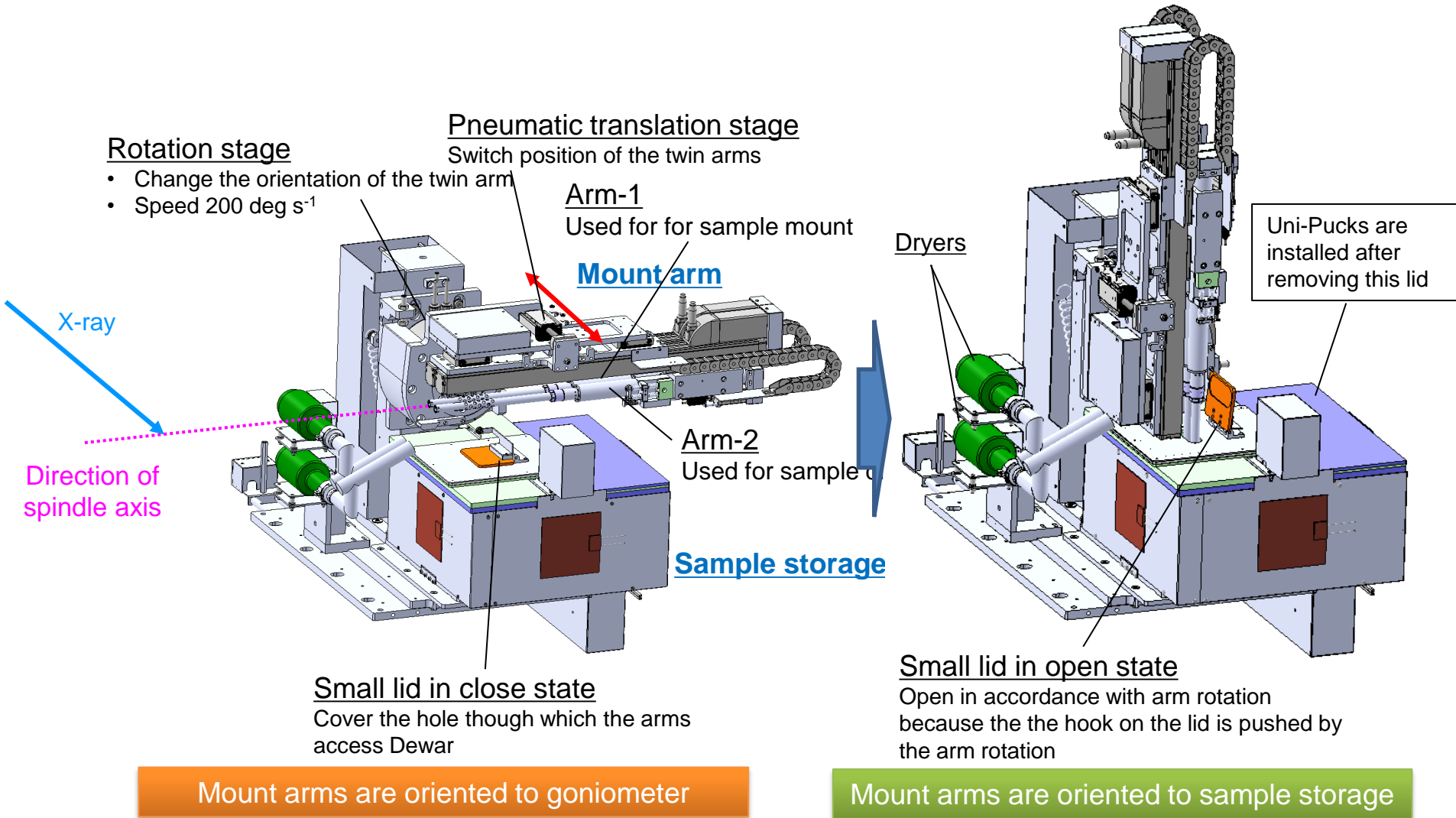
Open in accordance with arm rotation because the the hook on the lid is pushed by the arm rotation

Small lid in close state

Cover the hole though which the arms access Dewar

Mount arms are oriented to goniometer

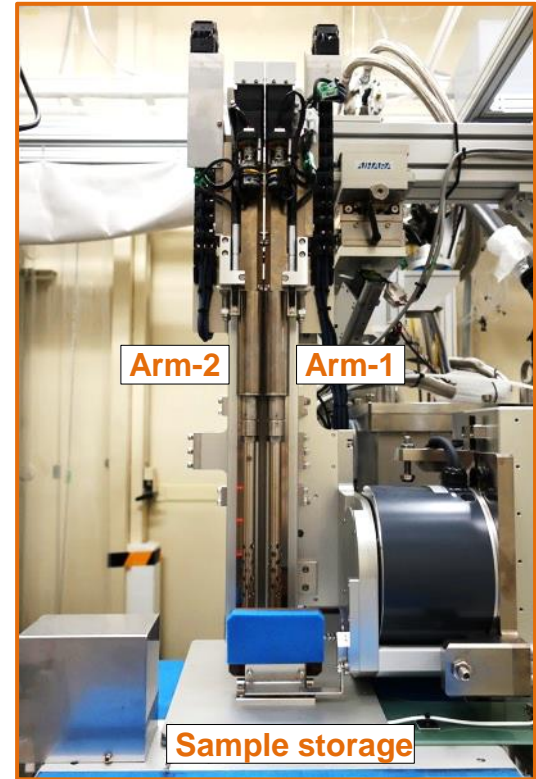
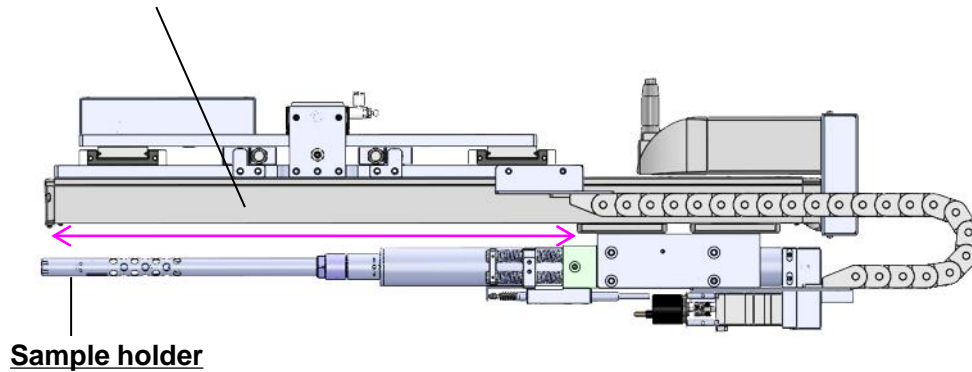
Mount arms are oriented to sample storage



Mount arm

Translation stage

- The stroke of 550 mm allows us to locate SPACE-II distant enough so as not to interfere with the detector
- The speed is 465 mm s^{-1}

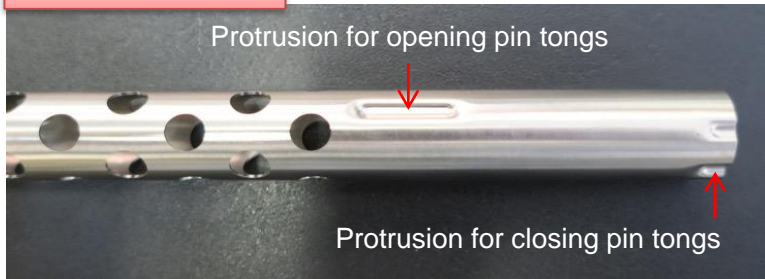


Each mount arm has a translational axis to independently access the goniometer/Uni-puck.

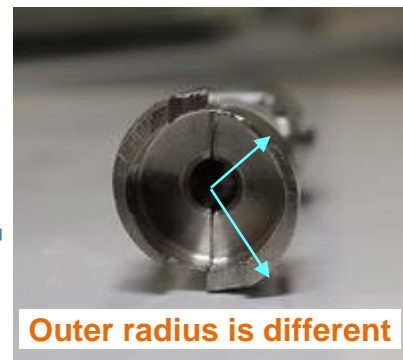
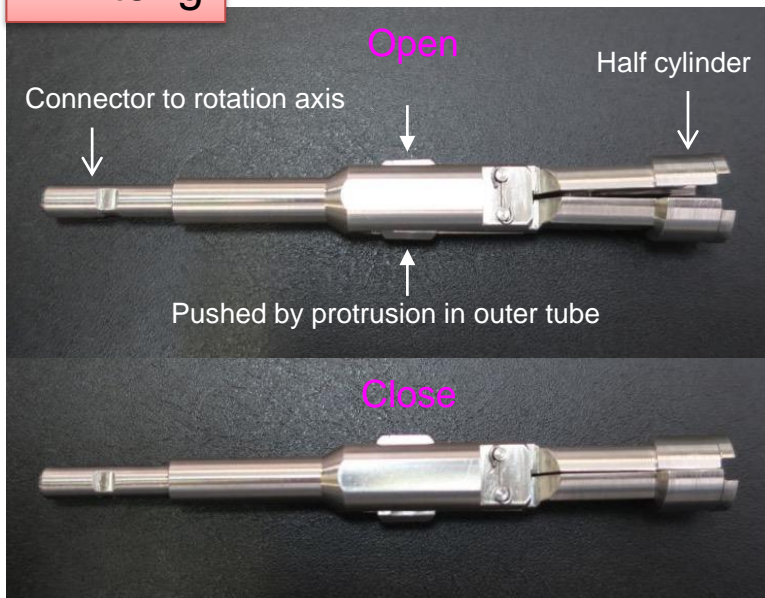
Sample holder

Composed of the outer tube and pin-tong

Outer tube



Pin-tong



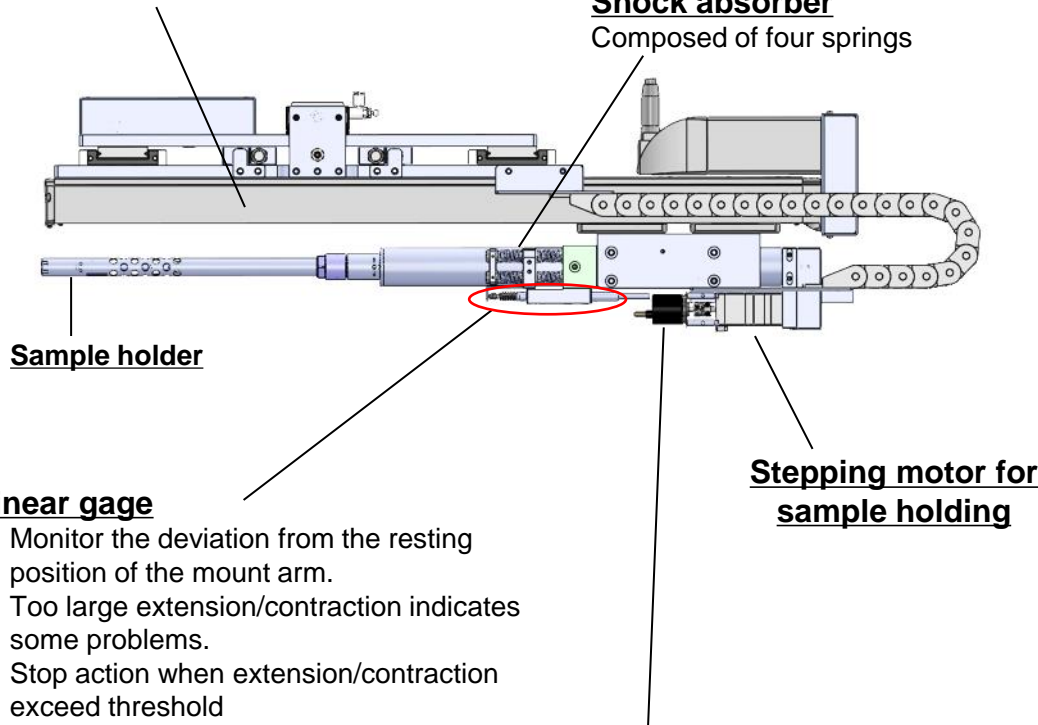
Mount arm

Translation stage

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- The speed is 465 mm s^{-1}

Shock absorber

Composed of four springs

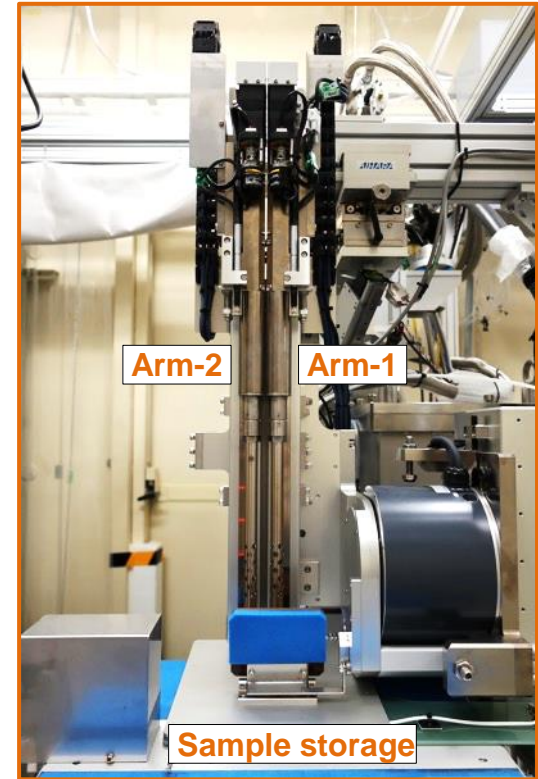


Linear gage

- Monitor the deviation from the resting position of the mount arm.
- Too large extension/contraction indicates some problems.
- Stop action when extension/contraction exceed threshold

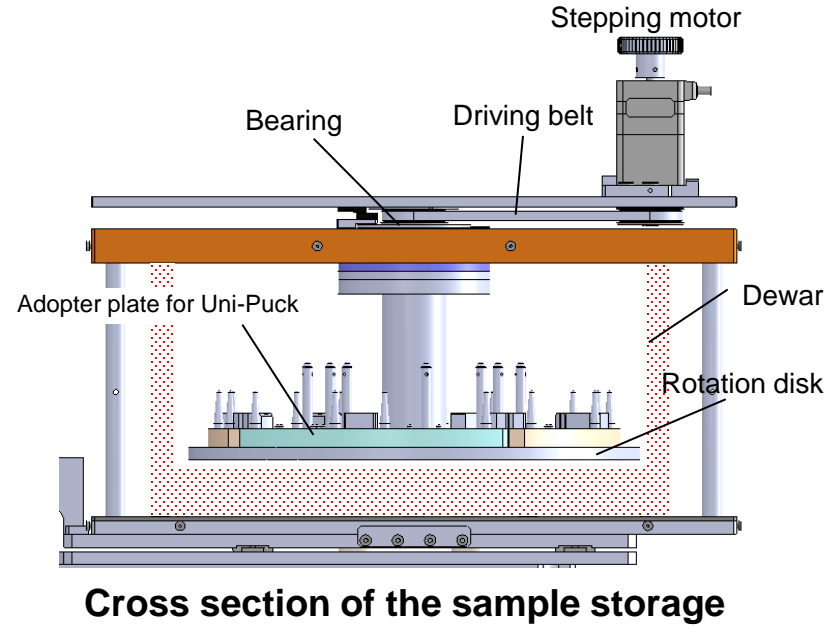
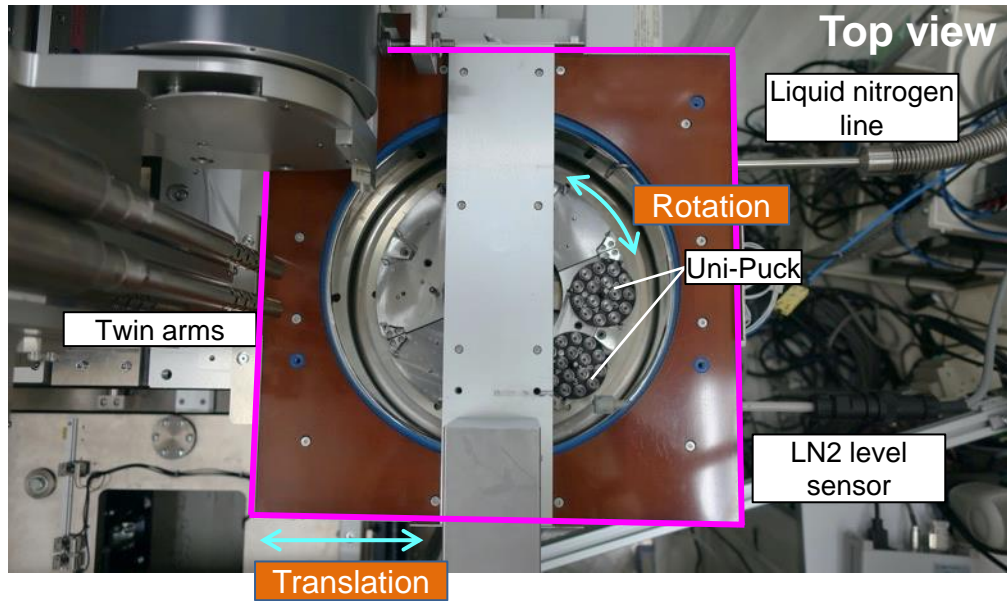
Rotary encoder

- Monitor rotation angle of the pin tongs because it directly relates to the open/close of the pin-tongs.
- Too much rotation means that no sample pin is gripped
- Too little rotation means that open/close of the pin-tongs fails.

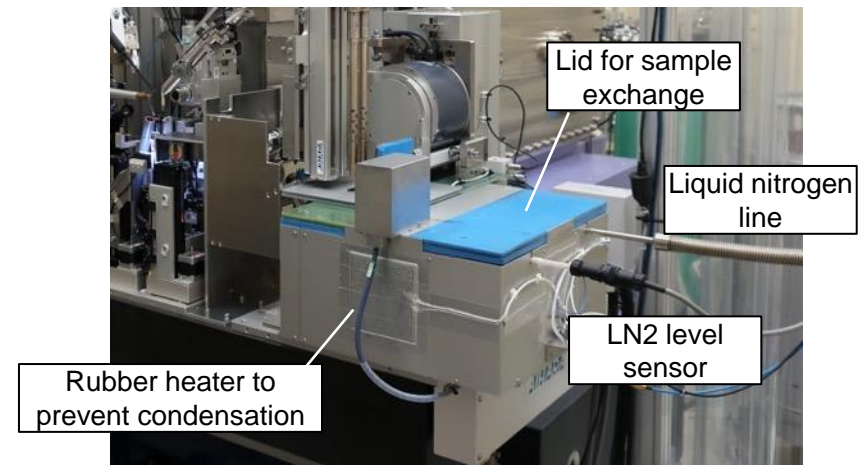


Each mount arm has a translational axis to independently access the goniometer/Uni-puck.

Sample storage

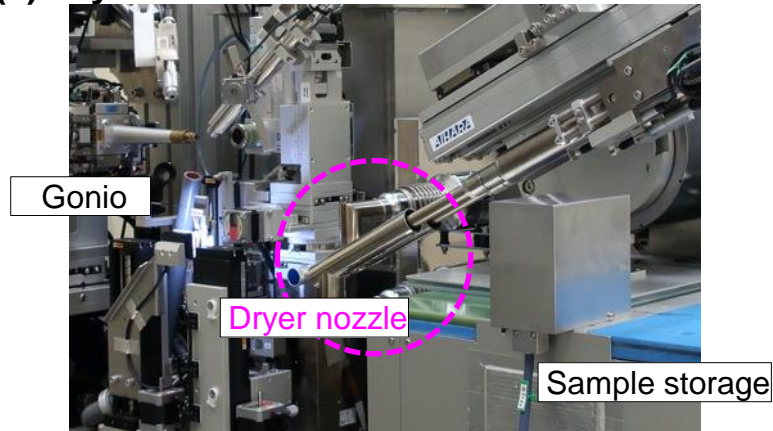


- Dewar is enclosed in a square chasis of $400 \times 400 \times 210$ mm
- The specified sample is conveyed to the position of mount arm by the combination of translation stage and rotation disc.
- Eight Uni-Pucks can be installed at once



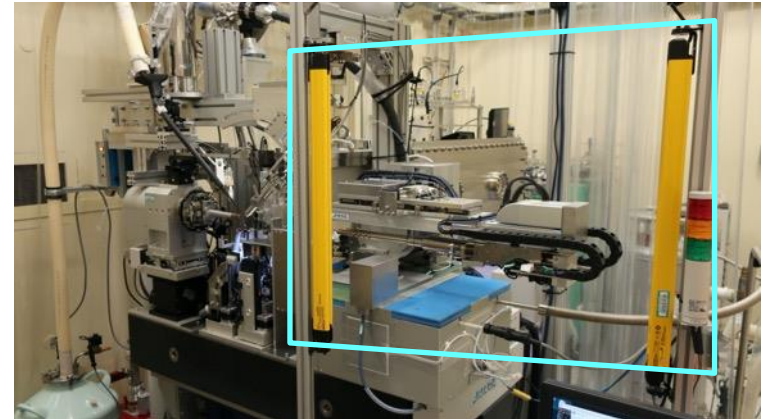
Ancillary equipments for SPACE-II

(1) Dryers



- Remove frost attached on the sample holder.
- Drying every one hour is recommended.
- It takes 2 min. But, can be conducted during sample centering or data collection; not affect the throughput.

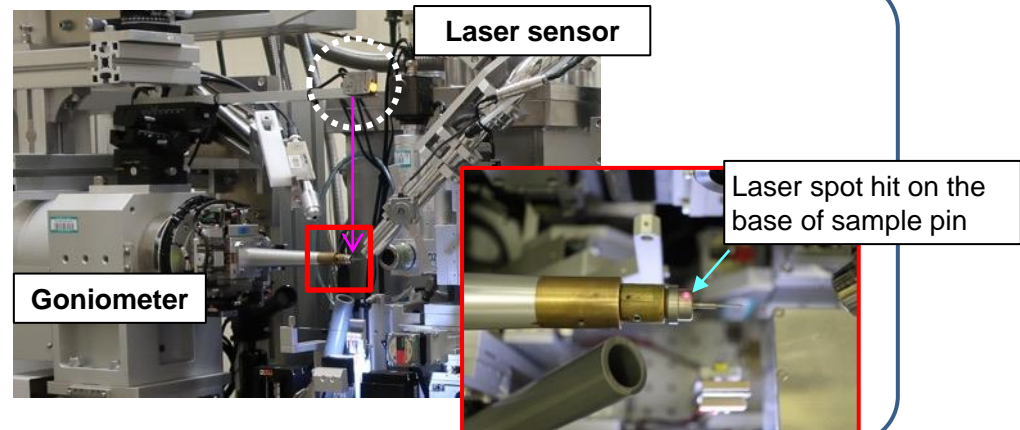
(2) Safety light curtain



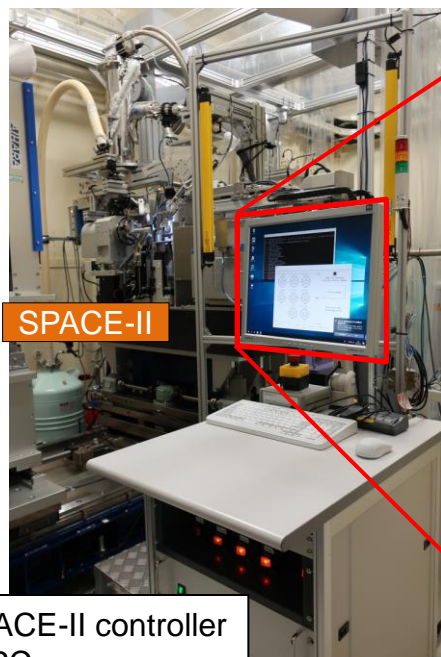
- SPACE-II stopped immediately when something crosses between the two yellow bars.
- We implemented this, because the motion of SPACE-II is so rapid that it is dangerous for a user to come nearby while it is moving.

(3) Lase CMOS sensor

- Confirm the successful mount/dismount of a sample pin on/from gonio.
- In case of failure, a retry sequence proceeds automatically.



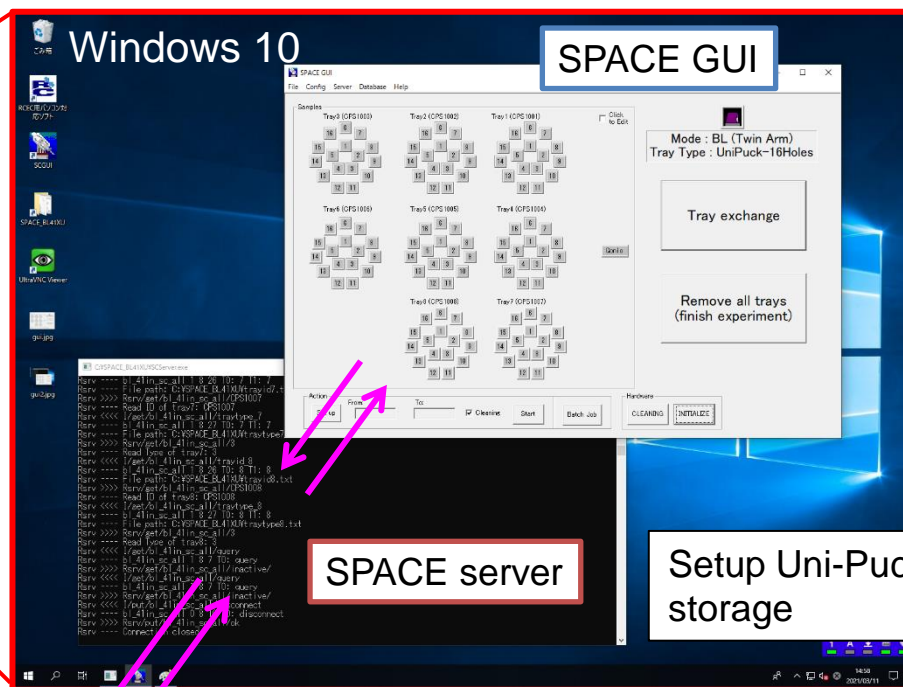
Controller and software



SPACE-II

SPACE-II controller

- PC
- Motor controller
- Dryer controller
- etc



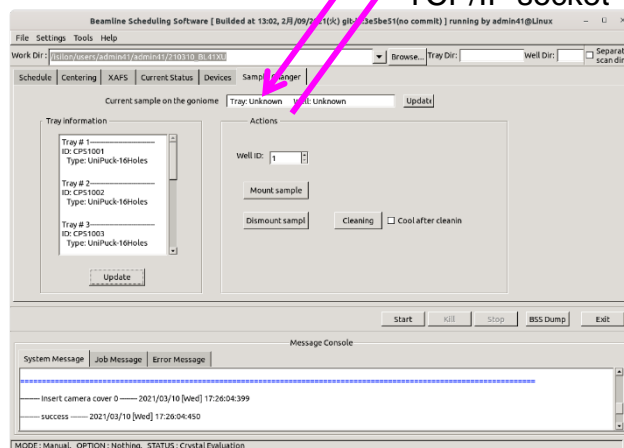
Windows 10

SPACE GUI

SPACE server

Setup Uni-Puck in sample storage

TCP/IP socket



Exchange sample on the goniometer

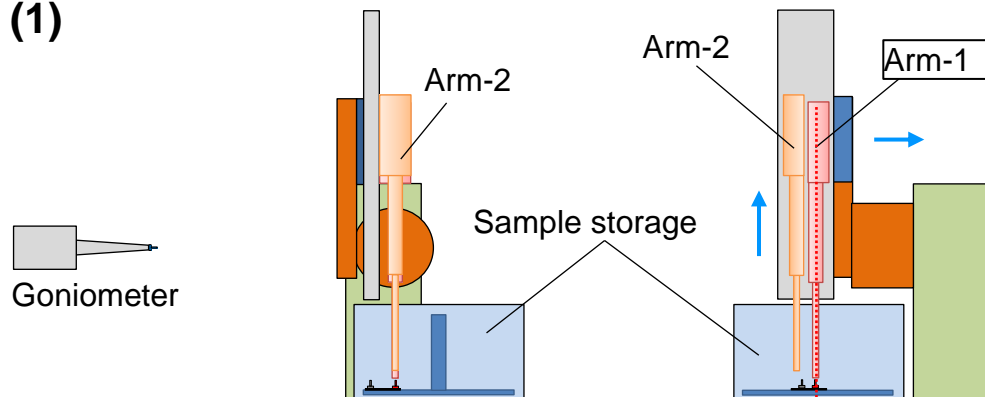
Data collection software (BSS)

Sequence of sample exchange

View toward incident X-ray

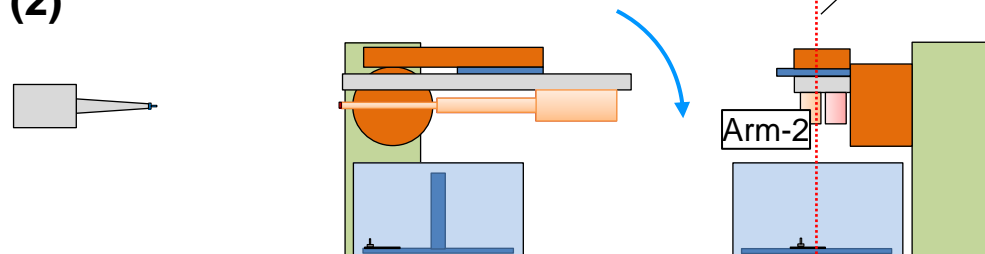
View toward goniometer

(1)



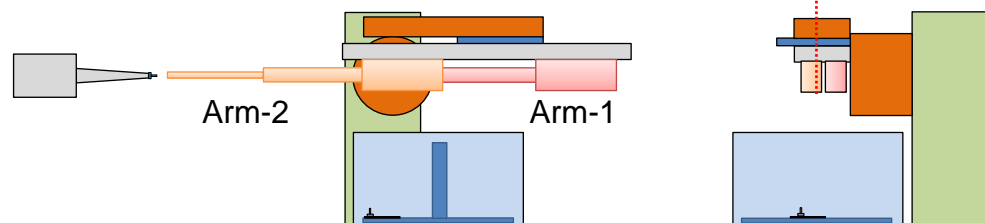
- Specified sample pin is moved to mounting position in Dewar.
- Arm-1 picks up the sample pin.
- Twin arms are pulled up, then their position is switched.

(2)



- Twin arms are rotated by 90° to direct them to goniometer

(3)

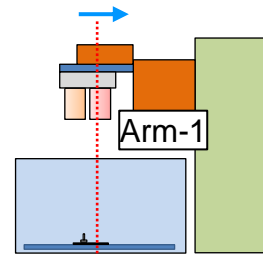
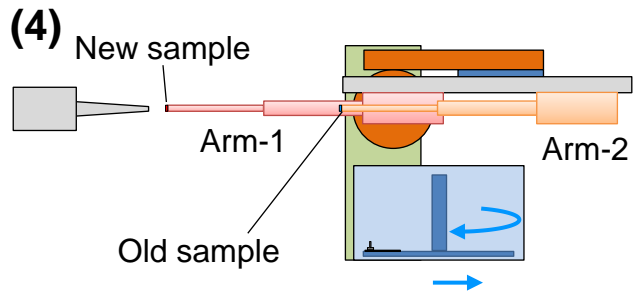


- Sample pin on goniometer is dismantled by extending Arm-2.
- Position of twin arms is switched.

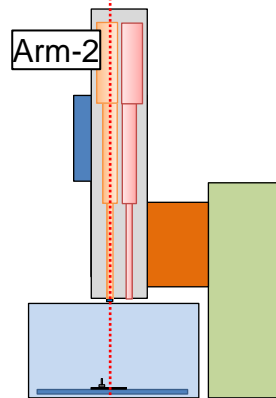
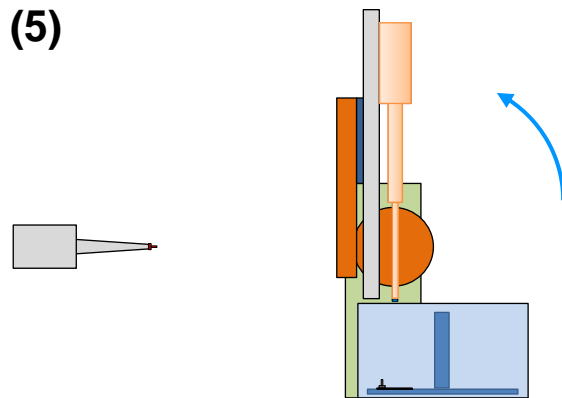
Sequence of sample exchange

View toward incident X-ray

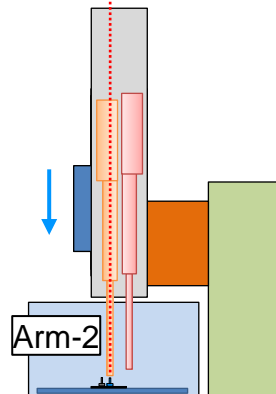
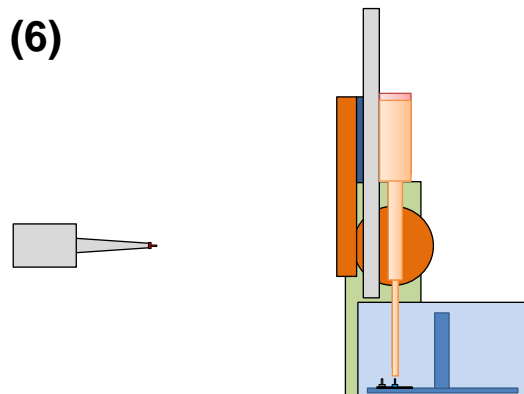
View toward goniometer



- New sample pin is mounted by extending Arm-1.
- While Arm-1 moving back, position of Uni-Puck is changed to return dismantled sample pin to original position.
- Positions of twin arms are switched.

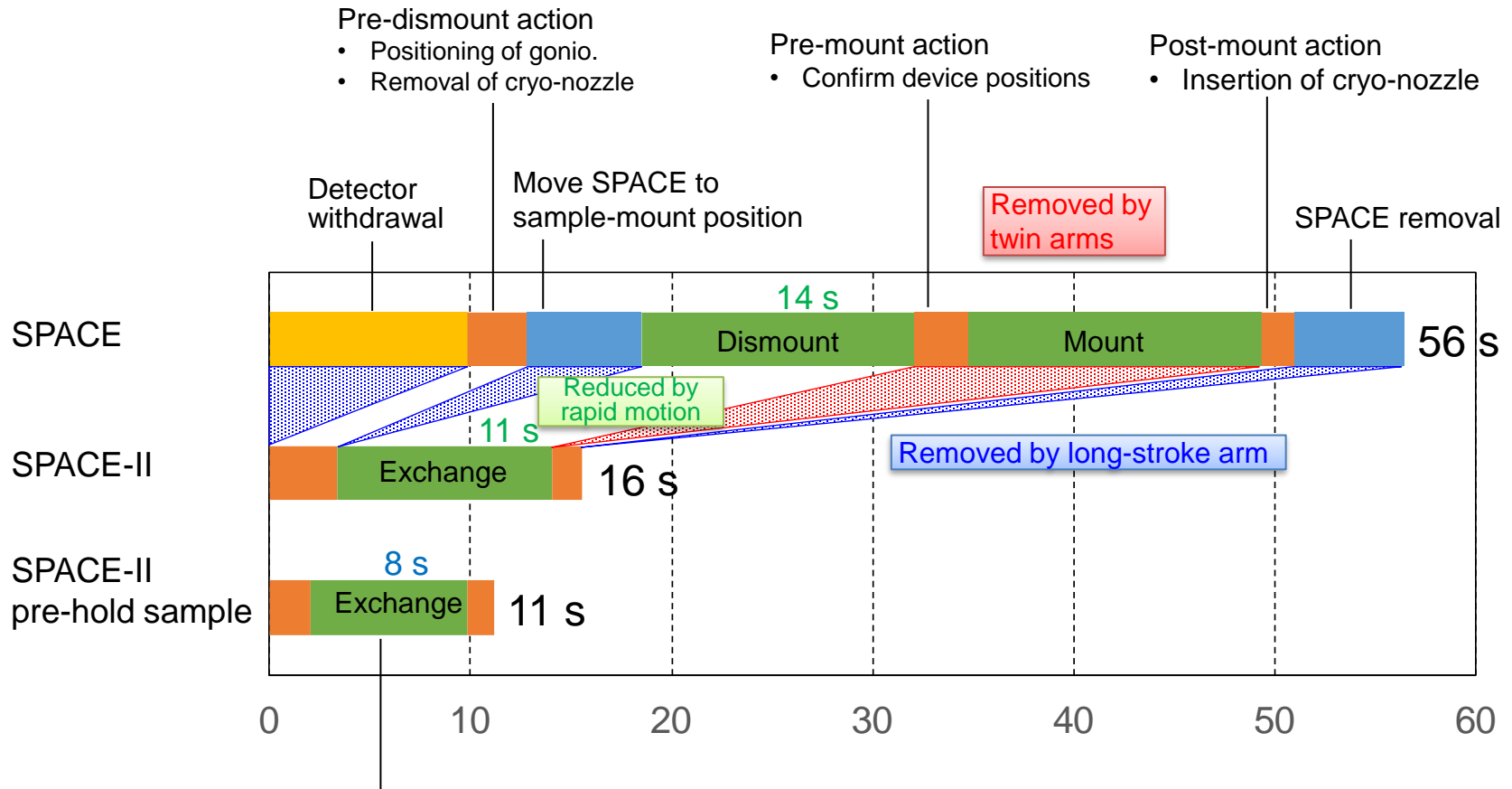


- Twin arms are rotated by 90° to direct them to sample storage.



- Dismounted sample pin is transferred to Uni-Puck.

Timeline of sample exchange of SPACE and SPACE-II



Implementation of the twins arms allows pre-hold of a new sample in the case of automatic data collection.

Performance of SPACE-II

	SPACE	SPACE-II
Period	FY2016 (Apr. 2016 to Dec. 2016)	FY2018 (Apr. 2018 to Feb. 2019)
No. of days	127	130
Total no. of samples	16,708	23,525
Average	132/day	185/day
Maximum	290/day	371/day
No. of error	13	29
Percentage of error	0.078%	0.12%

Data collection efficiency was Improved by 40%

Reason of error

Reason of error	No.
Fail to release the sample pin on the goniometer or Uni-Puck Caused by ice at the tip of arm; it happens in continuous operation without drying more than one hours.	9
Fail to pick up sample pins from Uni-Pucks Caused by ice between the sample pin and Uni-puck which might attached during loading sample pins on Uni-puck.	5
Improper loading Uni-Puck in the sample storage, use of broken Uni-Pucks, or use of defective sample pins Not a problem of SPACE-II	5
Improper setting of software or hard ware (bug of software, mis-alignment of sensor) Already fixed	3
Unknown error	7
Total	29 (21)
Percentage of error	0.12% (0.09%)

Summary

Development of SPACE-II

- Exchange sample in 16 s
- Improve data collection efficiency by 40%
- Error rate $< 1\%$
- Installed at four MX beamlines:
BL41XU, BL26B2, BL44XU, BL45XU

The remaining problem

Accommodate only 8 Uni-Puck at once; **which is a big problem in automatic data collection with ZOO.**

Summary

Development of SPACE-II

- Sample exchange in 16 s
- Failure rate ~ 1%
- Improve efficiency by 40%
- Installed at four MX beamlines:
BL26B2, BL41XU, BL44XU, BL45XU

The remaining problem

Accommodate only 8 Uni-Puck at once; big problem in automatic data collection, **which will be fixed soon.**

Acknowledgements

- JASRI SPring-8
 - Hironori Murakami
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 - Takahiko Hoshi
 - Masahiro Manoda
 - Makoto Toyama
 - Yasufumi Torizuka
- Users at SPring-8 MX BLs



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