

Scanning 3D X-ray Diffraction Microscopy of Non-Cubic Au Microcrystallite

Summer Student:

Ihor Svynarskyi

Supervisor:

Chaitali Sow

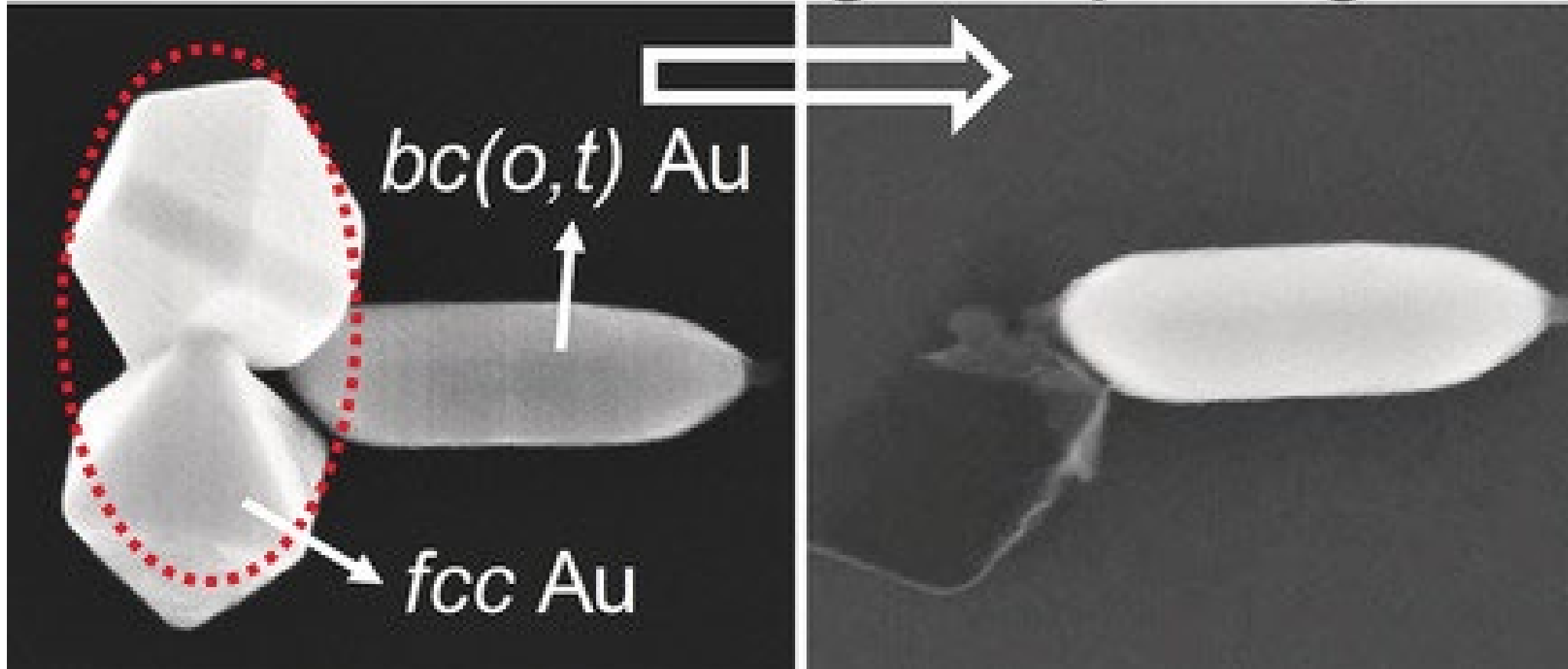
DESY FS-PETRA (PETRA III)

HELMHOLTZ



Non-Cubic Au Microcrystallite

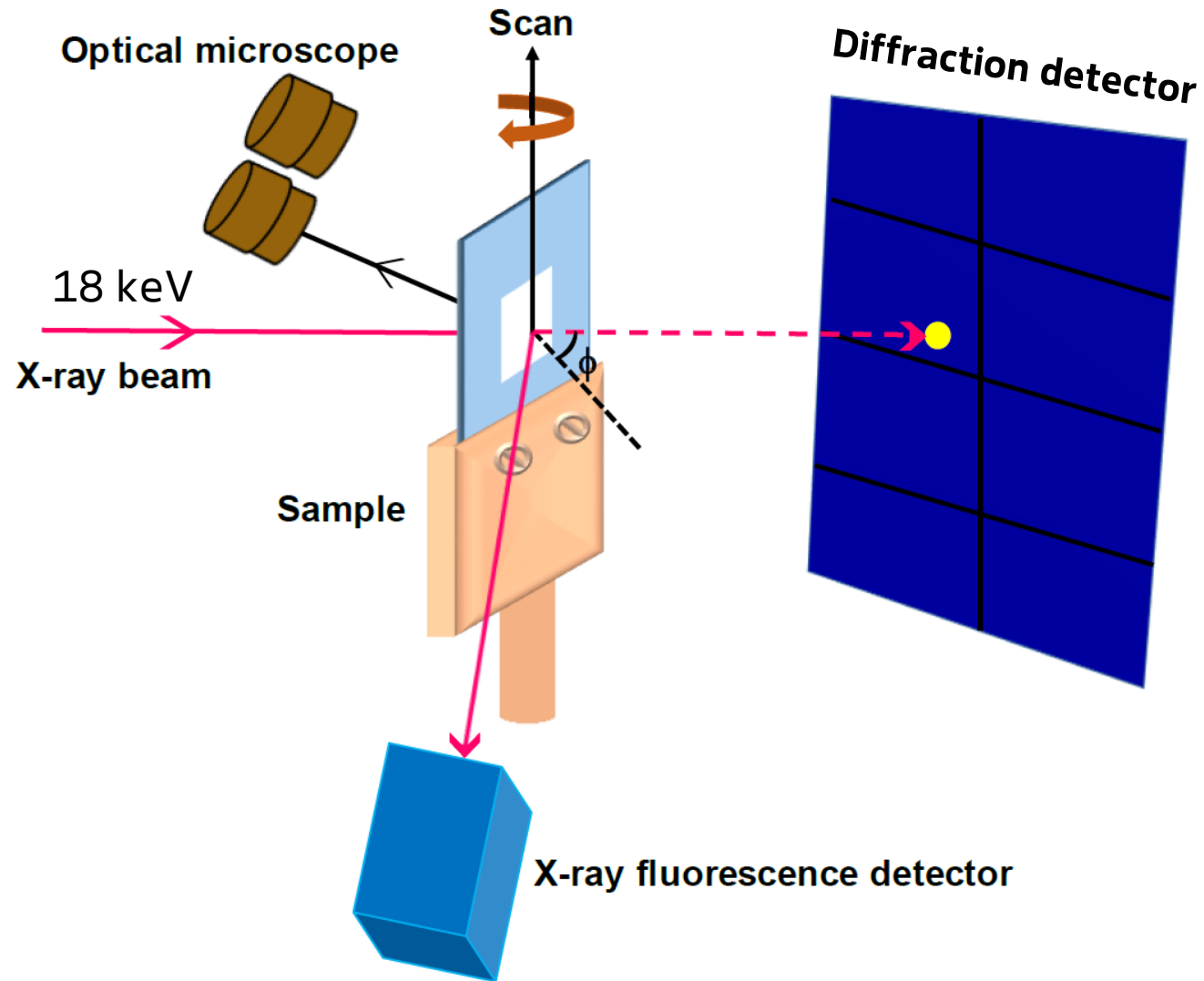
treatment with Hg or aqua regia



Mettela, G.; et al. *Angew. Chem., Int. Ed.* **2018**, 57, 9018

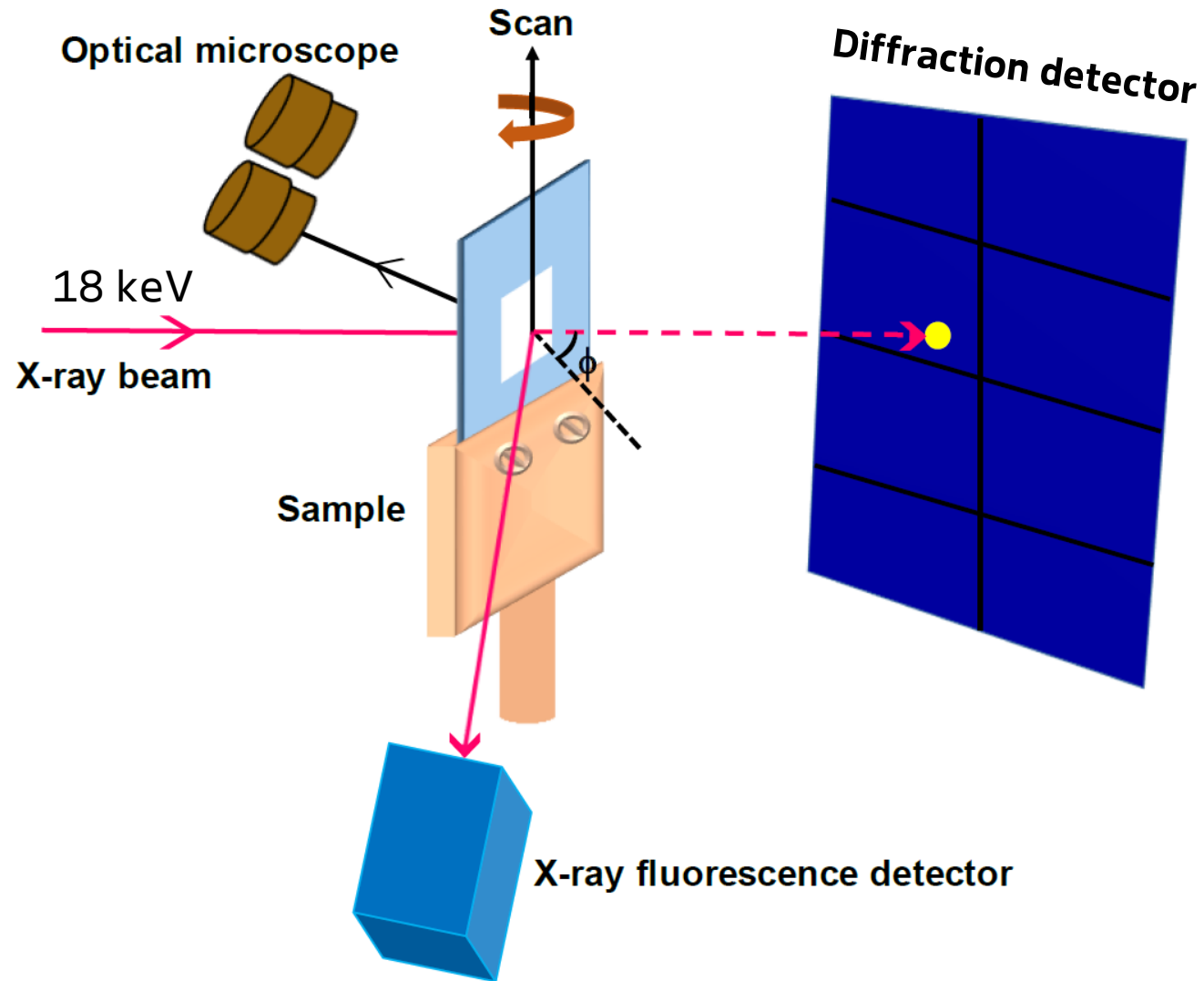
Mettela, G.; et al. *Nano Res.* **2017**, 10, 2271

Experimental Setup



Sow, C.; et al. *ACS Nano* **2020**, *14*, 9456–9465

Experimental Setup



Sow, C.; et al. *ACS Nano* **2020**, *14*, 9456–9465

DESY. Ihor Svytnarskyi | Scanning 3D X-ray Diffraction Microscopy | Summer Student Sessions | 11.09.2025

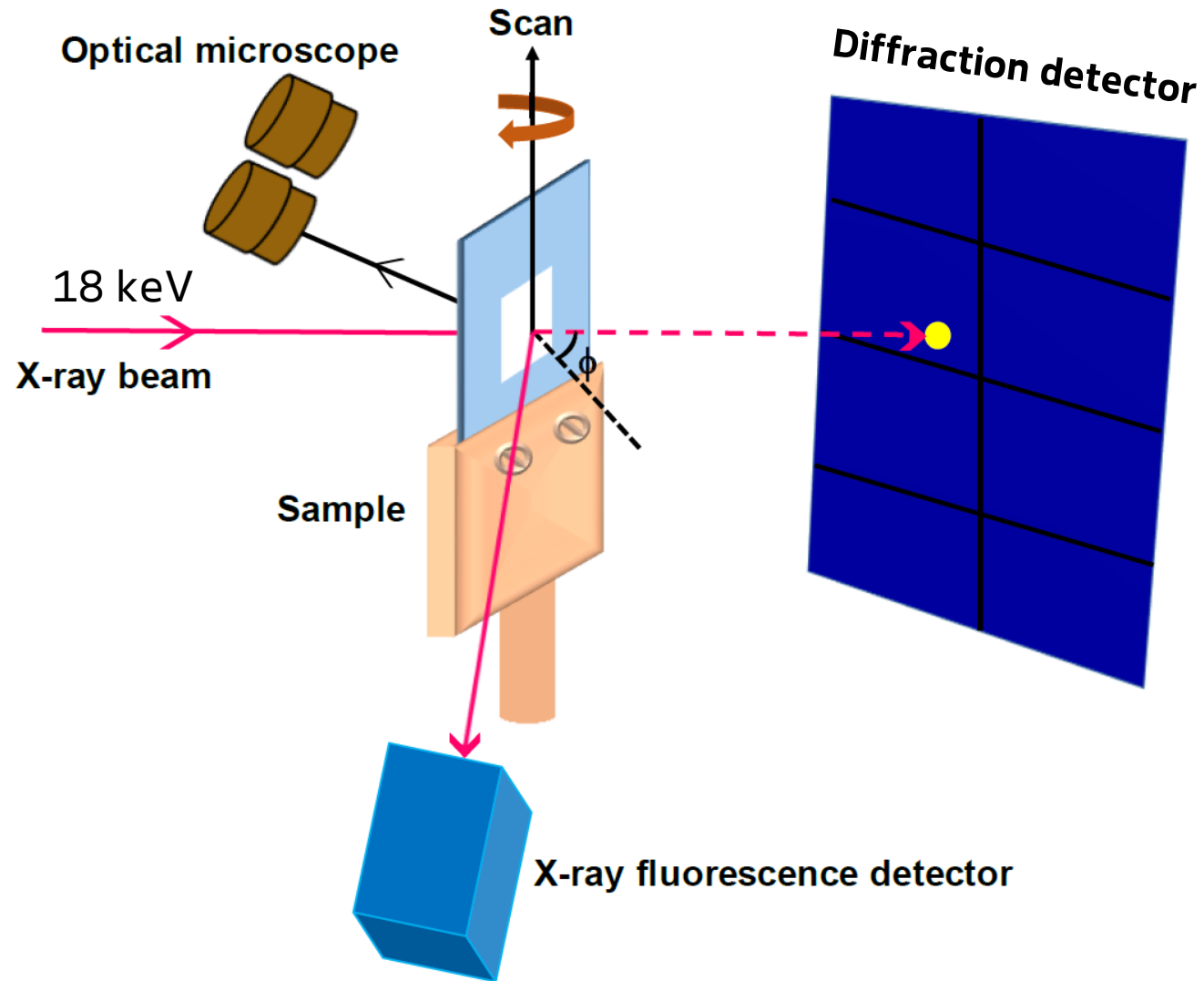
Photo of the sample



Experiment conducted
at P06, PETRA III, DESY

Unpublished 3

Experimental Setup



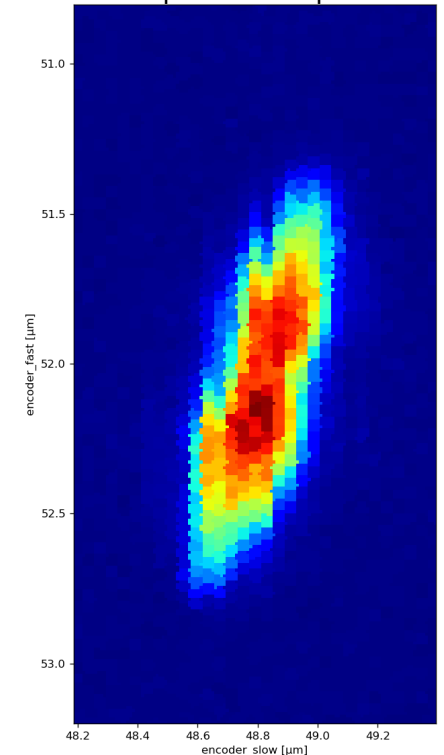
Sow, C.; et al. *ACS Nano* **2020**, *14*, 9456–9465

Photo of the sample



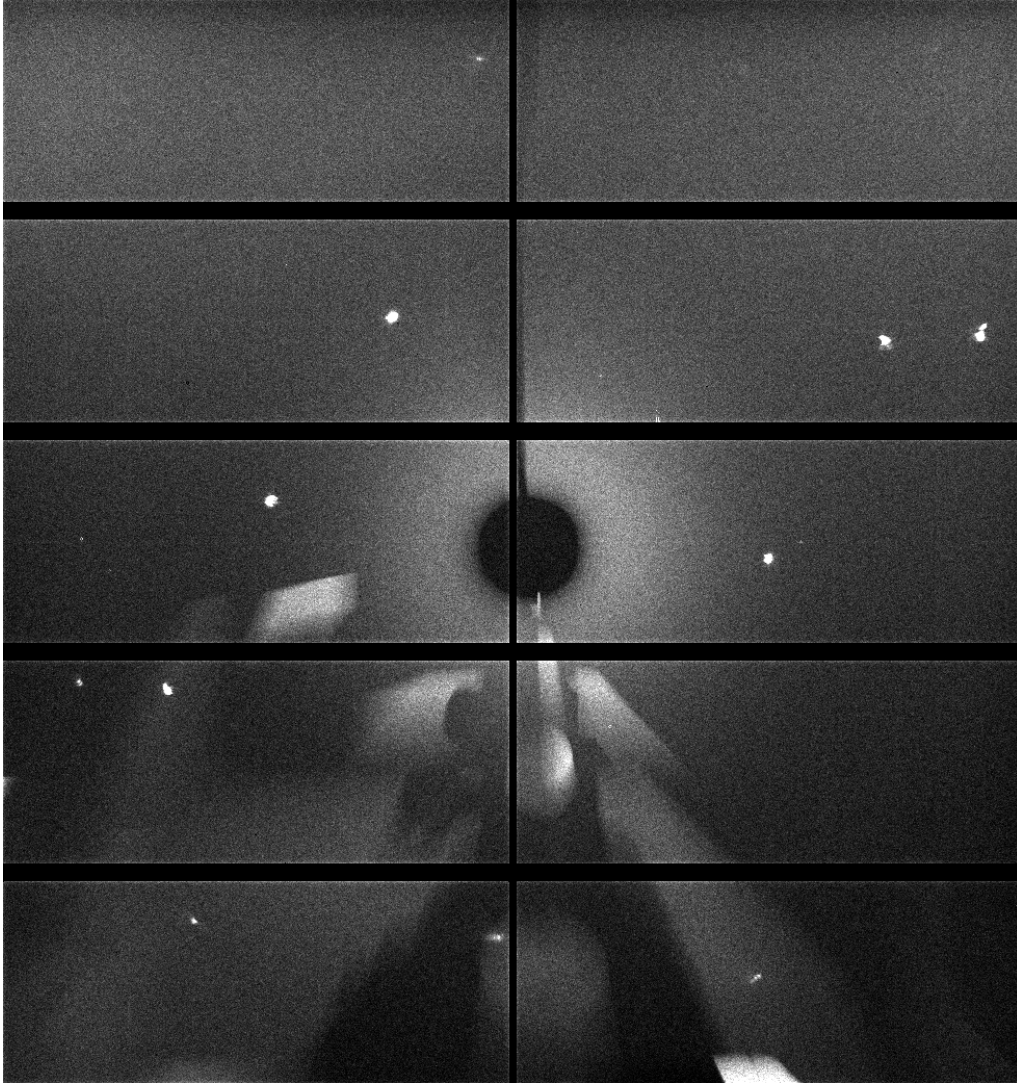
Experiment conducted
at P06, PETRA III, DESY

Interpolated map of Au



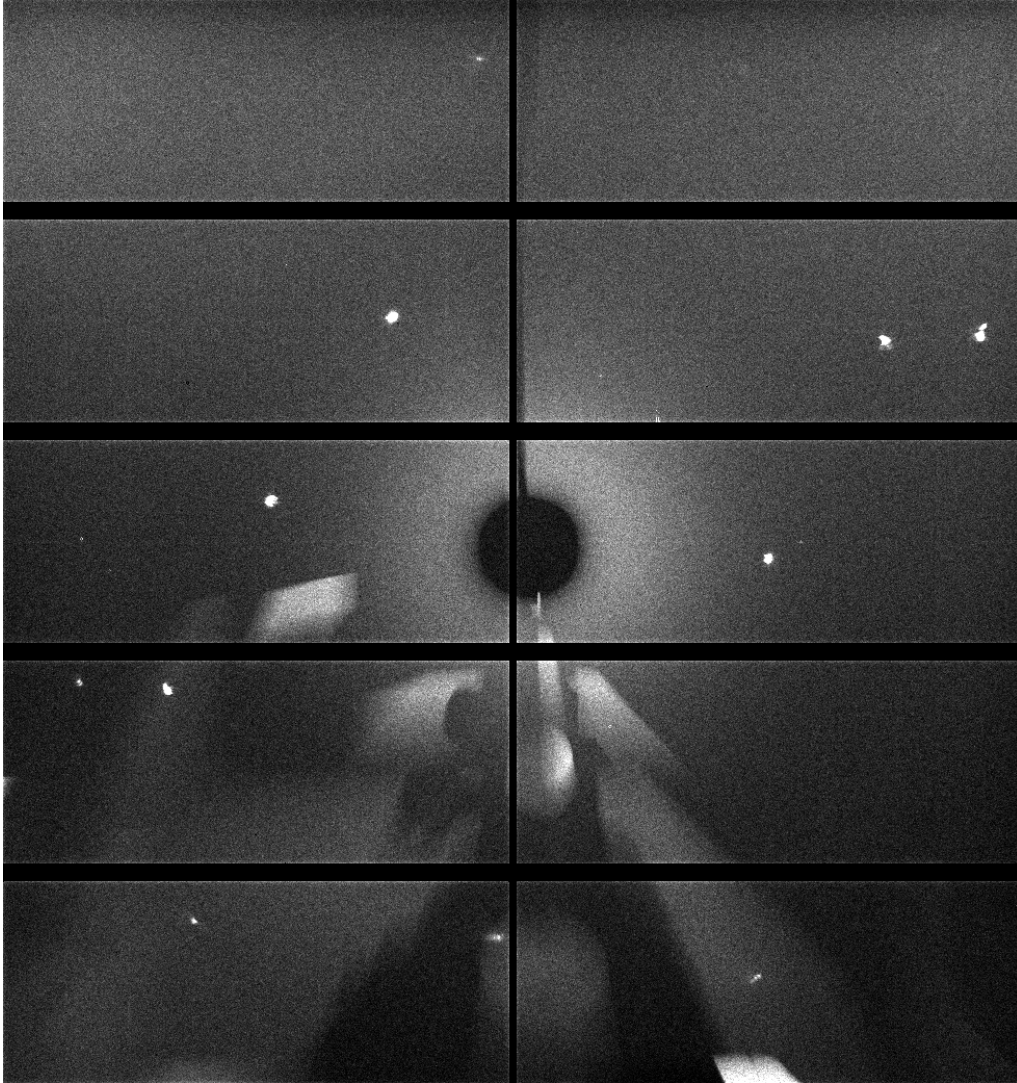
X-ray Diffraction Patterns

Individual scan

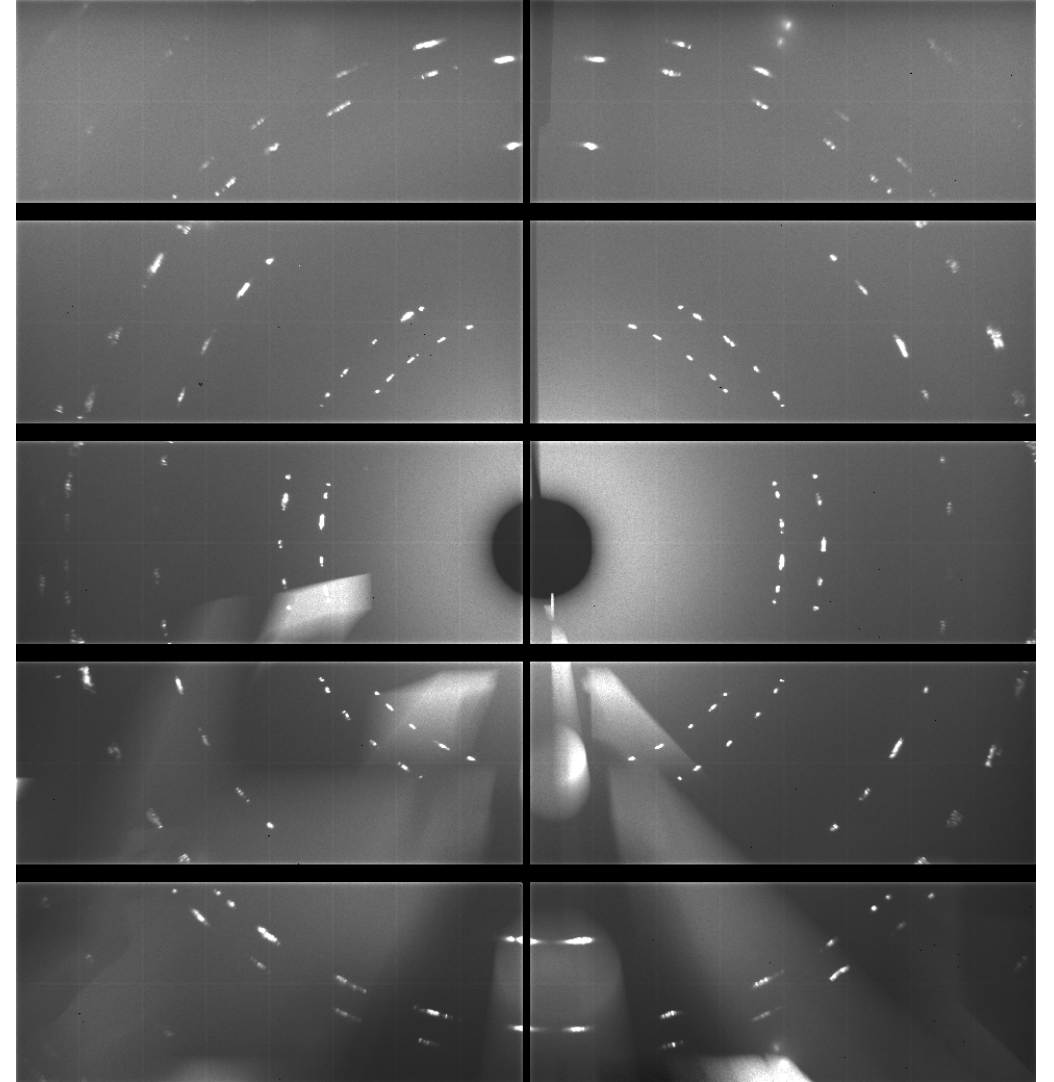


X-ray Diffraction Patterns

Individual scan

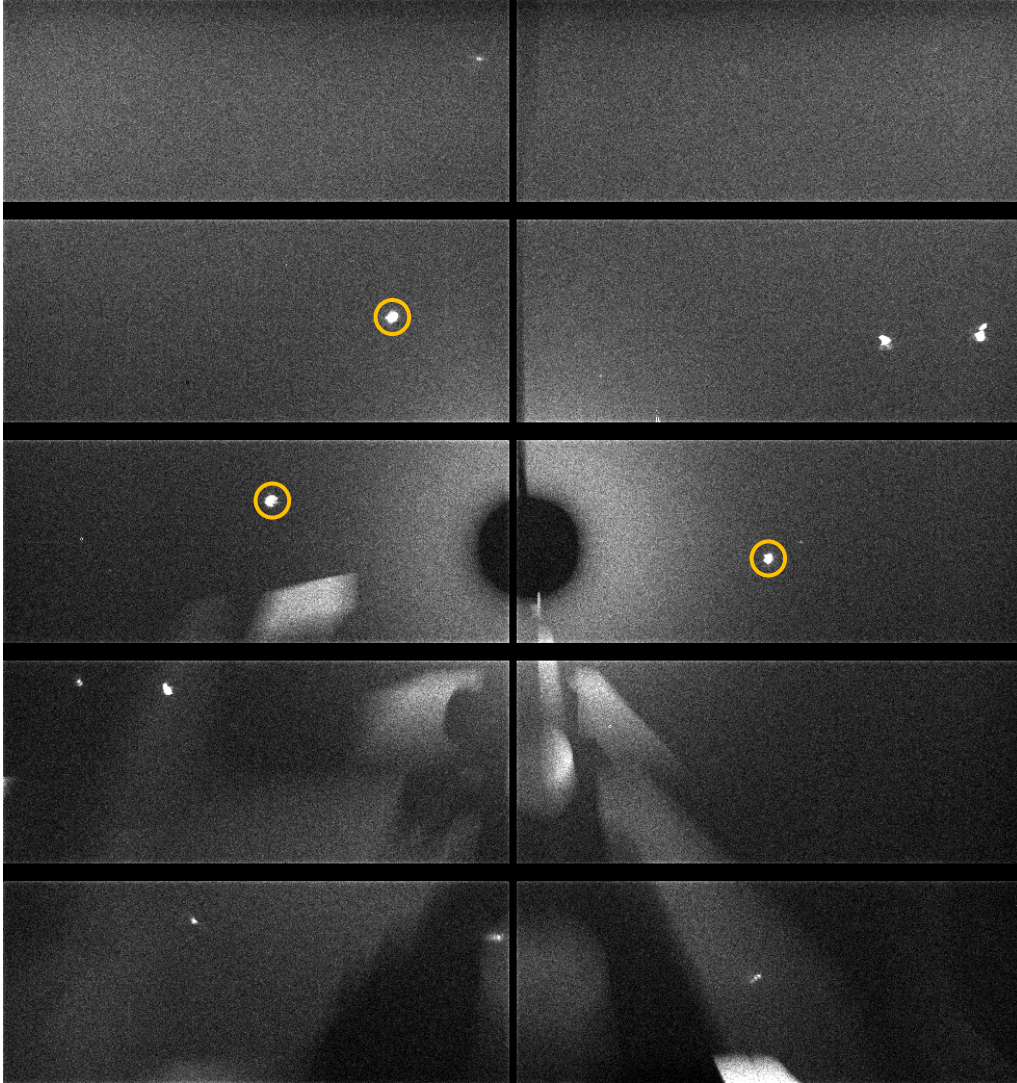


Diffraction pattern summed over all rotations

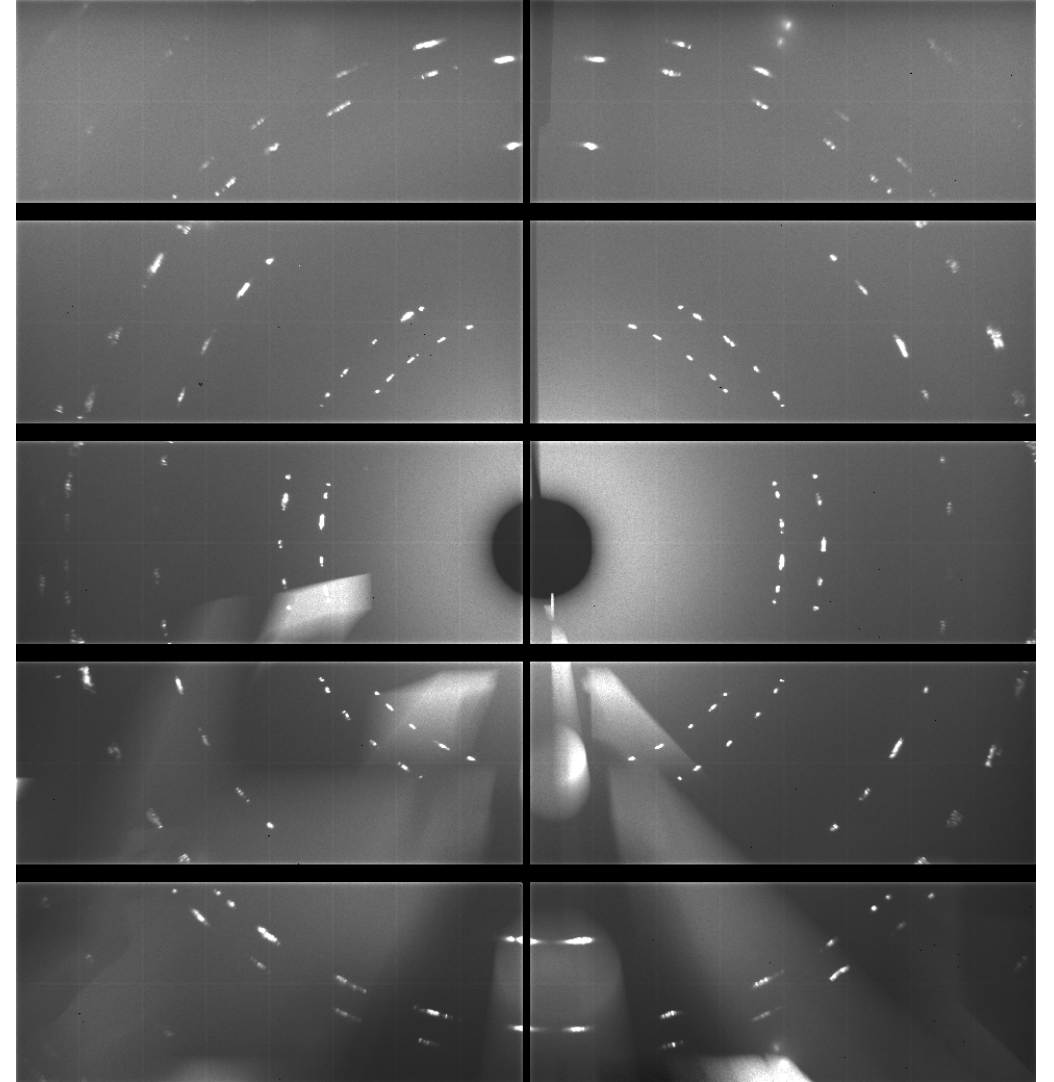


X-ray Diffraction Patterns

Individual scan

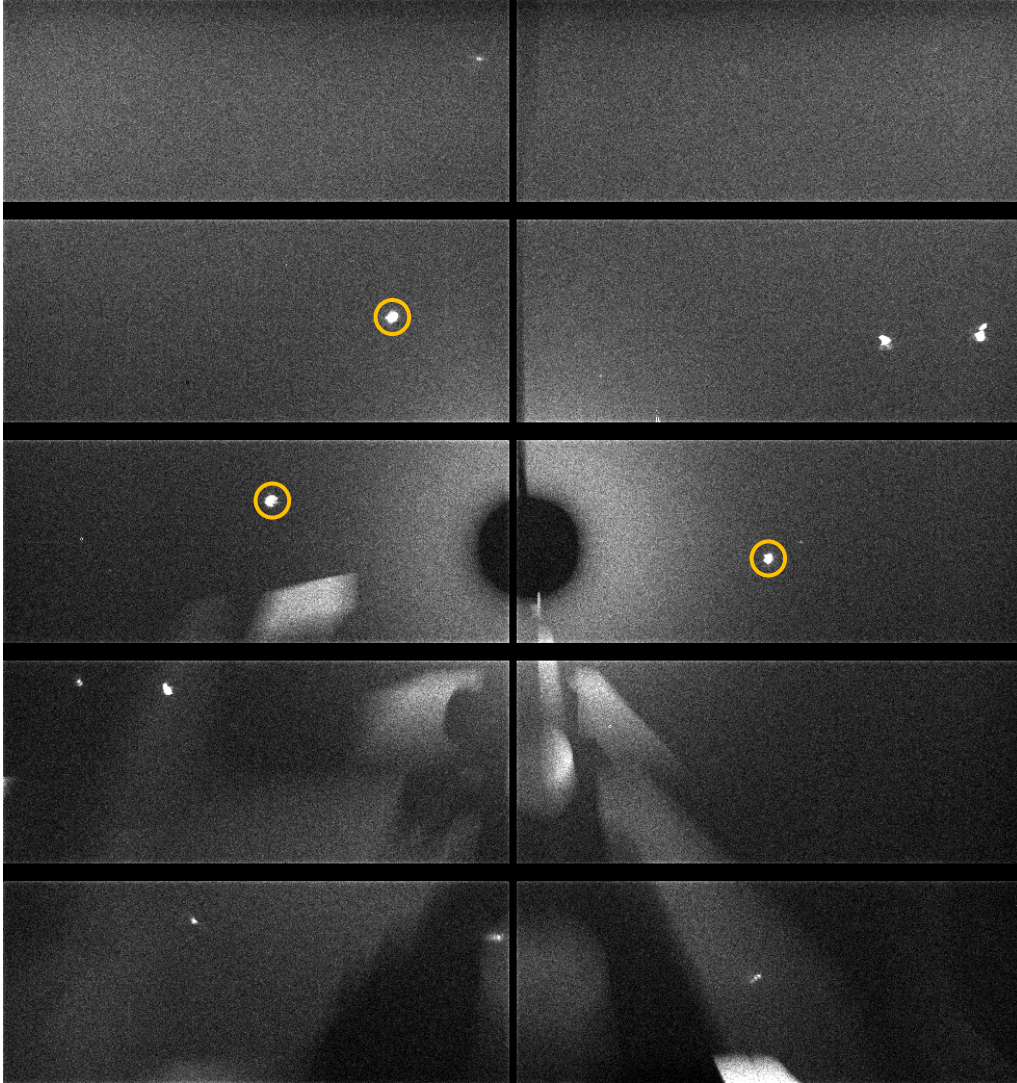


Diffraction pattern summed over all rotations

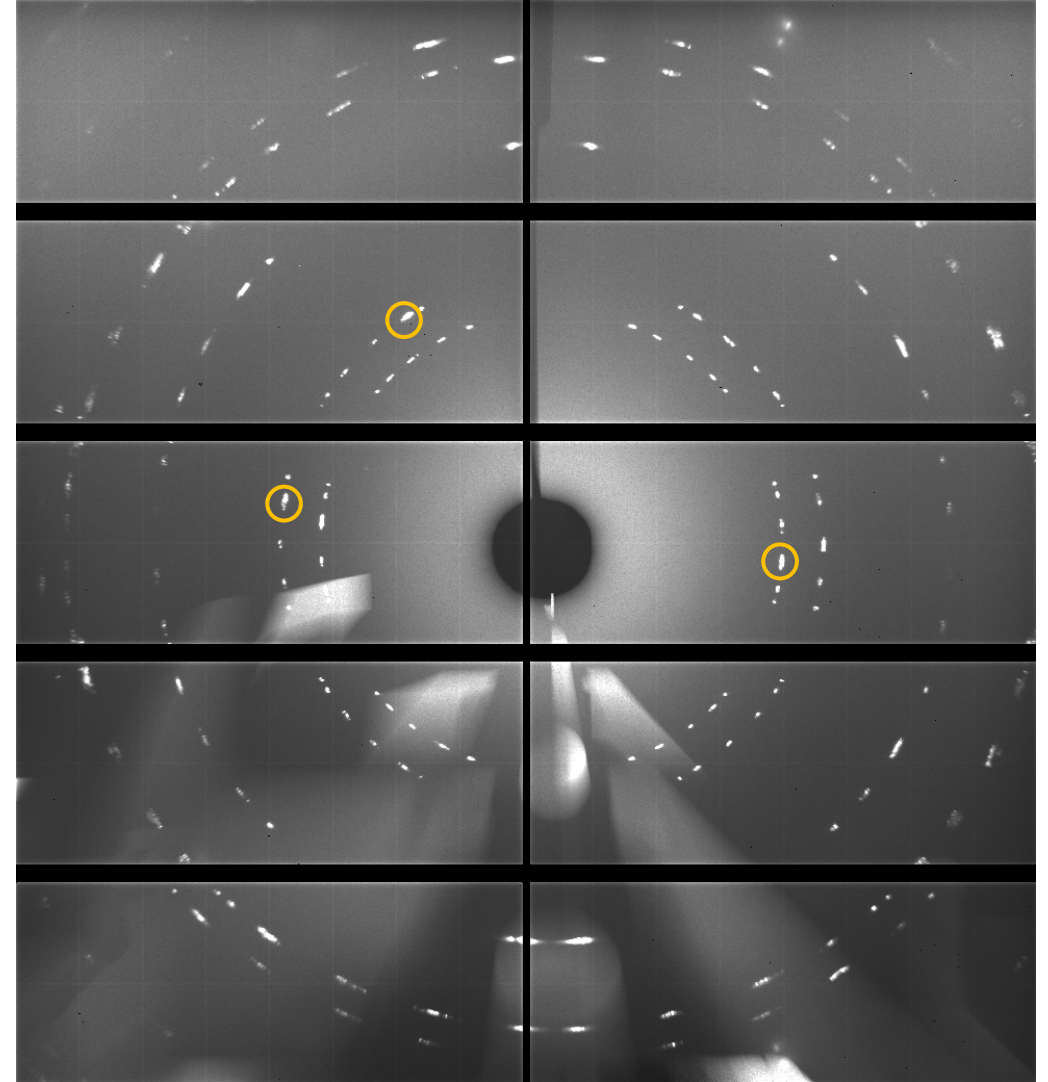


X-ray Diffraction Patterns

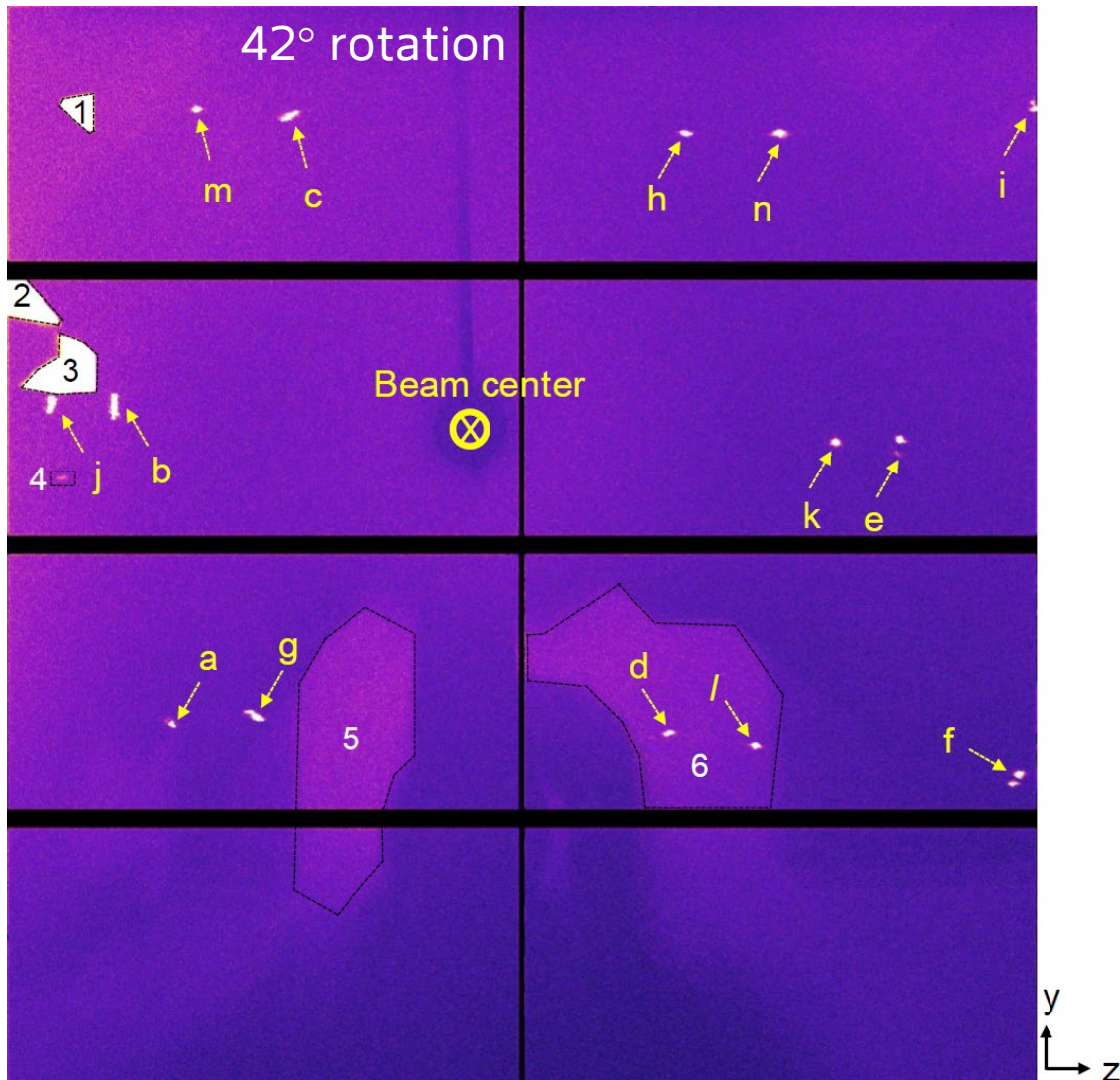
Individual scan



Diffraction pattern summed over all rotations

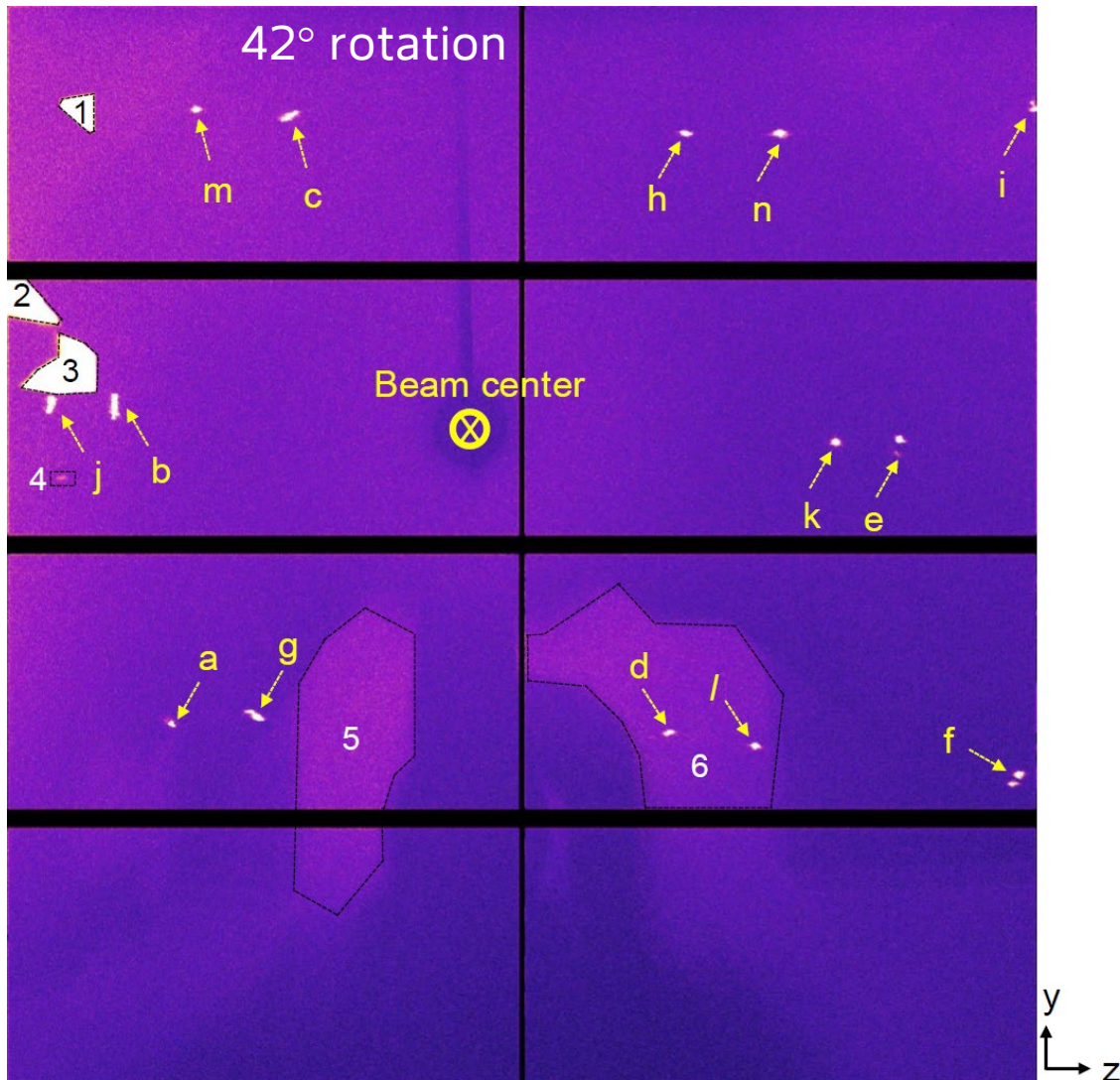


Comparison of Diffraction Patterns



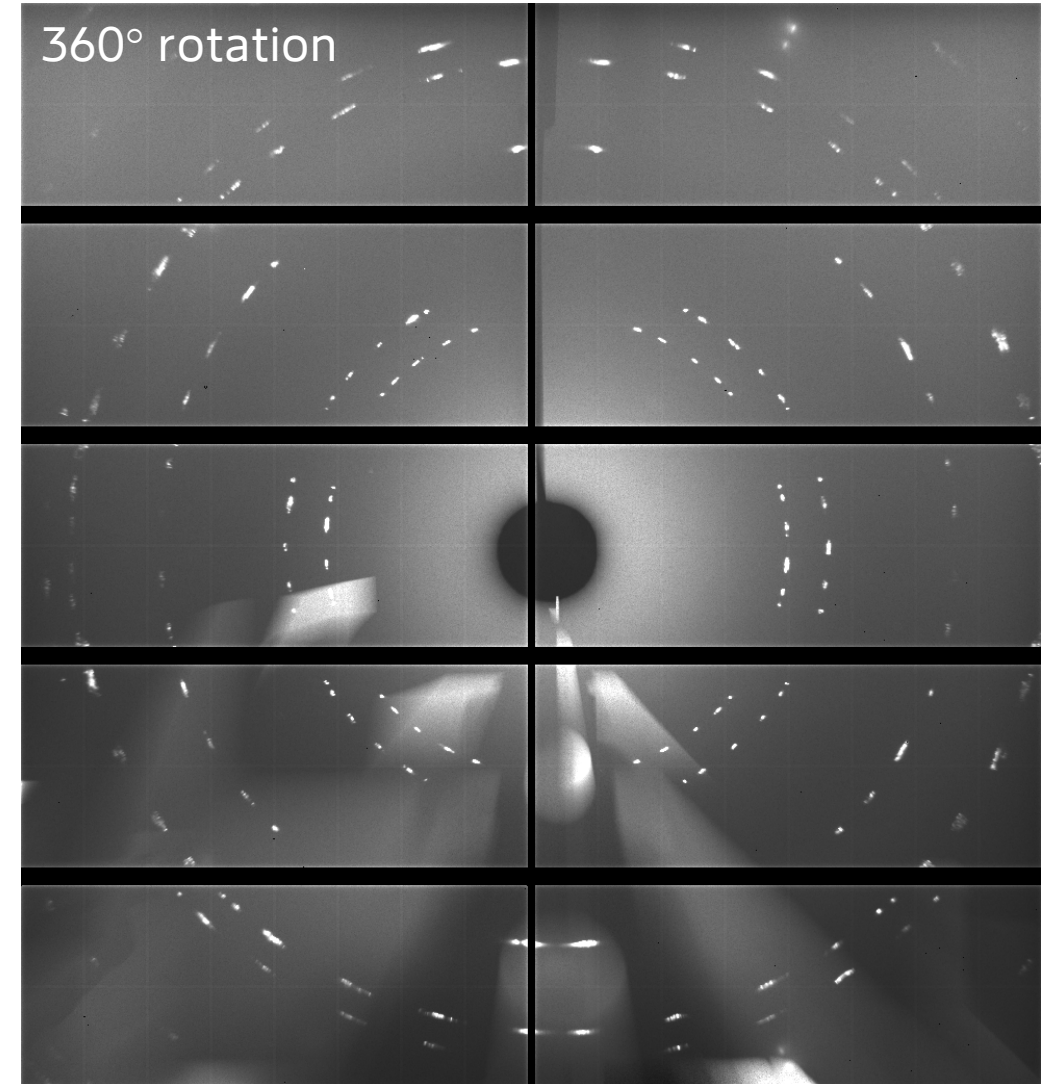
Sow, C.; et al. *ACS Nano* **2020**, *14*, 9456–9465

Comparison of Diffraction Patterns

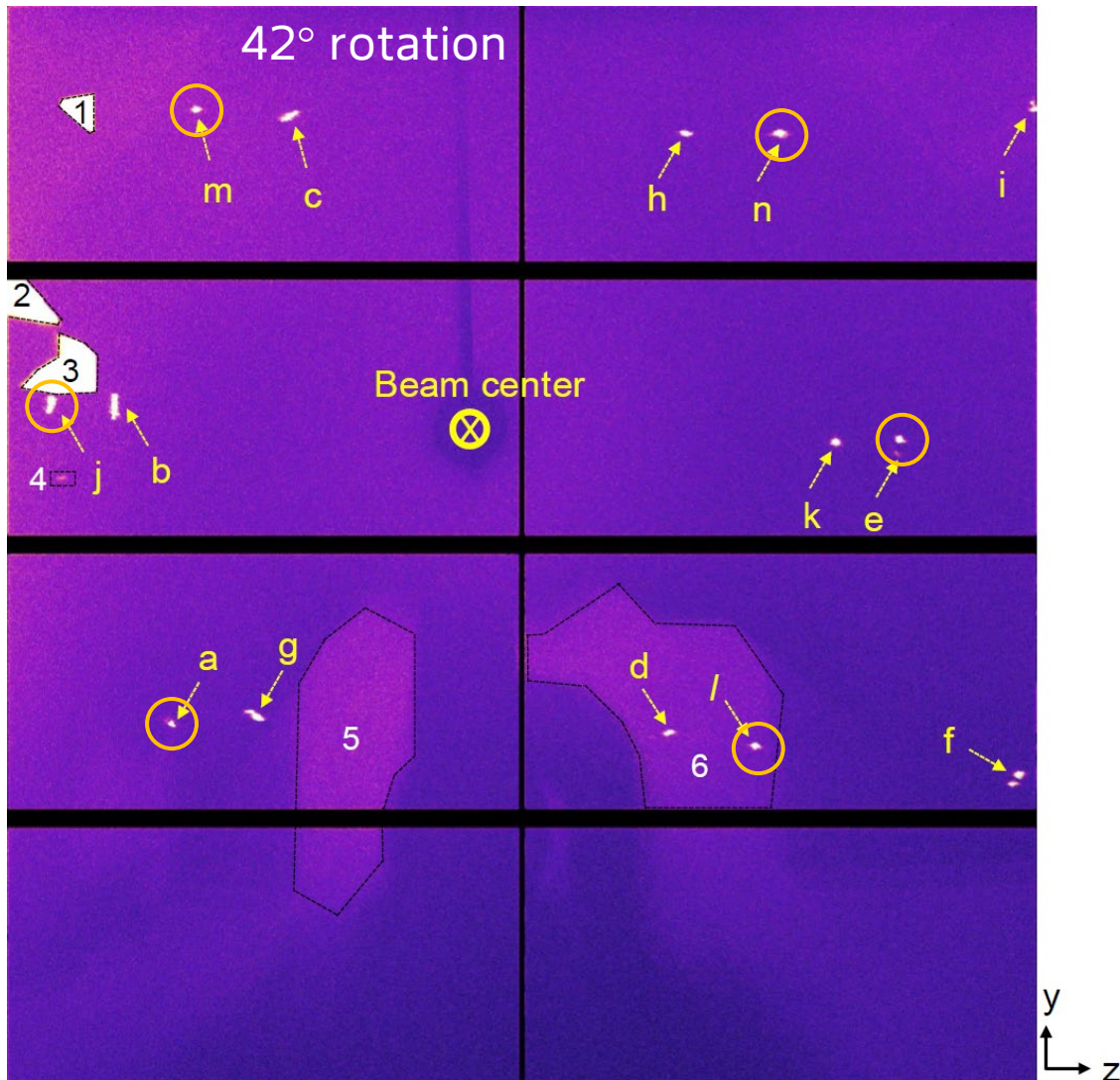


Sow, C.; et al. *ACS Nano* **2020**, *14*, 9456–9465

Diffraction pattern summed over all rotations

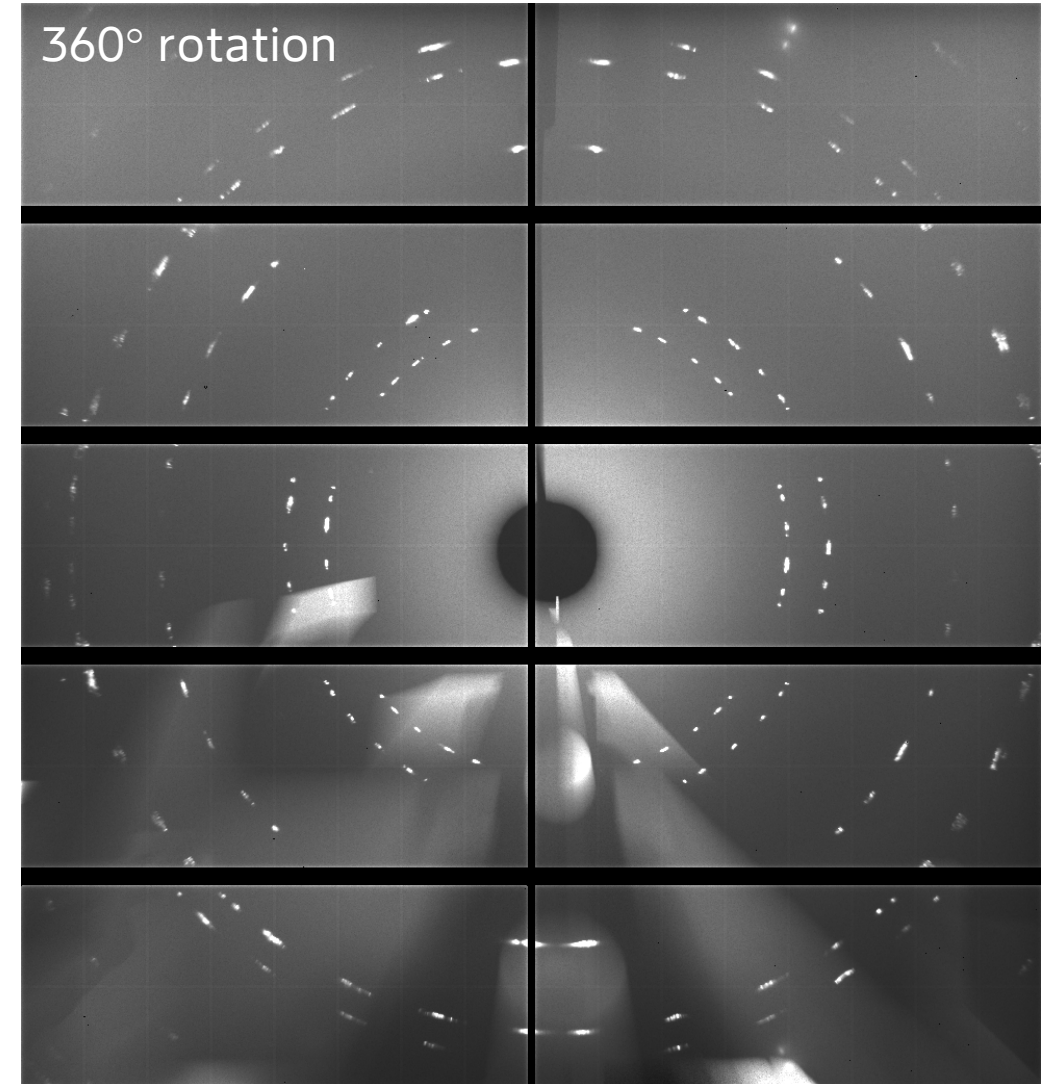


Comparison of Diffraction Patterns

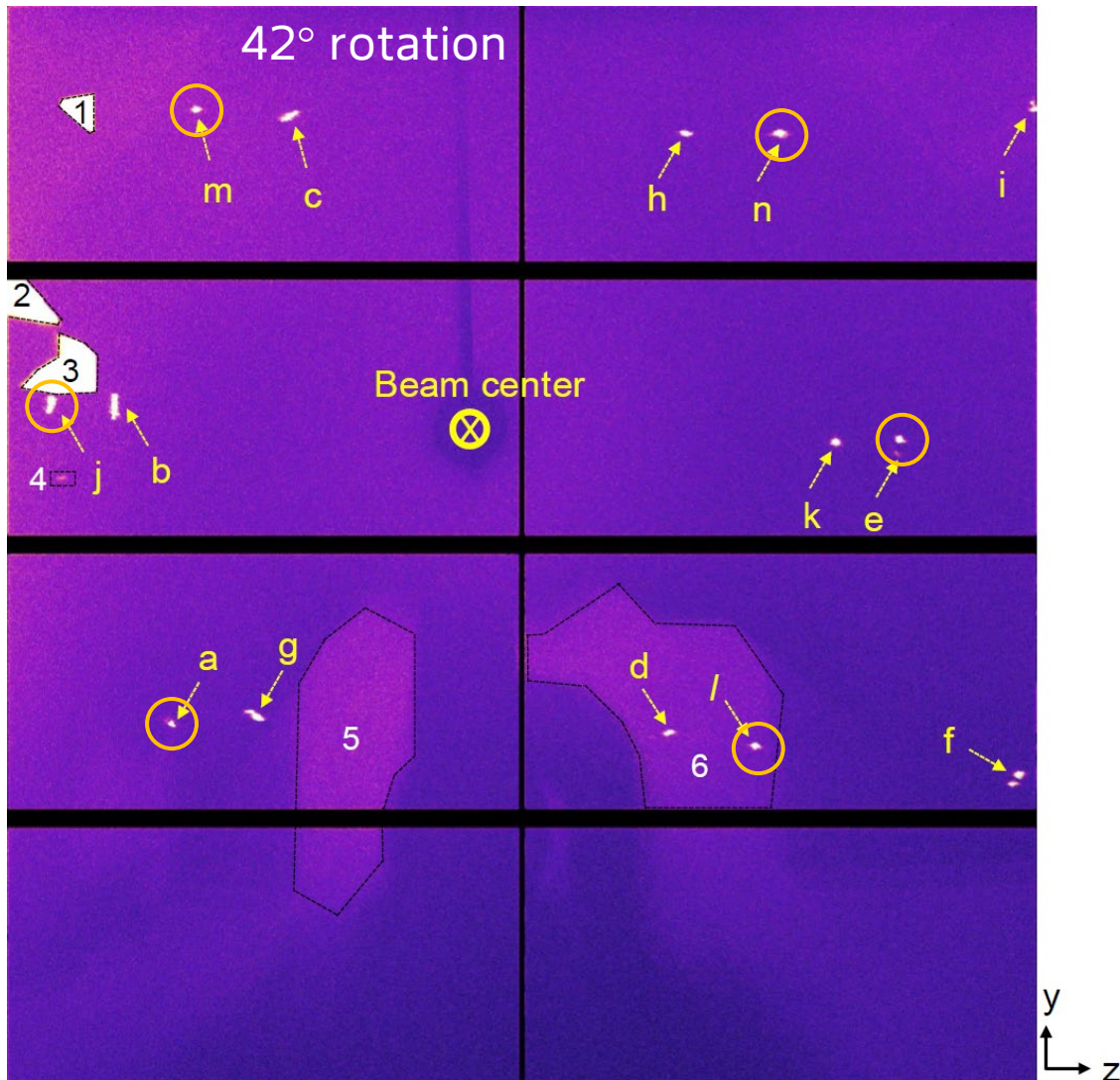


Sow, C.; et al. *ACS Nano* **2020**, *14*, 9456–9465

Diffraction pattern summed over all rotations

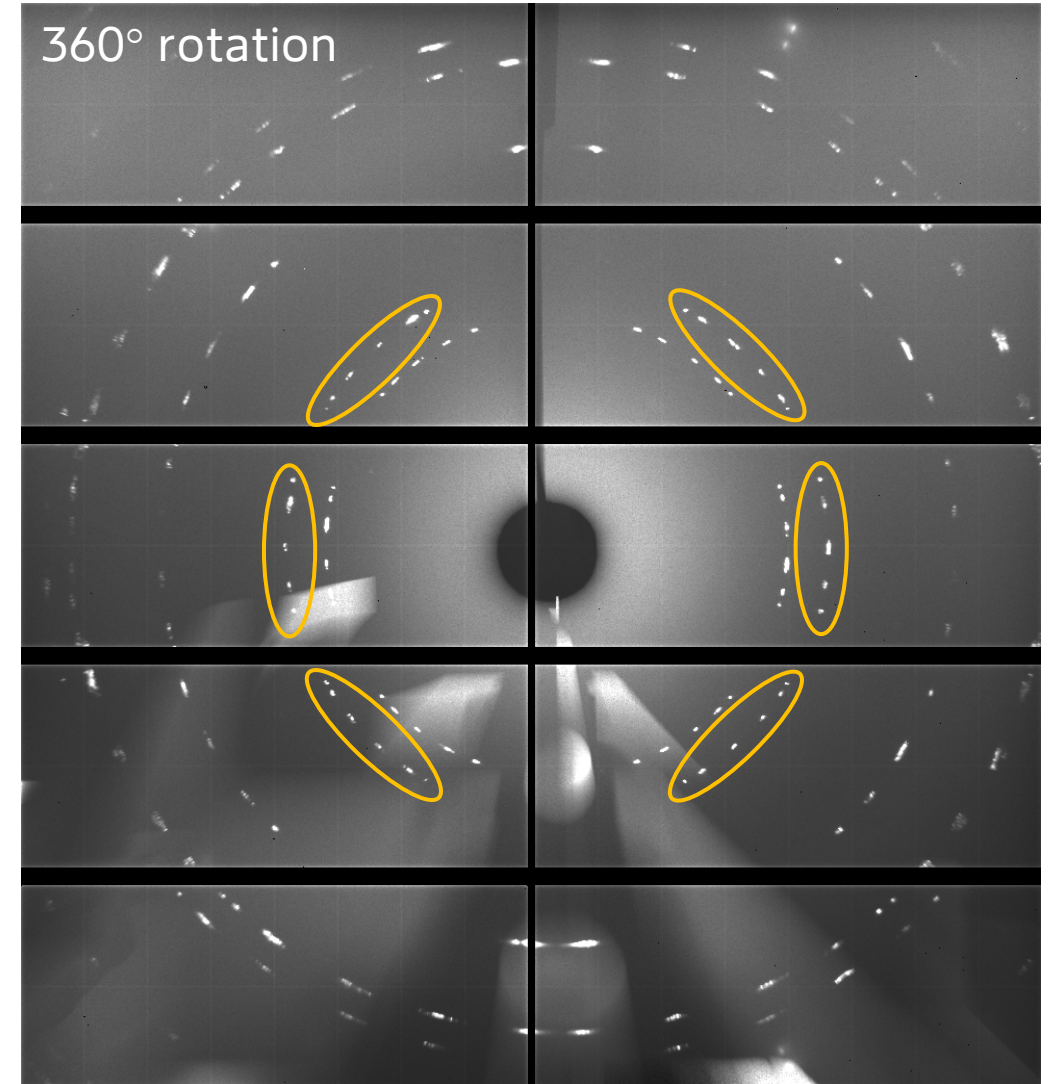


Comparison of Diffraction Patterns

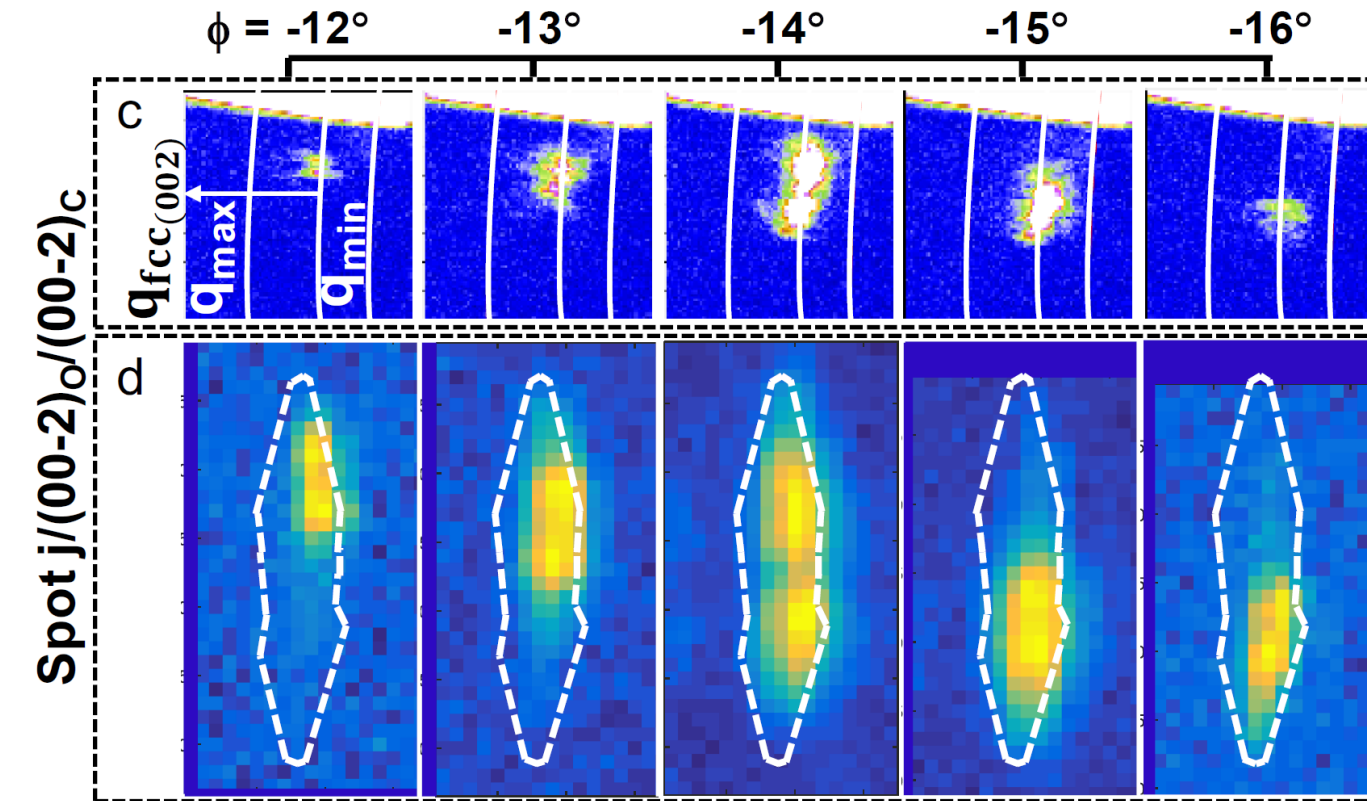


Sow, C.; et al. *ACS Nano* **2020**, *14*, 9456–9465

Diffraction pattern summed over all rotations

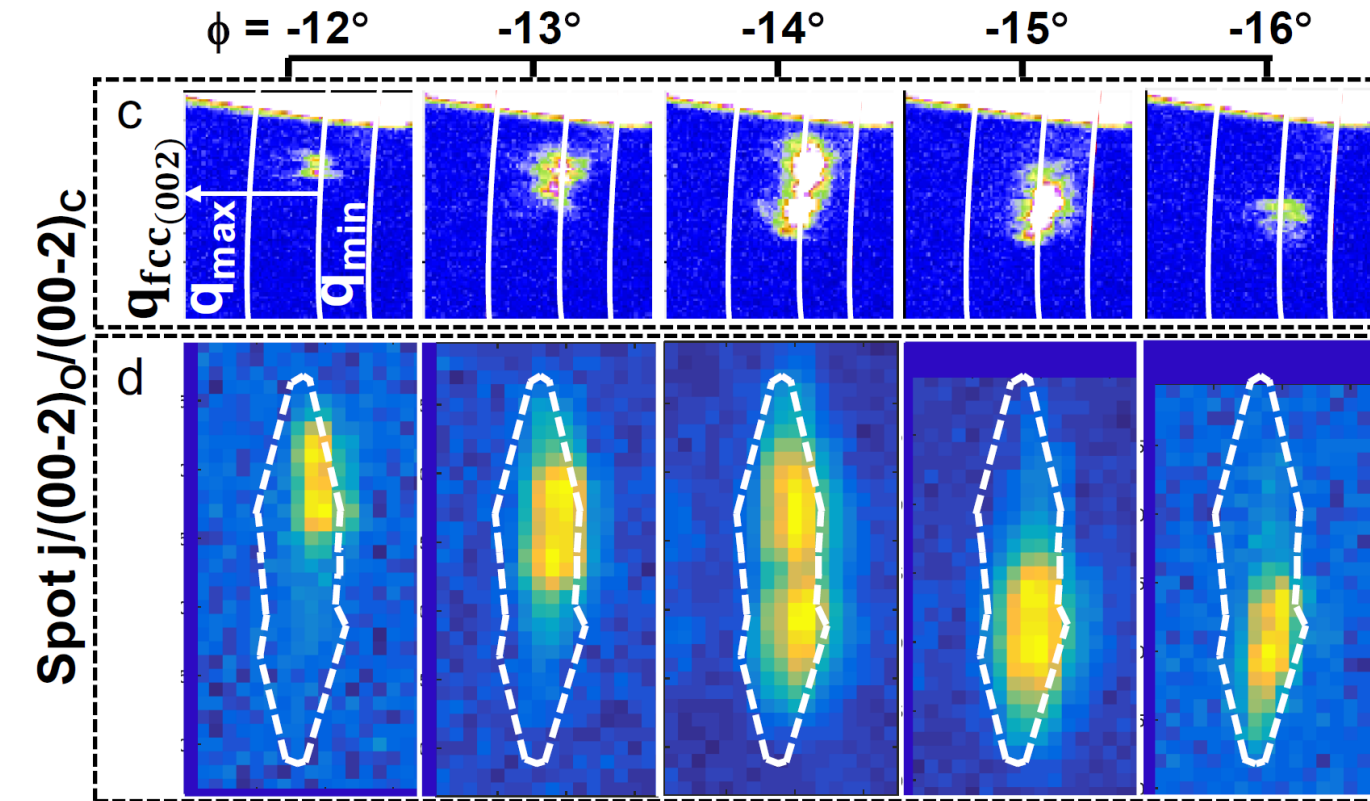


Presence of Twist from Previous Expt.



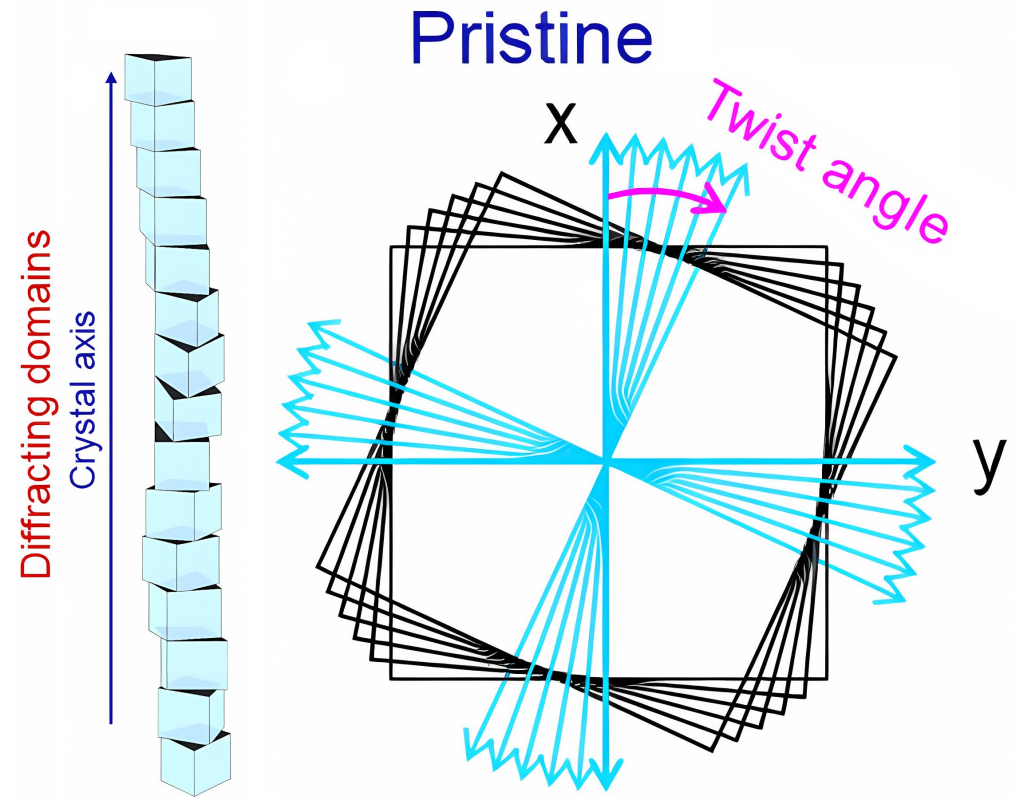
Sow, C.; et al. ACS Nano **2020**, 14, 9456–9465

Presence of Twist from Previous Expt.



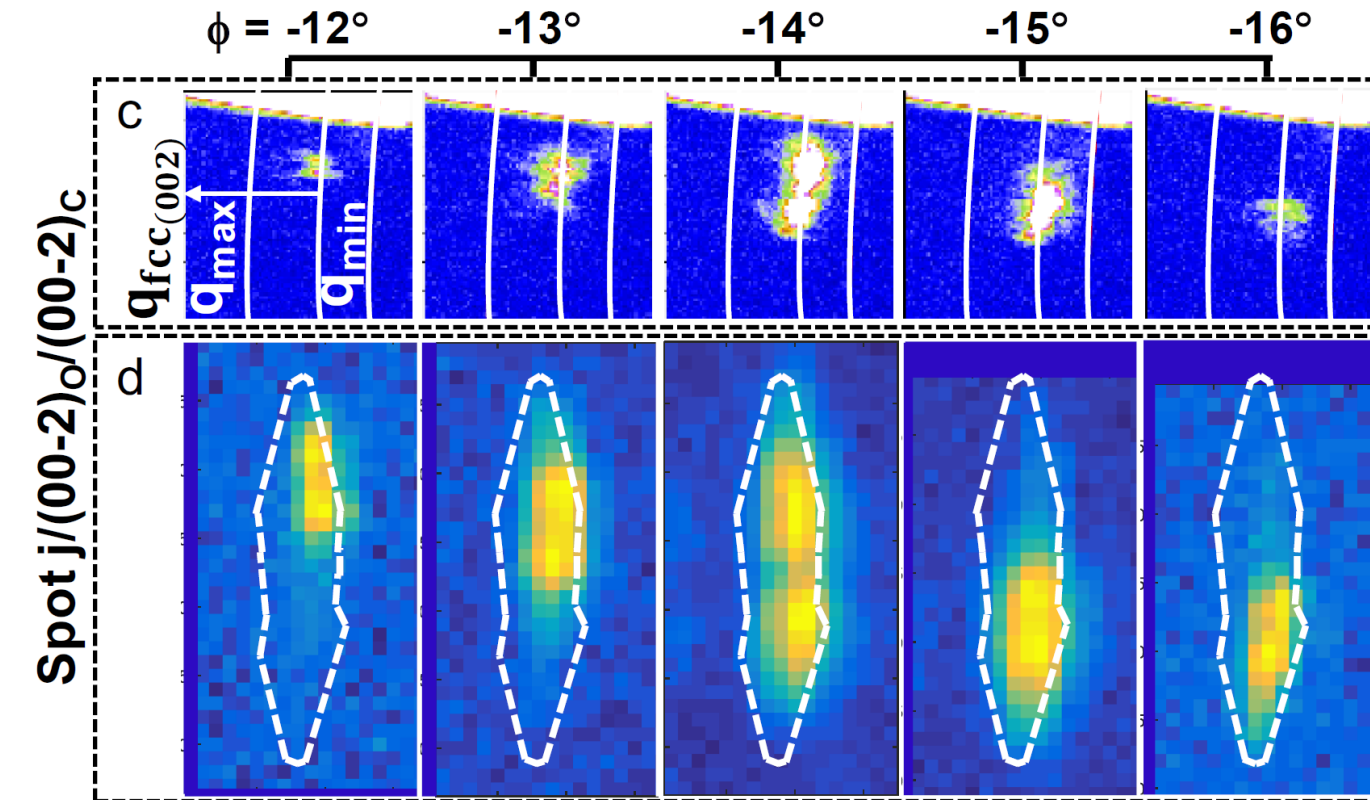
Sow, C.; et al. ACS Nano **2020**, 14, 9456–9465

✓ $\sim 6^\circ$ twist across the length

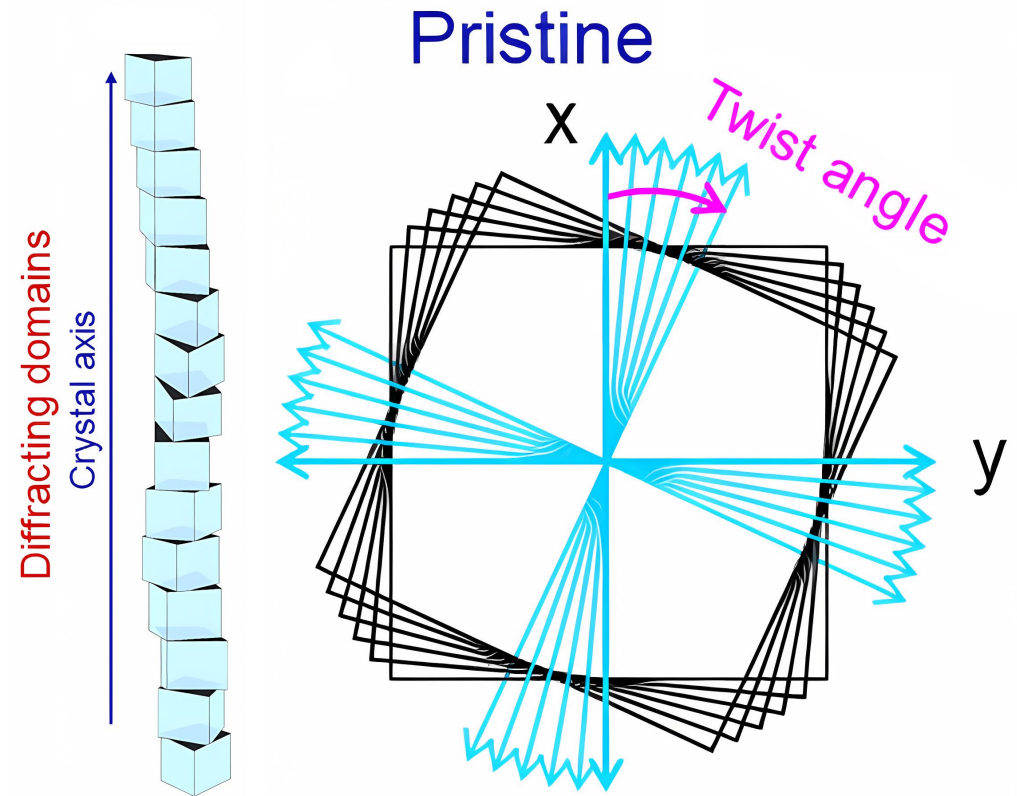


Sow, C.; et al. ACS Nano **2025**, 19, 19635–19645

Presence of Twist from Previous Expt.



Sow, C.; et al. ACS Nano **2020**, 14, 9456–9465

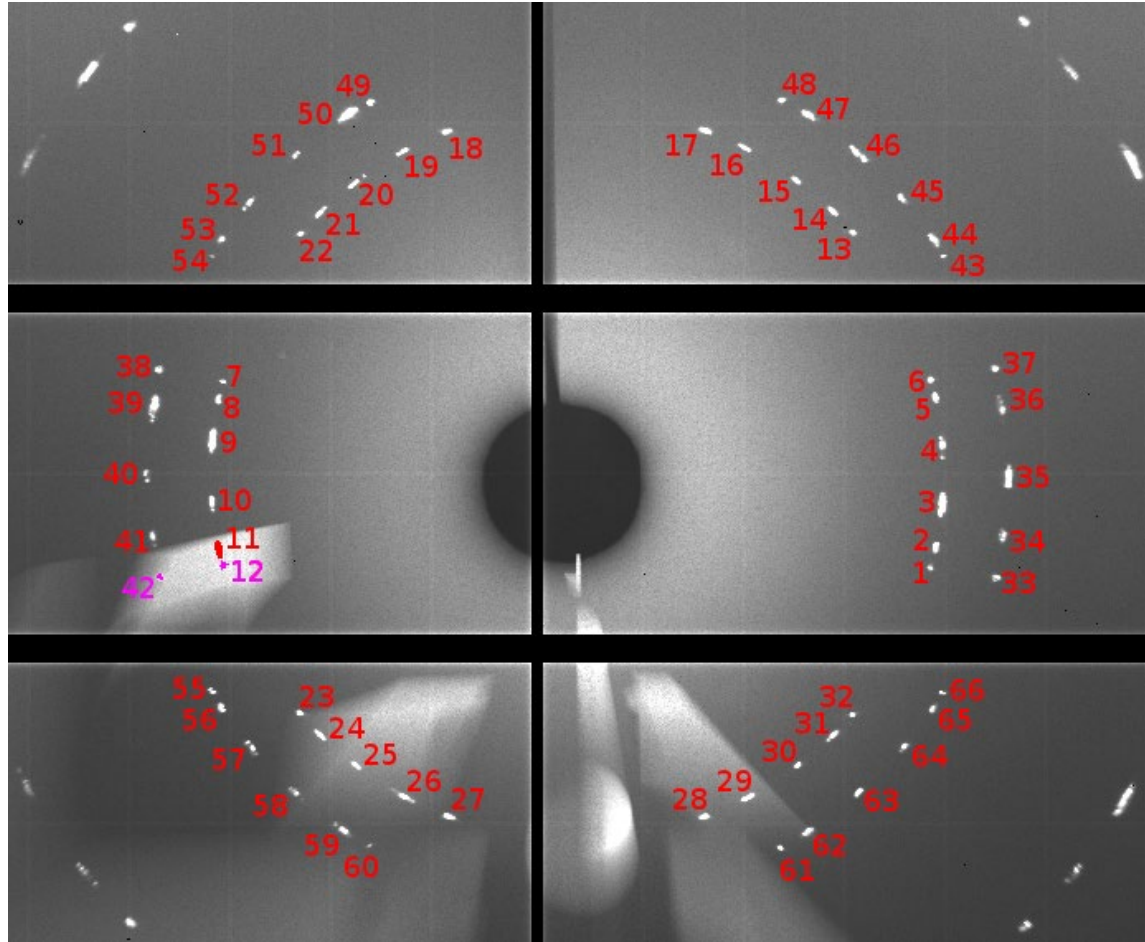


Sow, C.; et al. ACS Nano **2025**, 19, 19635–19645

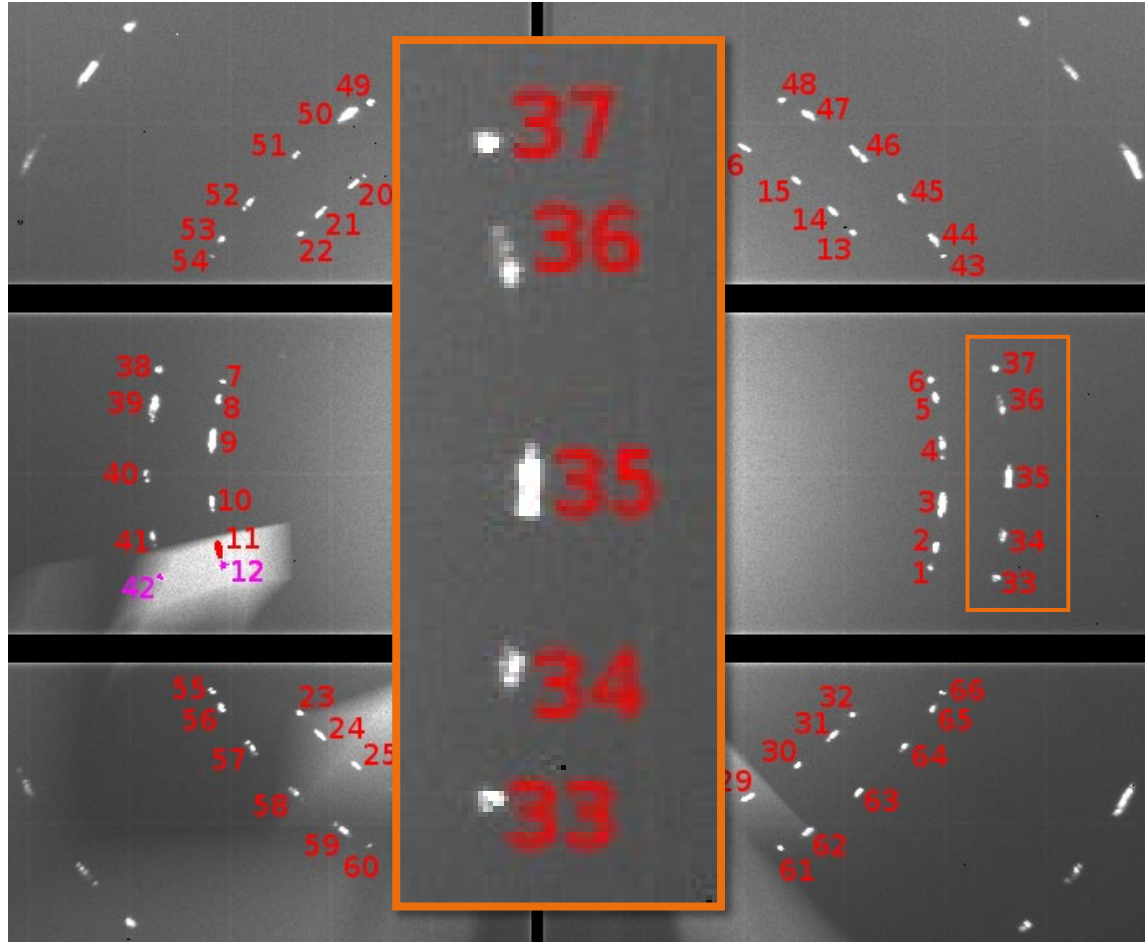
✓ $\sim 6^\circ$ twist across the length

✓ How is the twist in overall crystal?

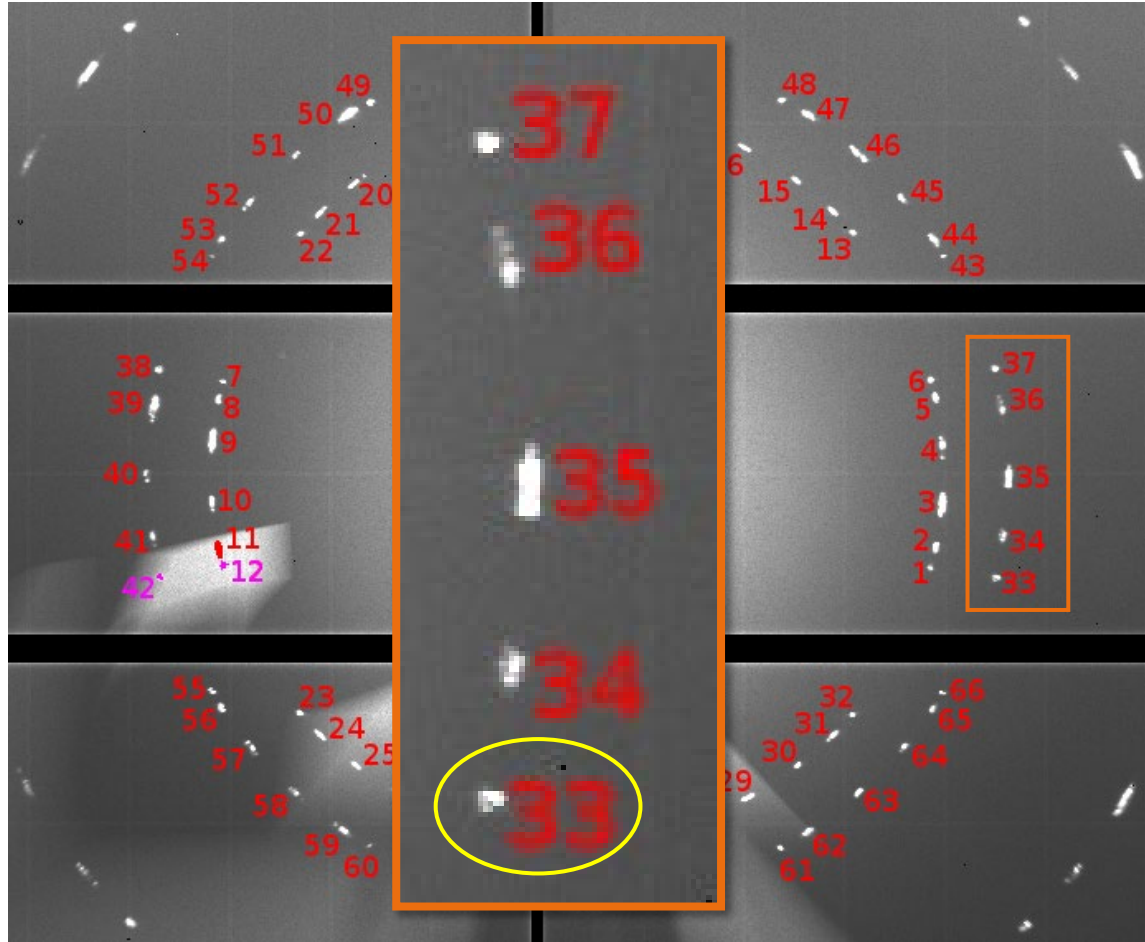
Diffraction Spots and Maps



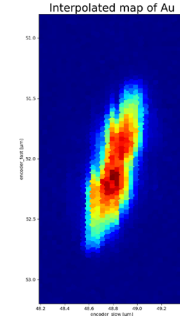
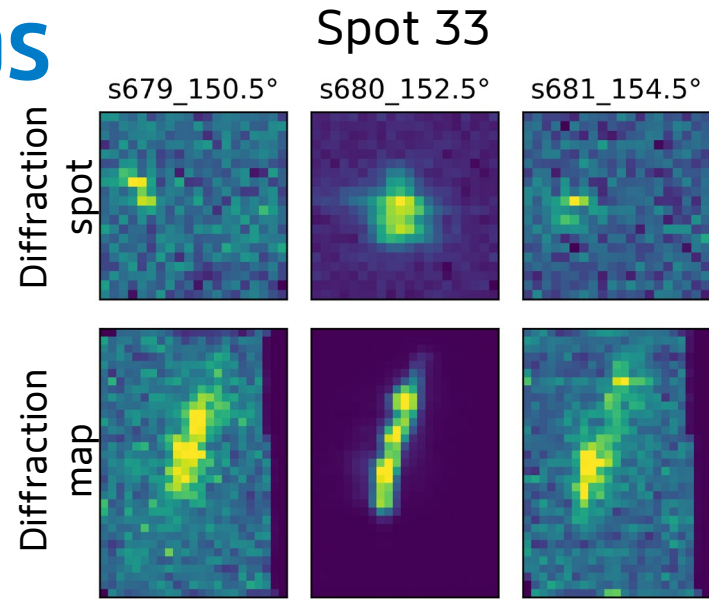
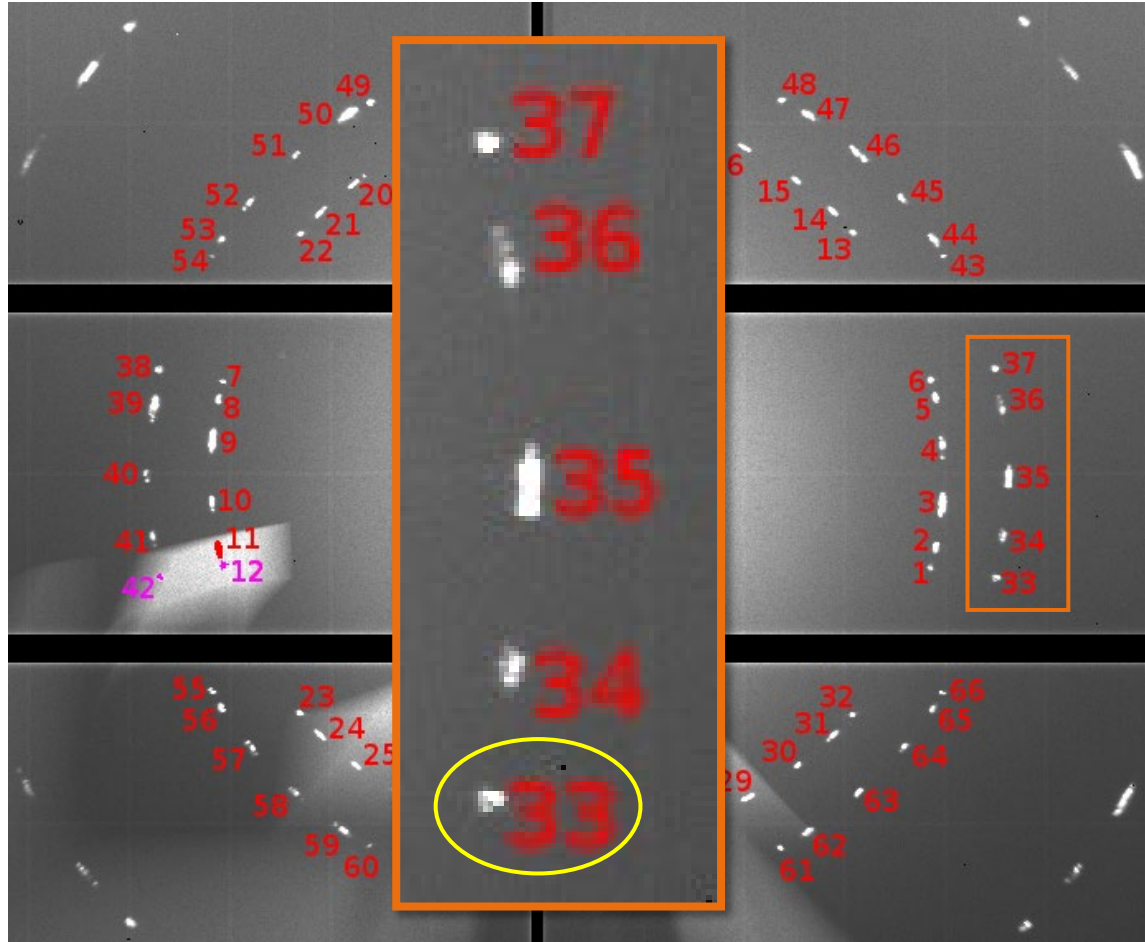
Diffraction Spots and Maps



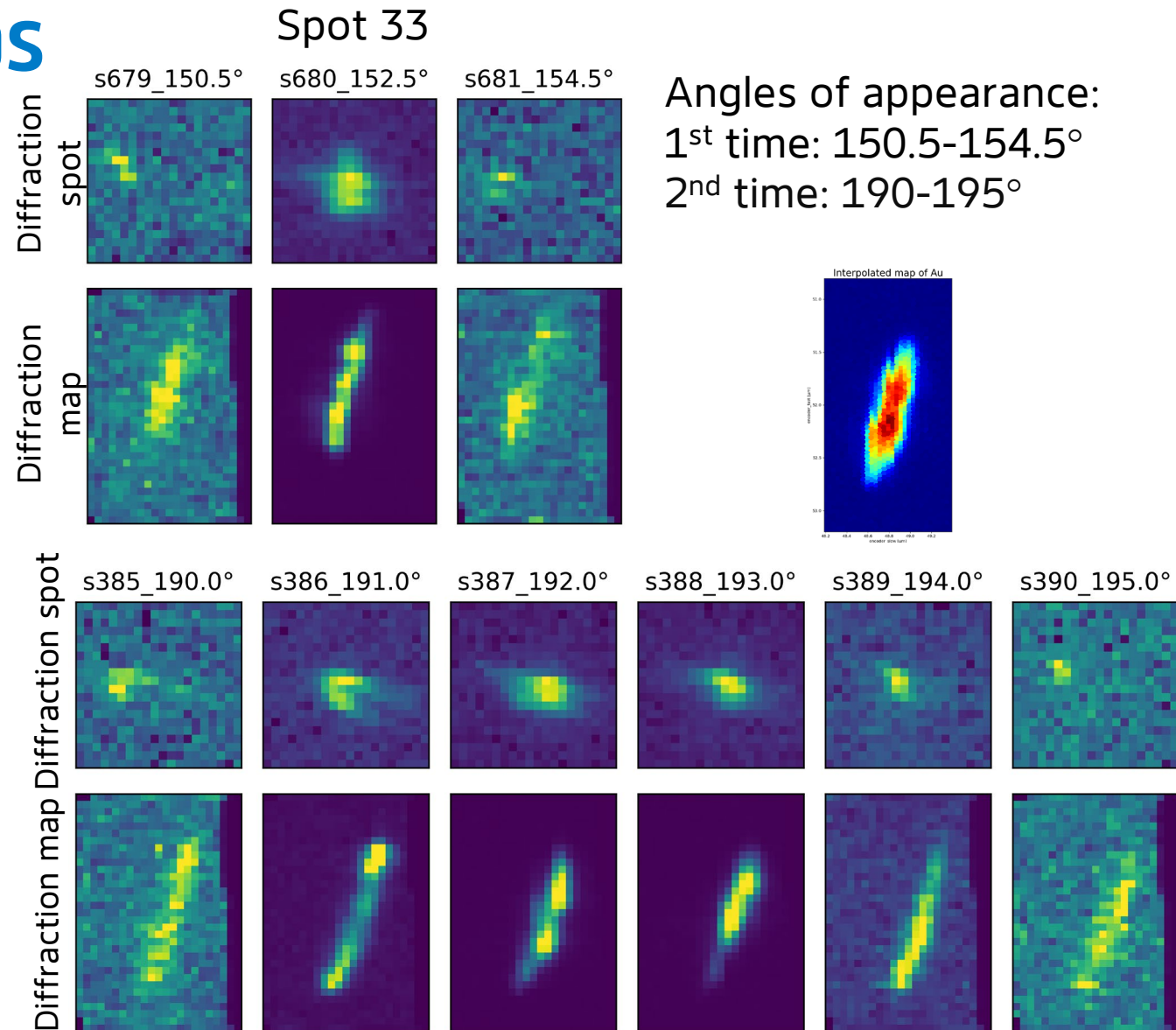
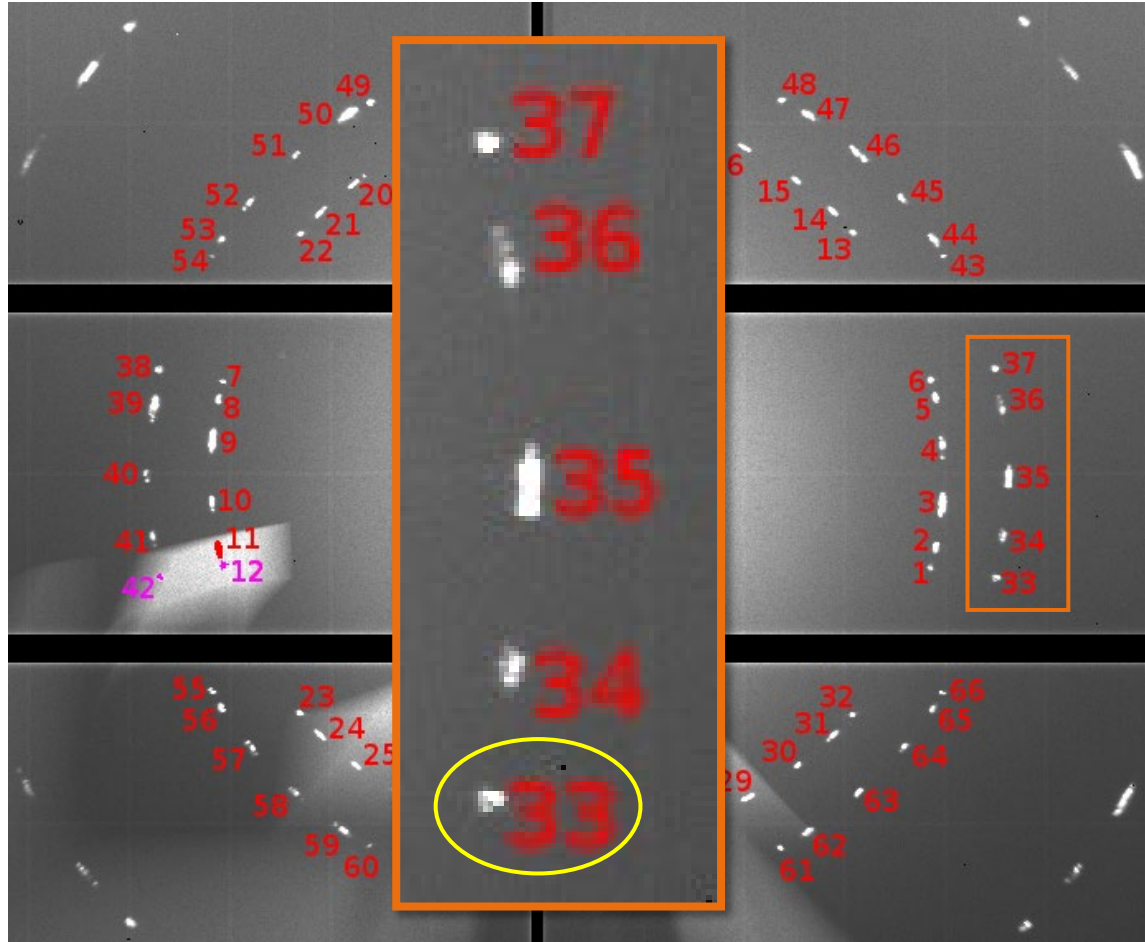
Diffraction Spots and Maps



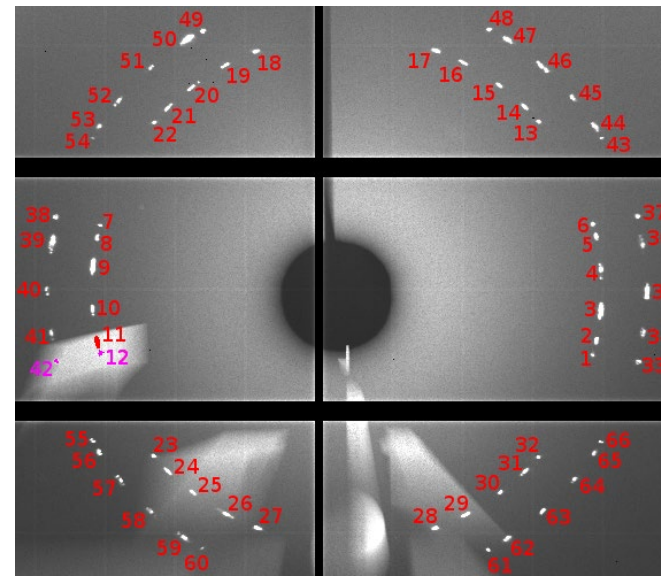
Diffraction Spots and Maps



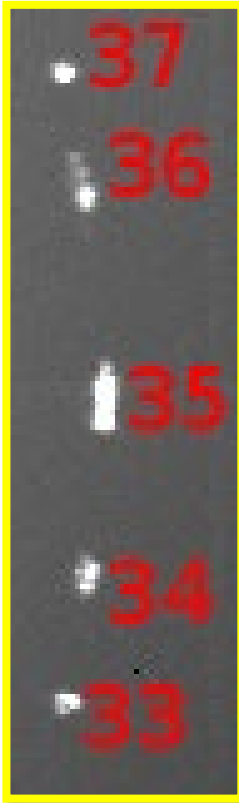
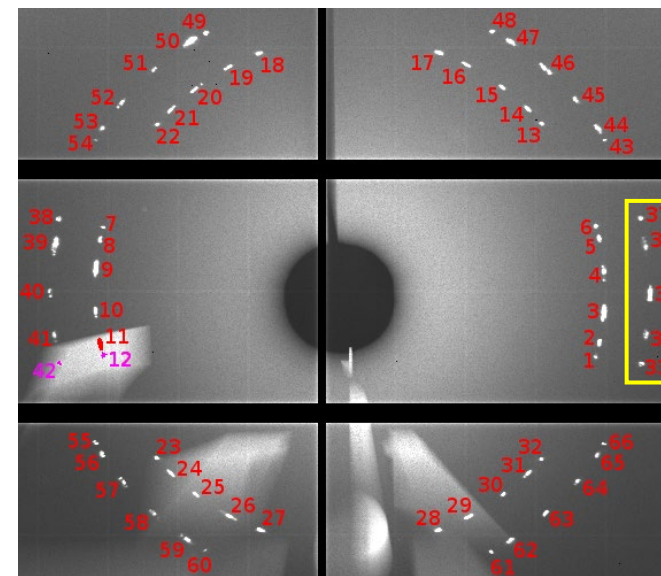
Diffraction Spots and Maps



Diffraction Spots and Maps

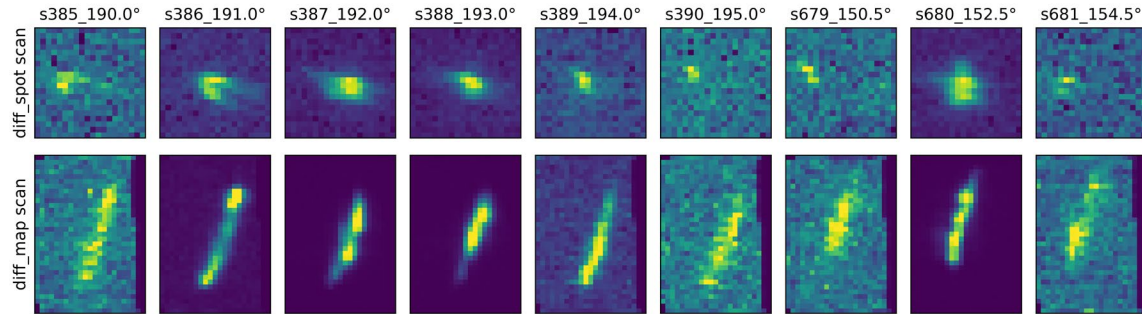


Diffraction Spots and Maps

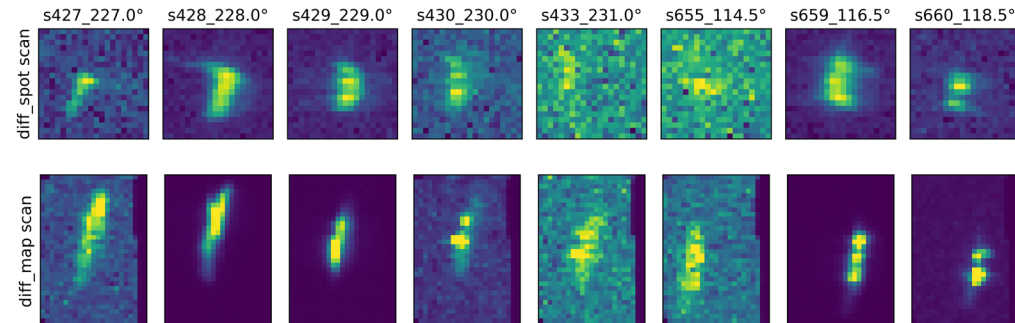


Diffraction Spots and Maps

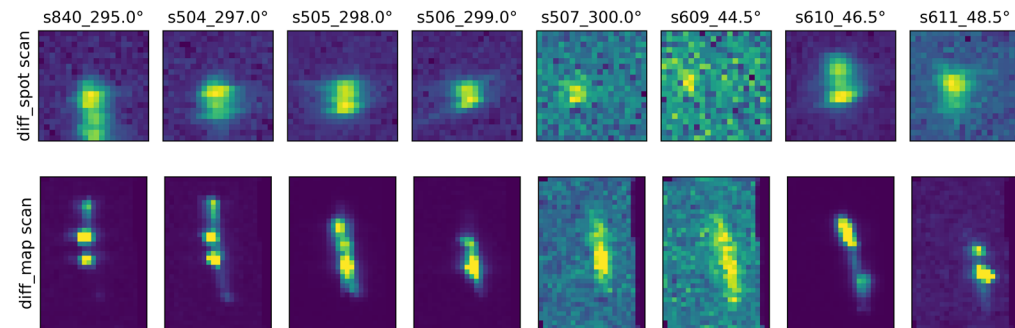
spot 33 (y=584, x=768)



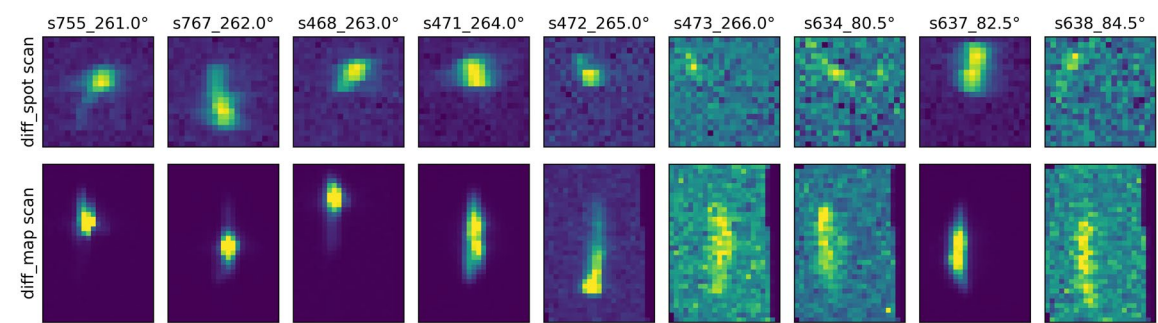
spot 34 (y=559, x=772)



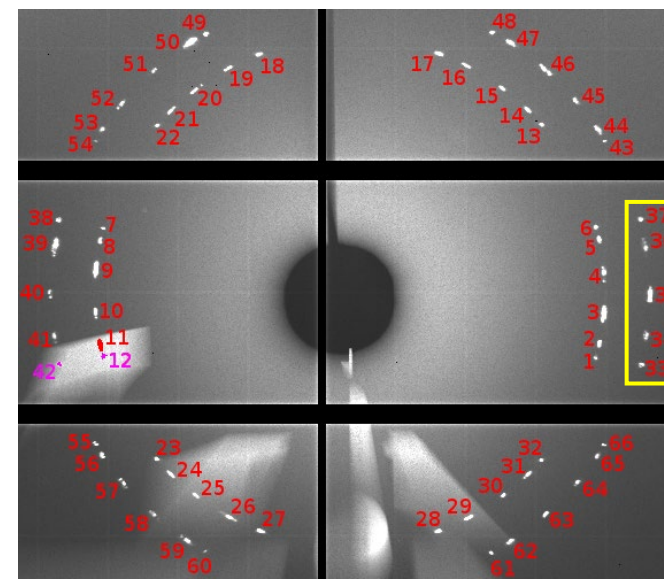
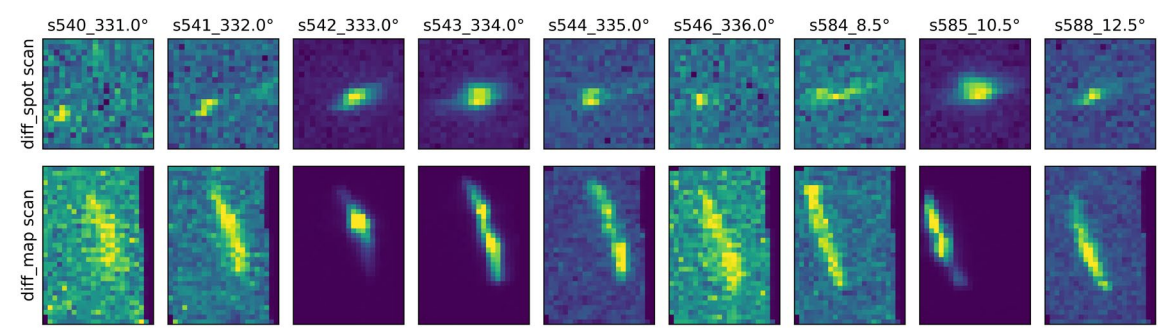
spot 36 (y=481, x=772)



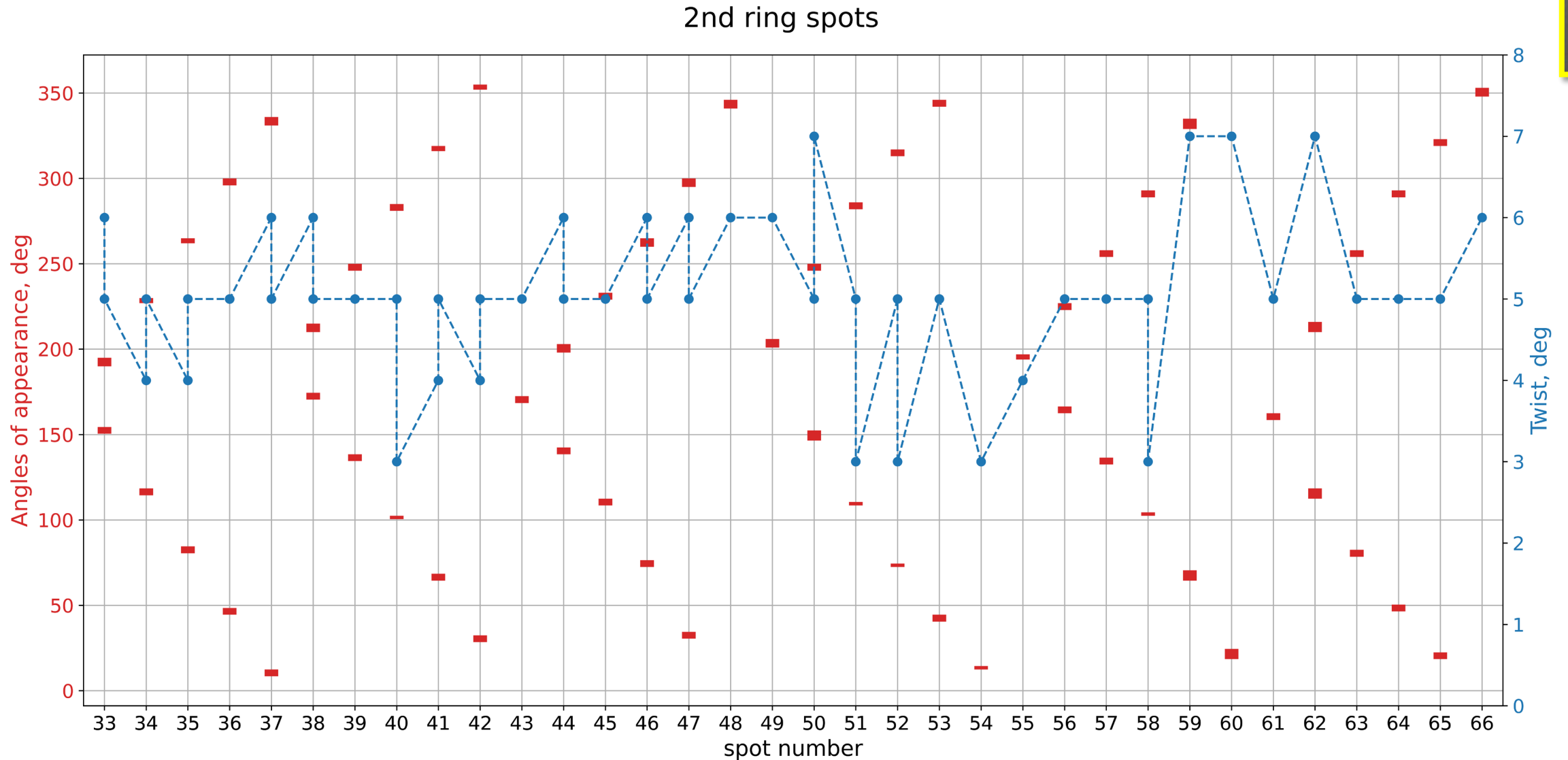
spot 35 (y=524, x=776)



spot 37 (y=458, x=767)

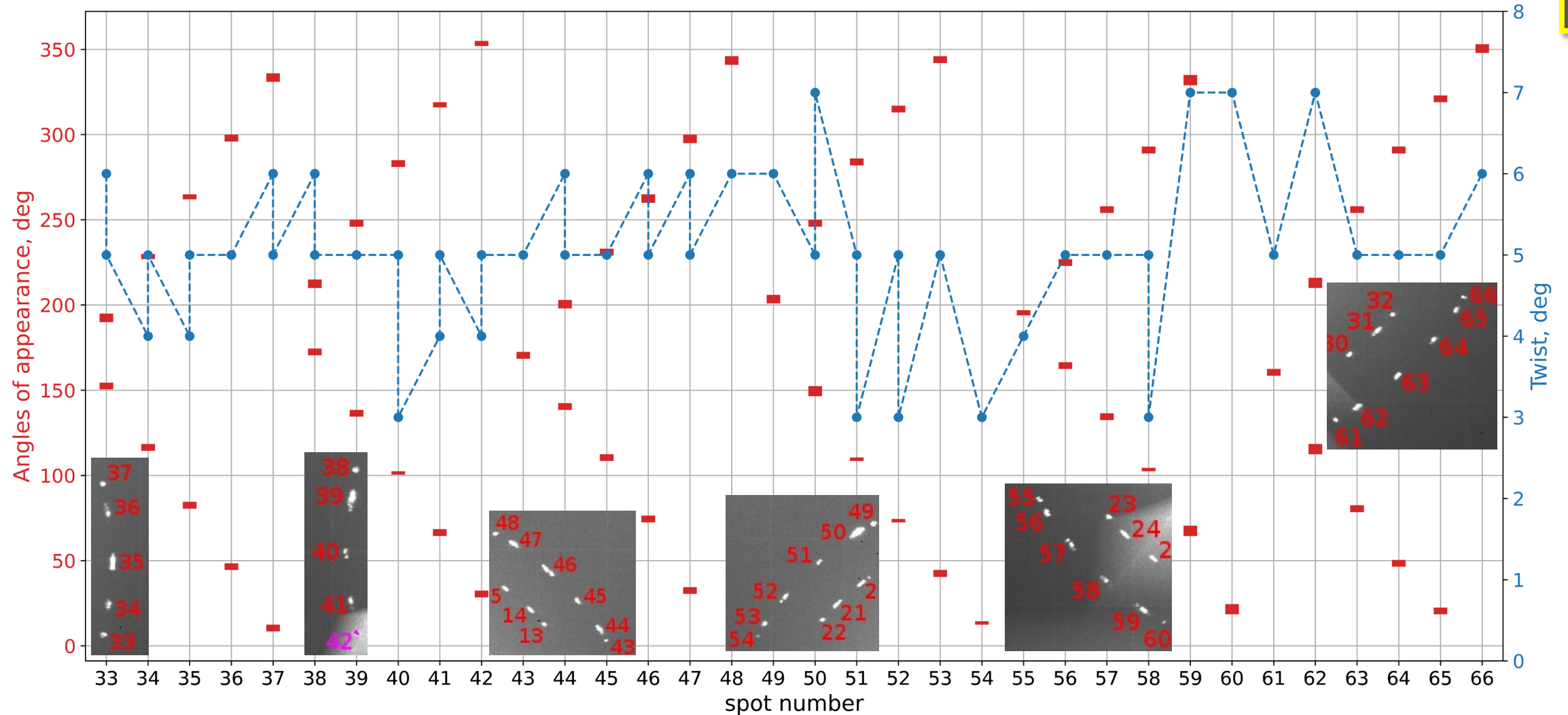


Angle of Appearance and Twist

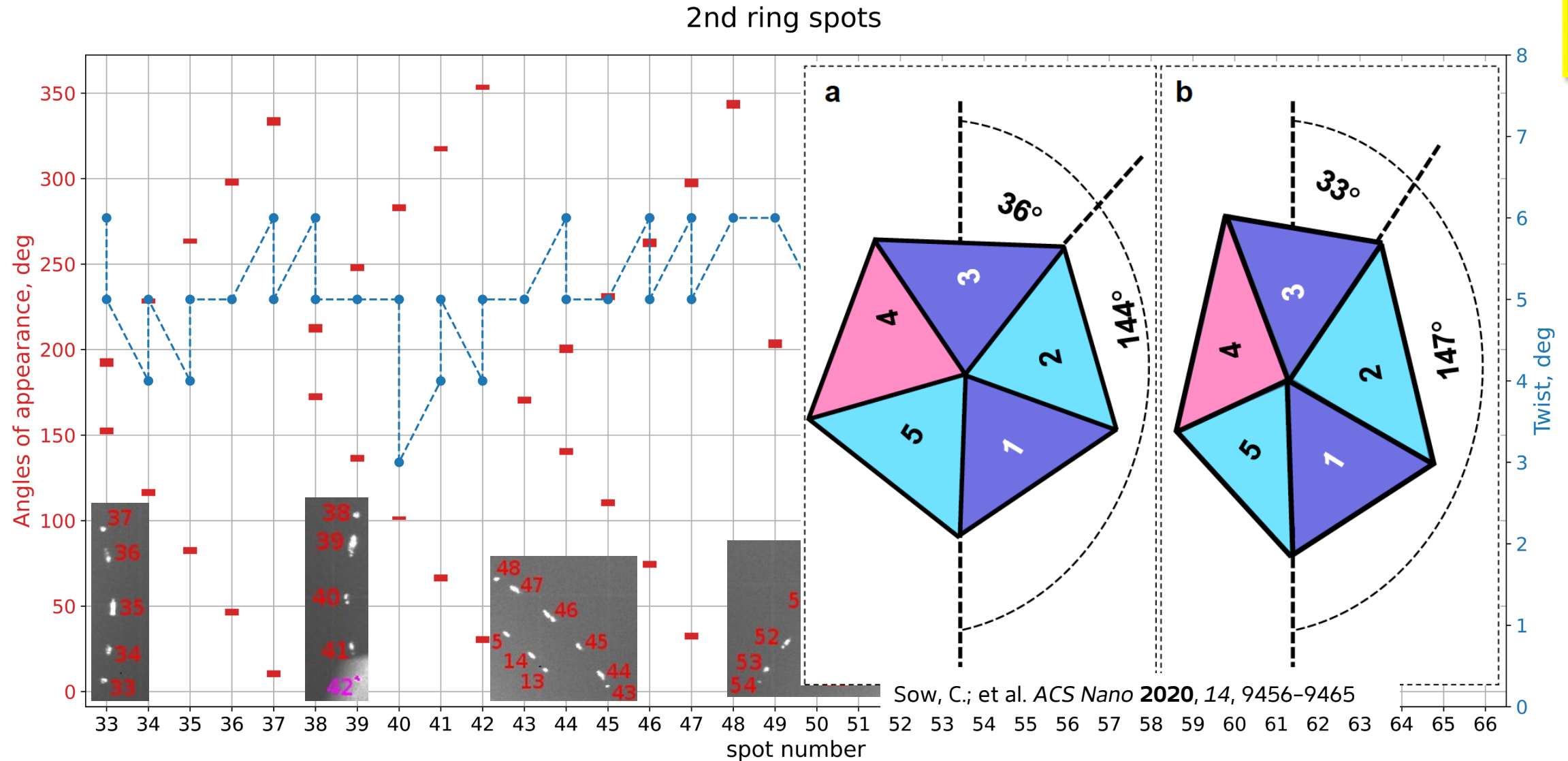


Angle of Appearance and Twist

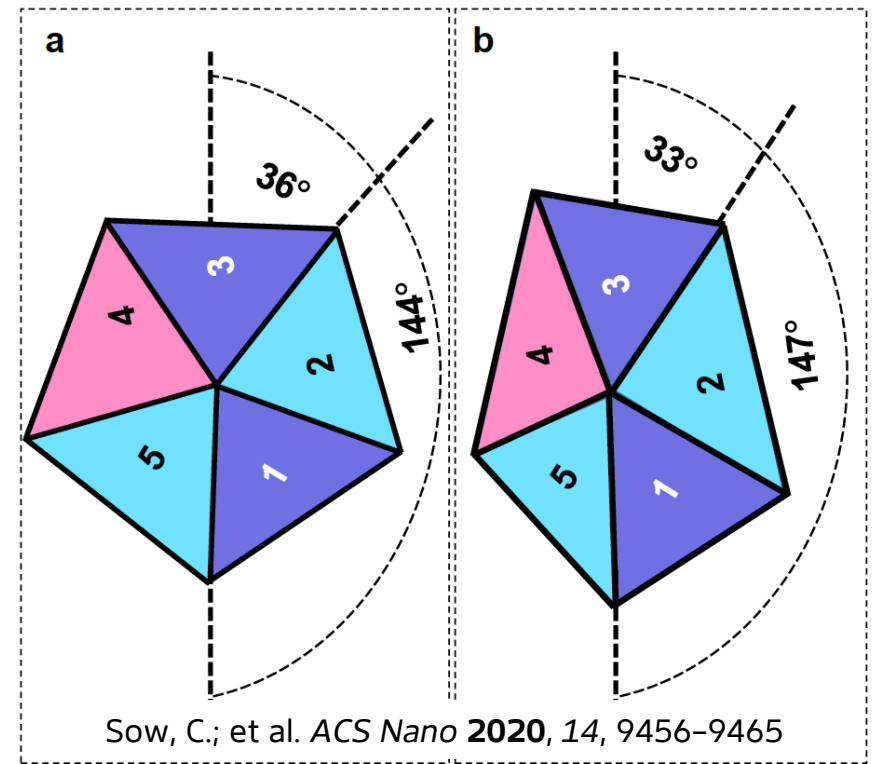
2nd ring spots



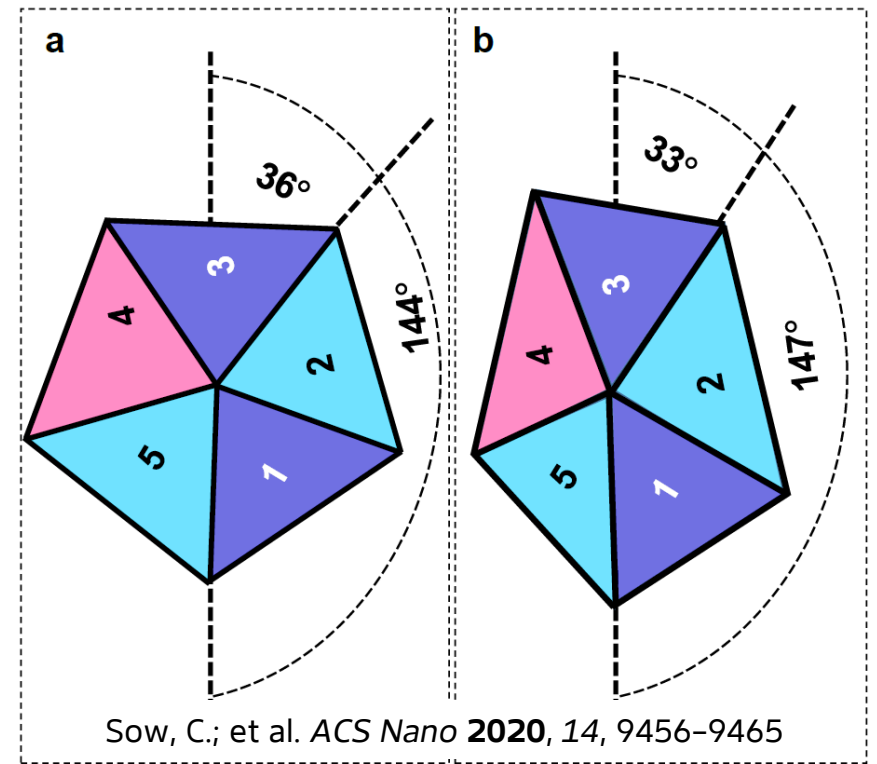
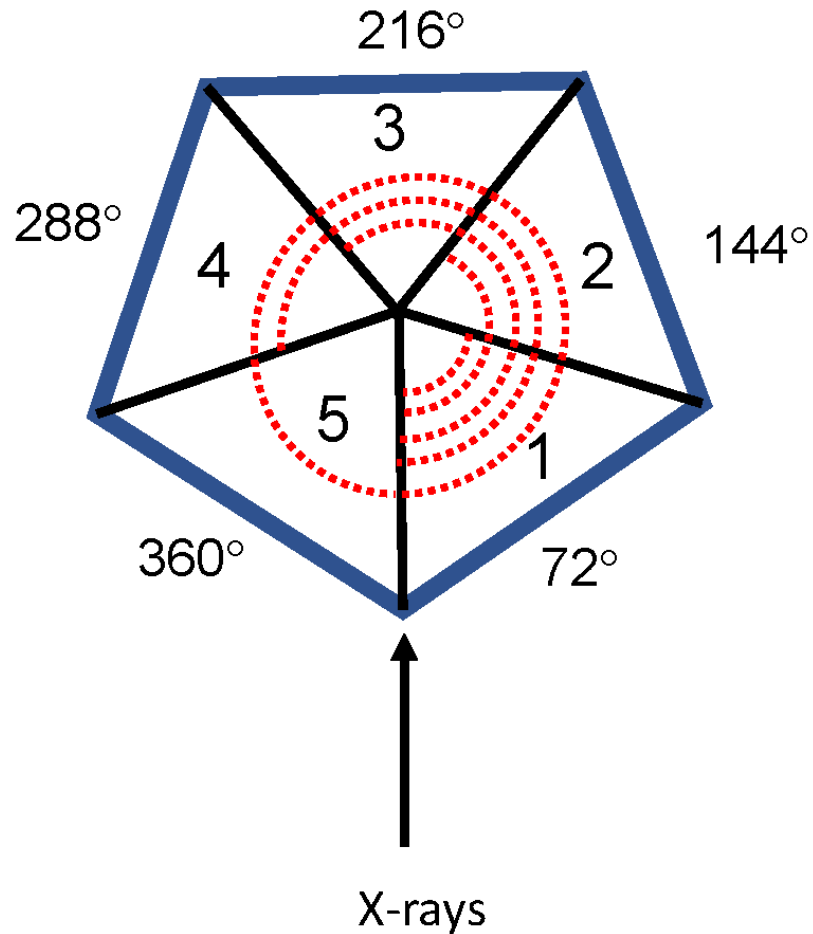
Angle of Appearance and Twist



Unveiling Five-Fold Symmetry

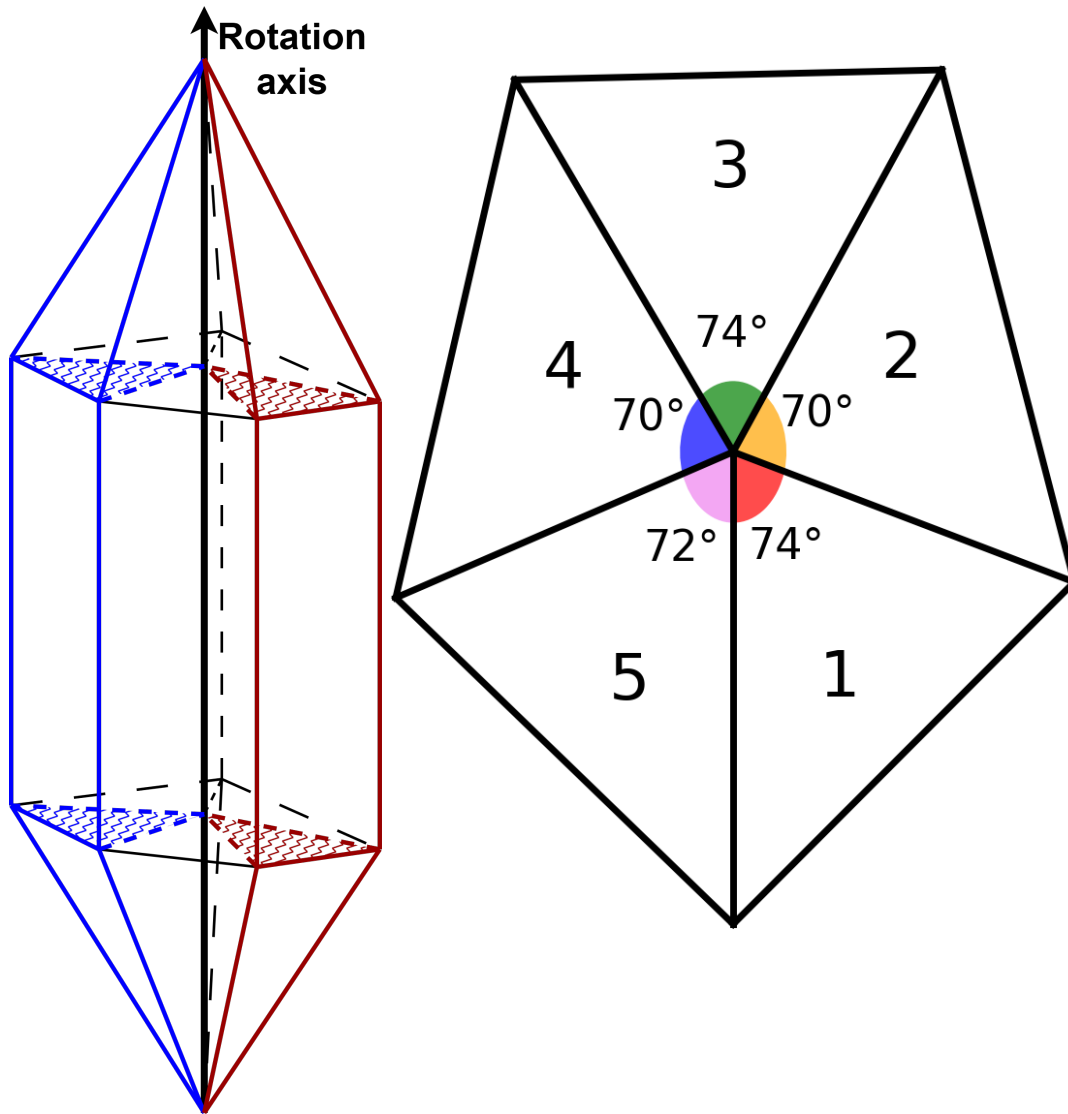


Unveiling Five-Fold Symmetry

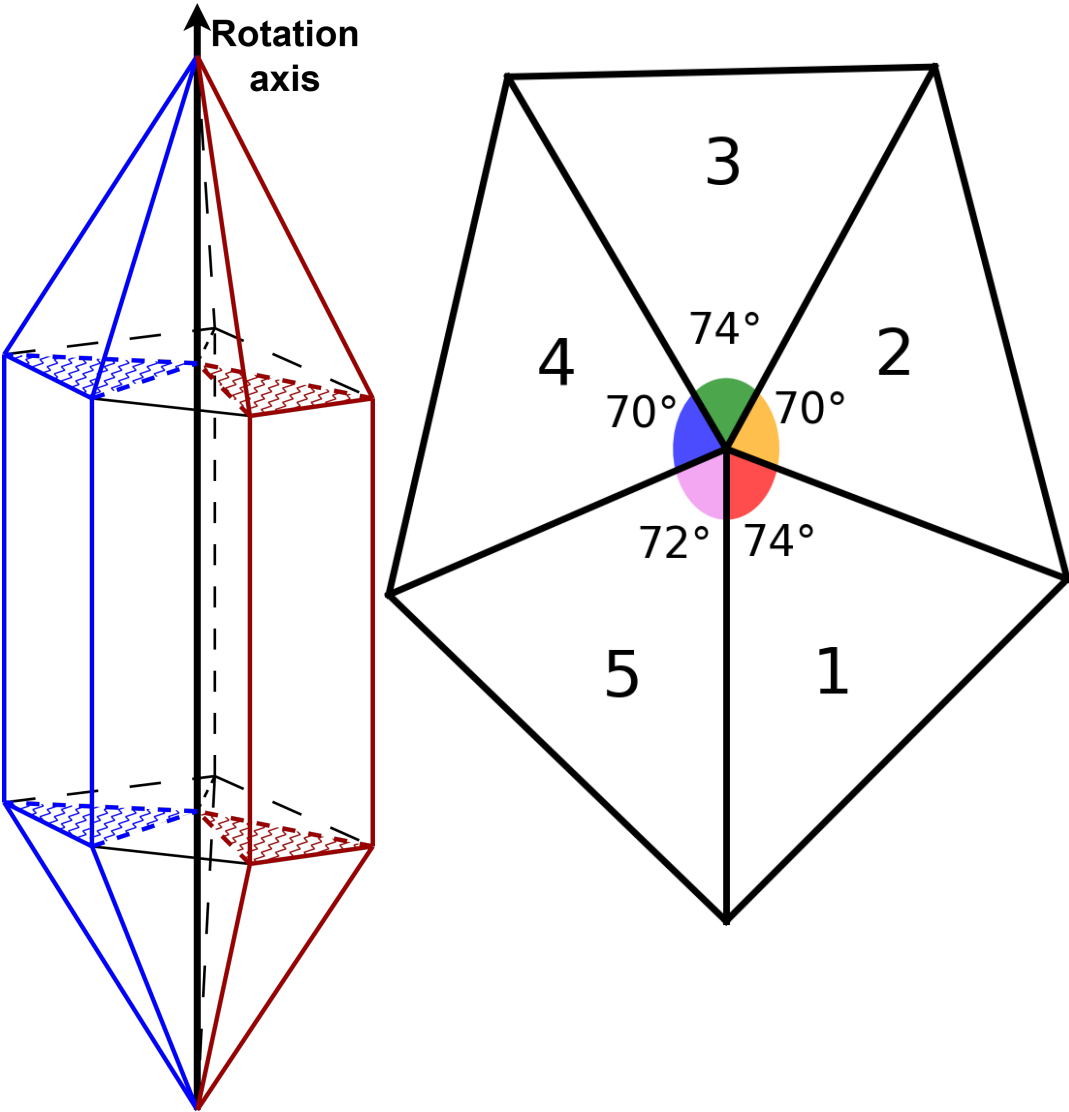


Domains into consideration	Angular rot. (ϕ°)	Angular relation with X-rays ($^\circ$)	Angle between the domains ($^\circ$)
(5, 1)	0	0	0
(2, 3)	36	$(144 + 36) = 180$	144
(4, 5)	72	$(288 + 72) = 360$	288
(1, 2)	108	$(72 + 108) = 180$	72
(3, 4)	144	$(216 + 144) = 360$	216

Angular Relations

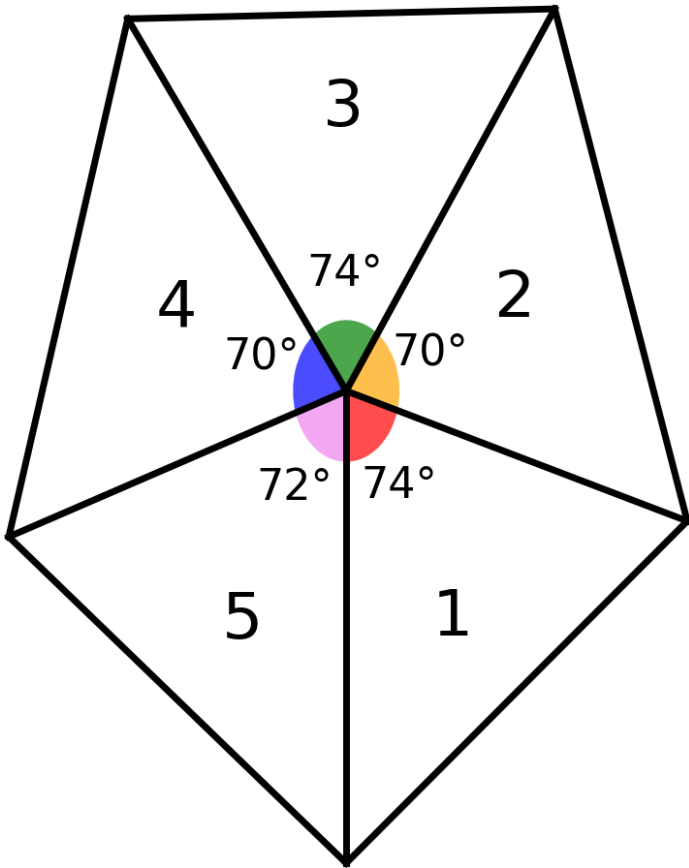
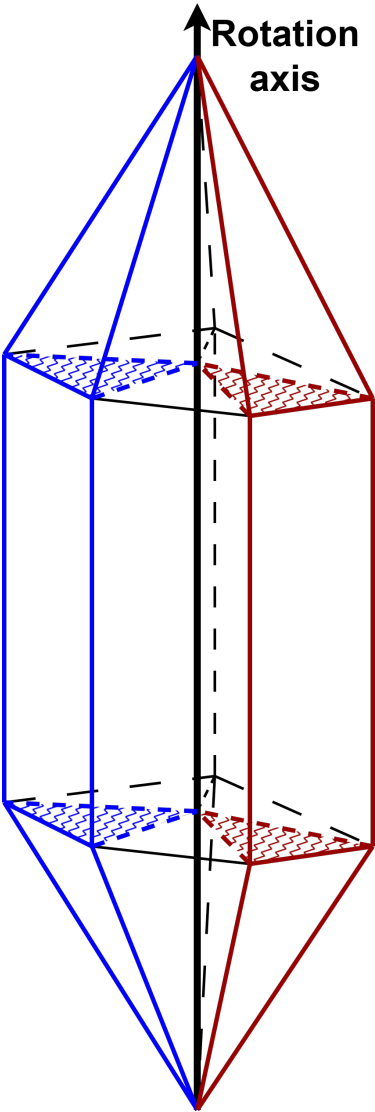


Angular Relations

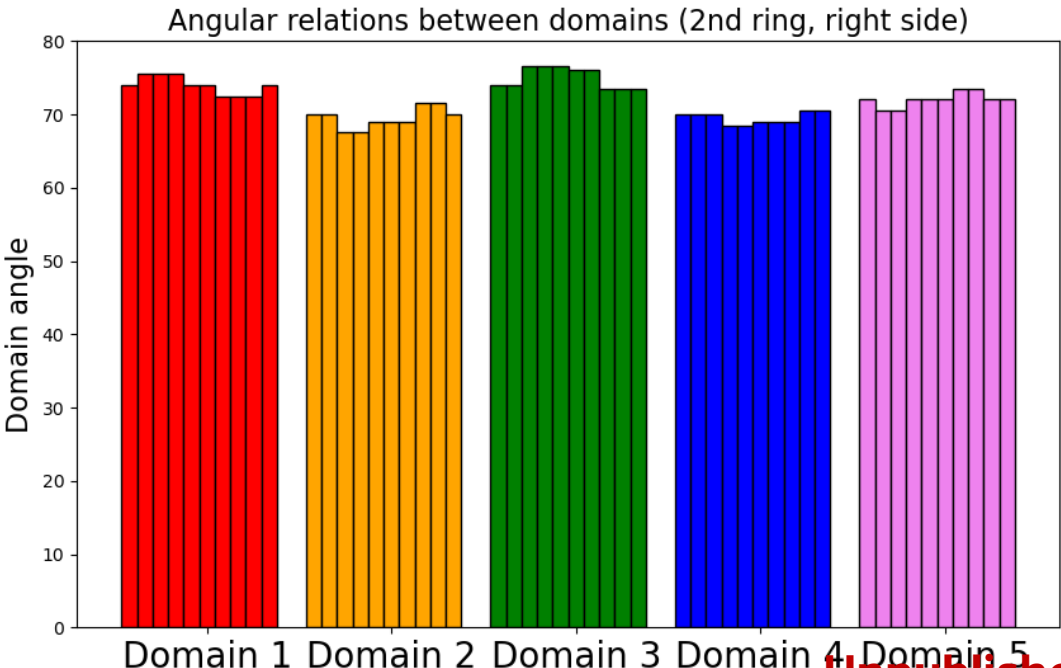


Angles under consideration	Domain 1	Domain 2	Domain 3	Domain 4	Domain 5
8.5, 44.5, 80.5, 114.5, 150.5	74	70	74	70	72
44.5, 80.5, 114.5, 150.5, 190	75.5	70	74	70	70.5
80.5, 114.5, 150.5, 190, 227	75.5	67.5	76.5	70	70.5
114.5, 150.5, 190, 227, 262	75.5	67.5	76.5	68.5	72
150.5, 190, 227, 262, 296	74	69	76.5	68.5	72
190, 227, 262, 296, 331	74	69	76	69	72
227, 262, 296, 331, 8.5	72.5	69	76	69	73.5
262, 296, 331, 8.5, 44.5	72.5	71.5	73.5	69	73.5
296, 331, 8.5, 44.5, 80.5	72.5	71.5	73.5	70.5	72
331, 8.5, 44.5, 80.5, 114.5	74	70	73.5	70.5	72

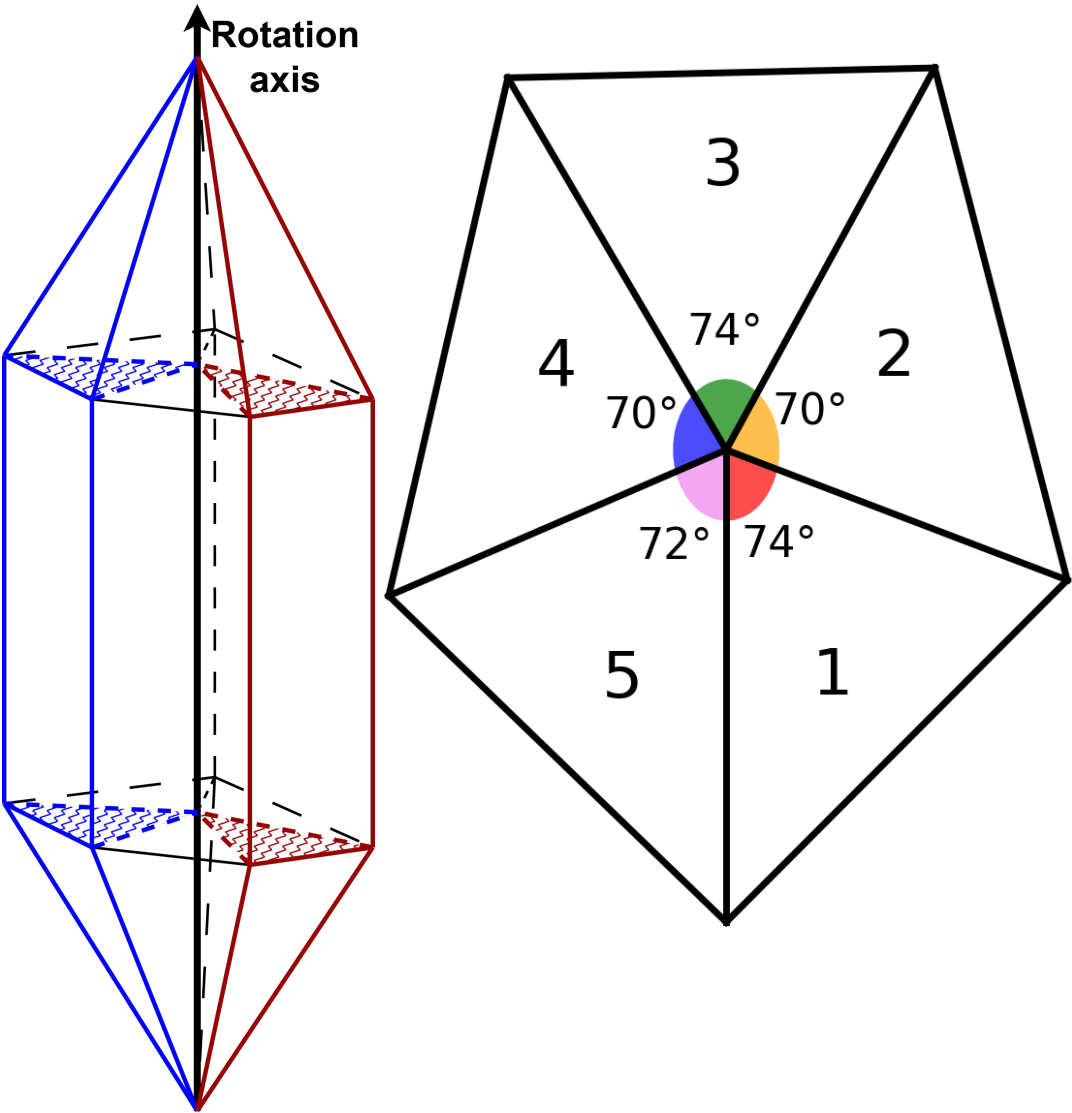
Angular Relations



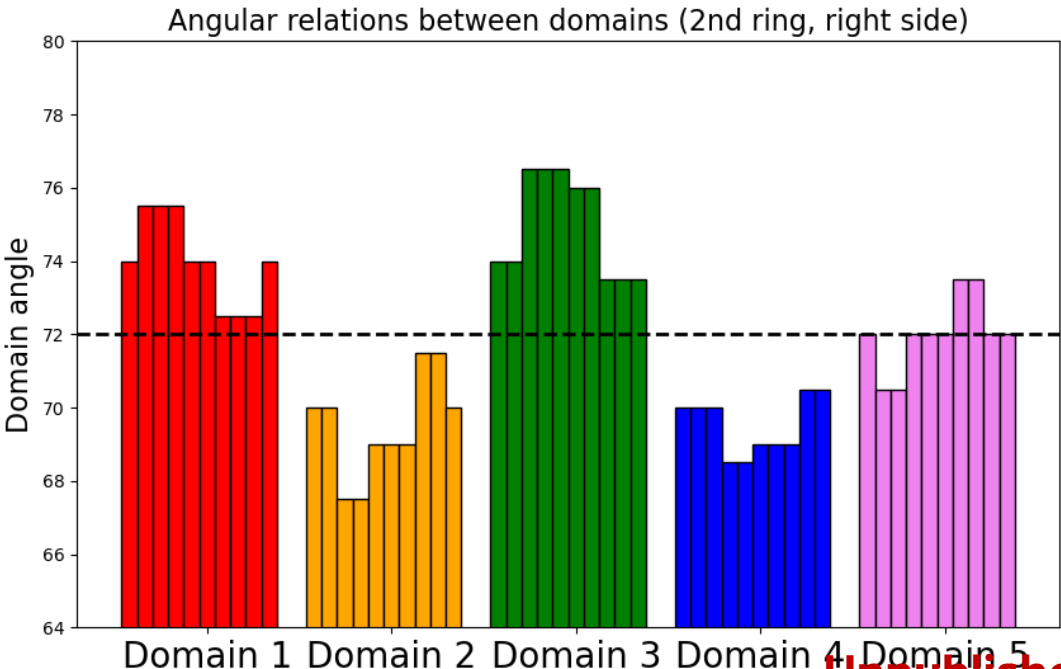
Angles under consideration	Domain 1	Domain 2	Domain 3	Domain 4	Domain 5
8.5, 44.5, 80.5, 114.5, 150.5	74	70	74	70	72
44.5, 80.5, 114.5, 150.5, 190	75.5	70	74	70	70.5
80.5, 114.5, 150.5, 190, 227	75.5	67.5	76.5	70	70.5
114.5, 150.5, 190, 227, 262	75.5	67.5	76.5	68.5	72
150.5, 190, 227, 262, 296	74	69	76.5	68.5	72
190, 227, 262, 296, 331	74	69	76	69	72
227, 262, 296, 331, 8.5	72.5	69	76	69	73.5
262, 296, 331, 8.5, 44.5	72.5	71.5	73.5	69	73.5
296, 331, 8.5, 44.5, 80.5	72.5	71.5	73.5	70.5	72
331, 8.5, 44.5, 80.5, 114.5	74	70	73.5	70.5	72



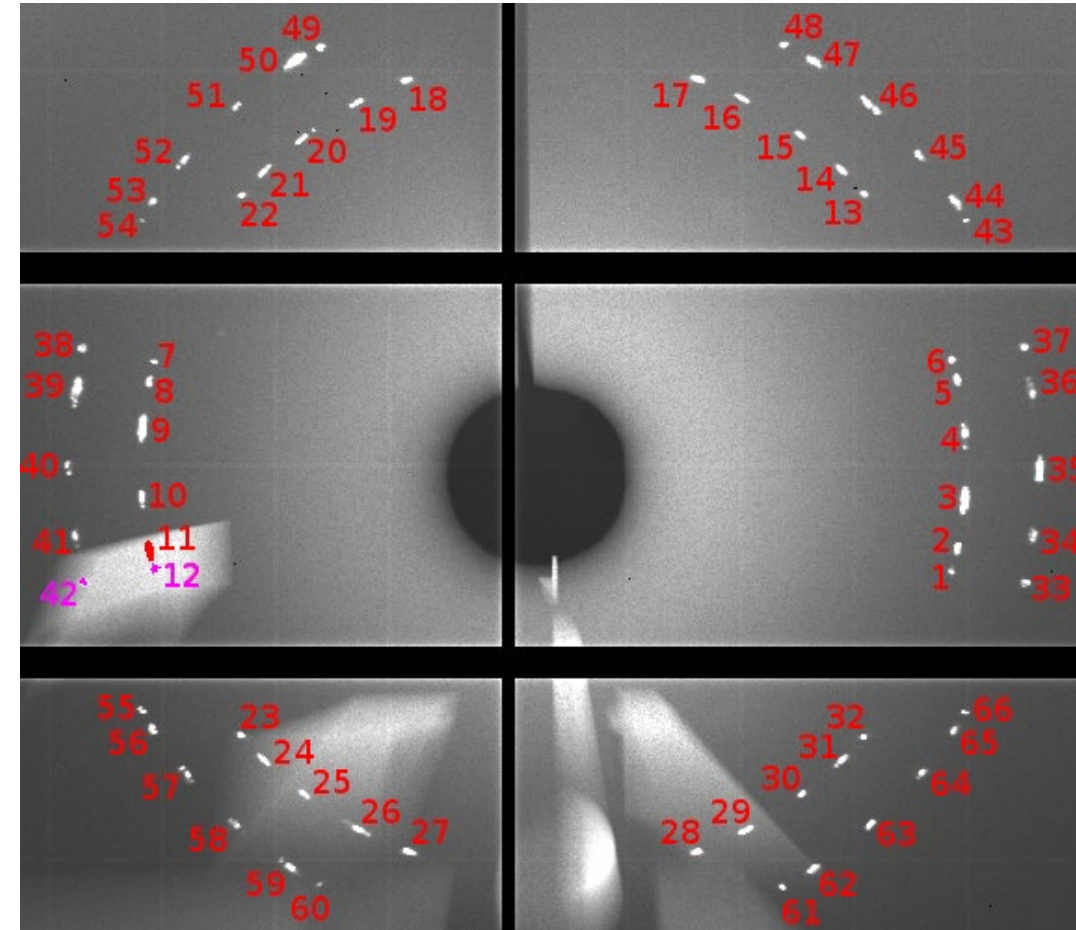
Angular Relations



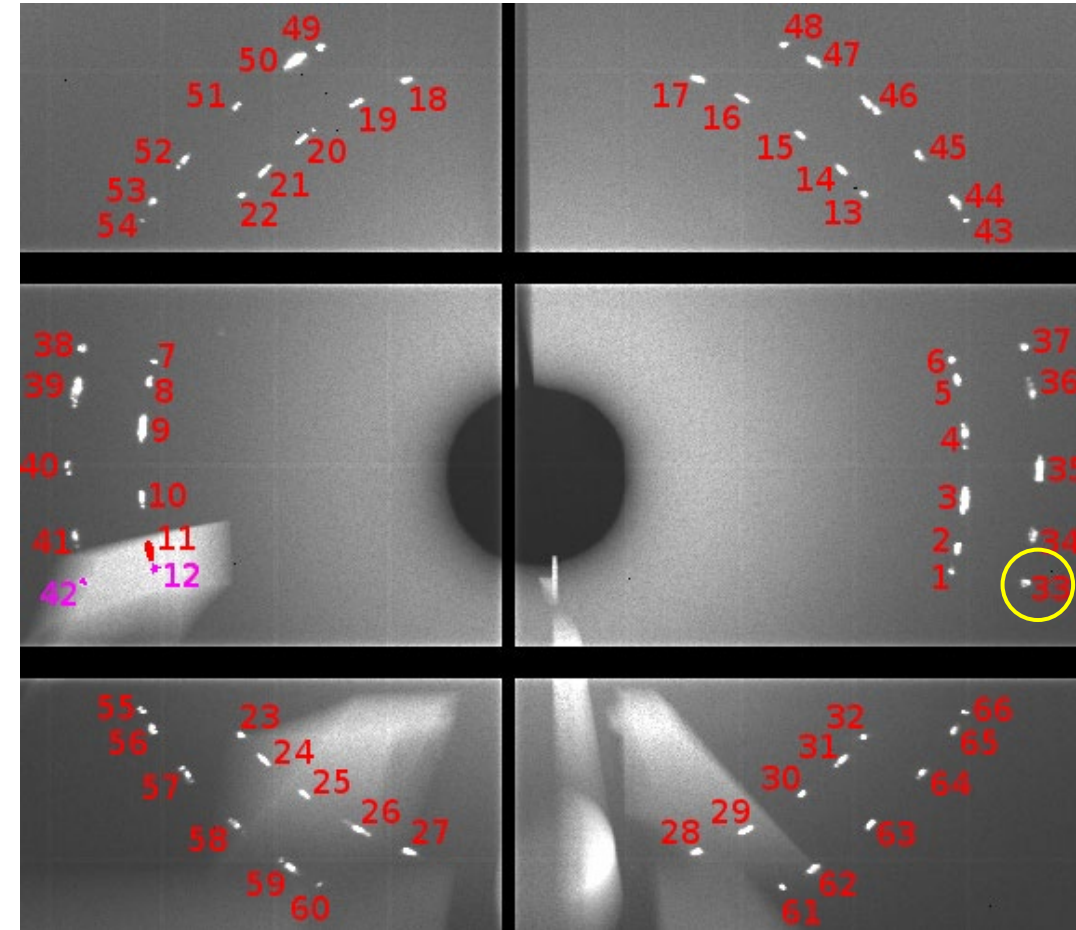
Angles under consideration	Domain 1	Domain 2	Domain 3	Domain 4	Domain 5
8.5, 44.5, 80.5, 114.5, 150.5	74	70	74	70	72
44.5, 80.5, 114.5, 150.5, 190	75.5	70	74	70	70.5
80.5, 114.5, 150.5, 190, 227	75.5	67.5	76.5	70	70.5
114.5, 150.5, 190, 227, 262	75.5	67.5	76.5	68.5	72
150.5, 190, 227, 262, 296	74	69	76.5	68.5	72
190, 227, 262, 296, 331	74	69	76	69	72
227, 262, 296, 331, 8.5	72.5	69	76	69	73.5
262, 296, 331, 8.5, 44.5	72.5	71.5	73.5	69	73.5
296, 331, 8.5, 44.5, 80.5	72.5	71.5	73.5	70.5	72
331, 8.5, 44.5, 80.5, 114.5	74	70	73.5	70.5	72



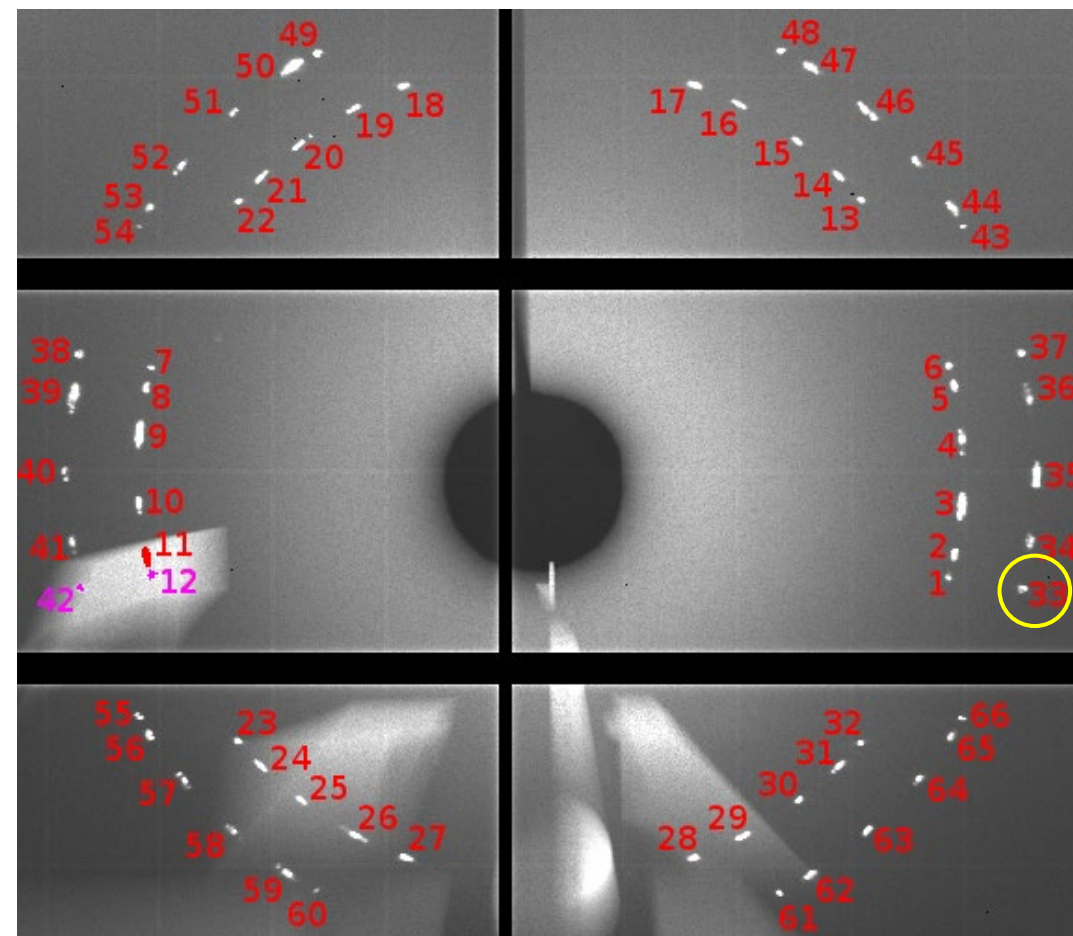
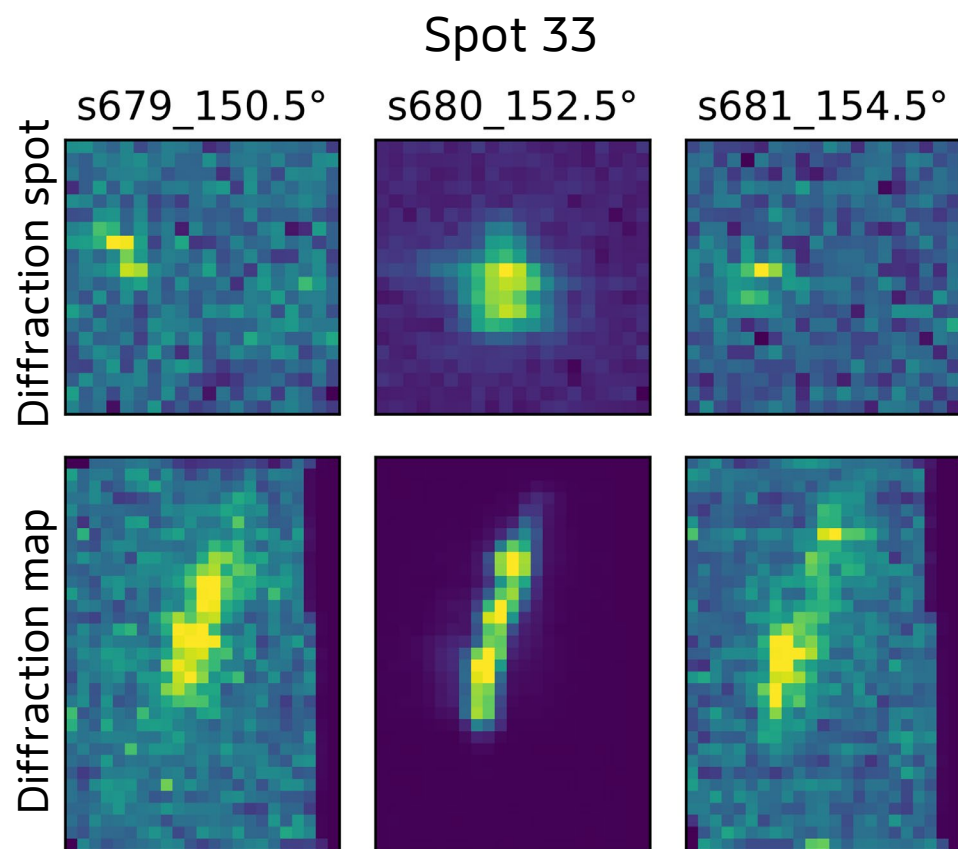
Visualization of Crystals



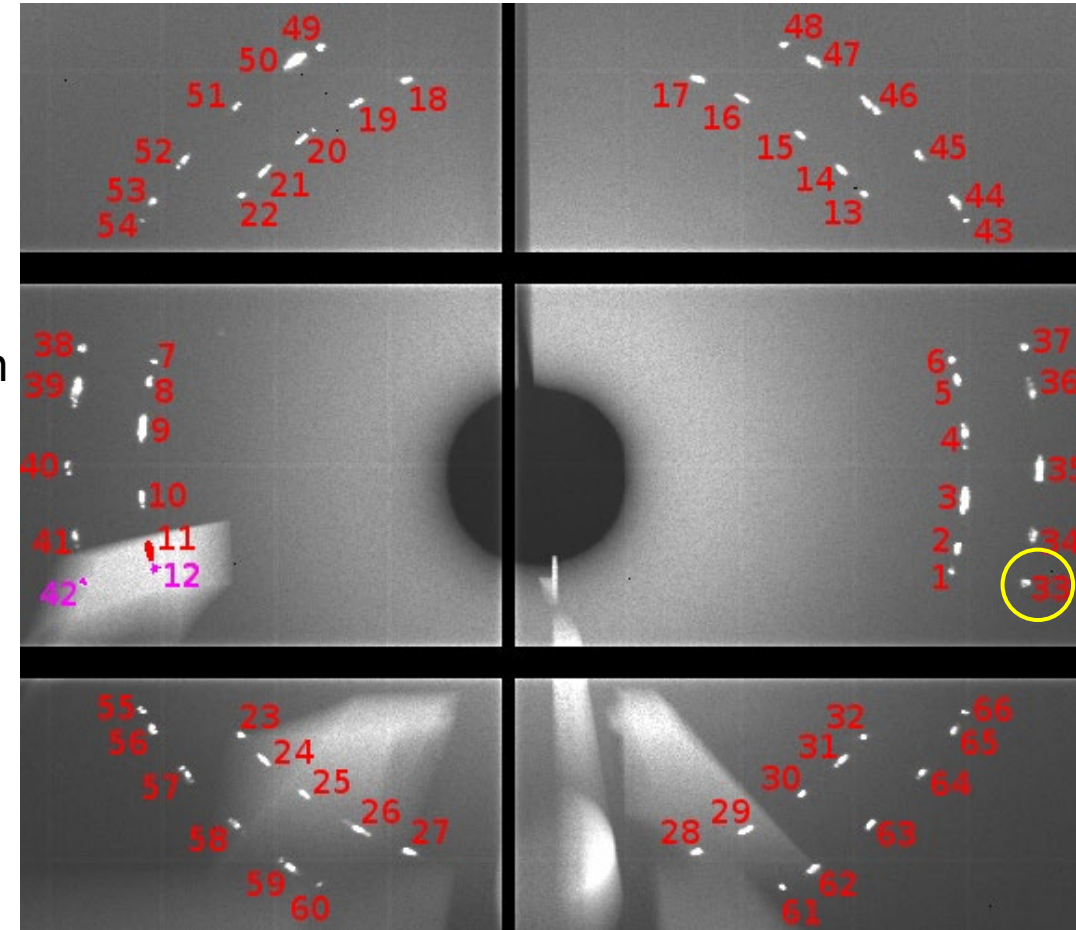
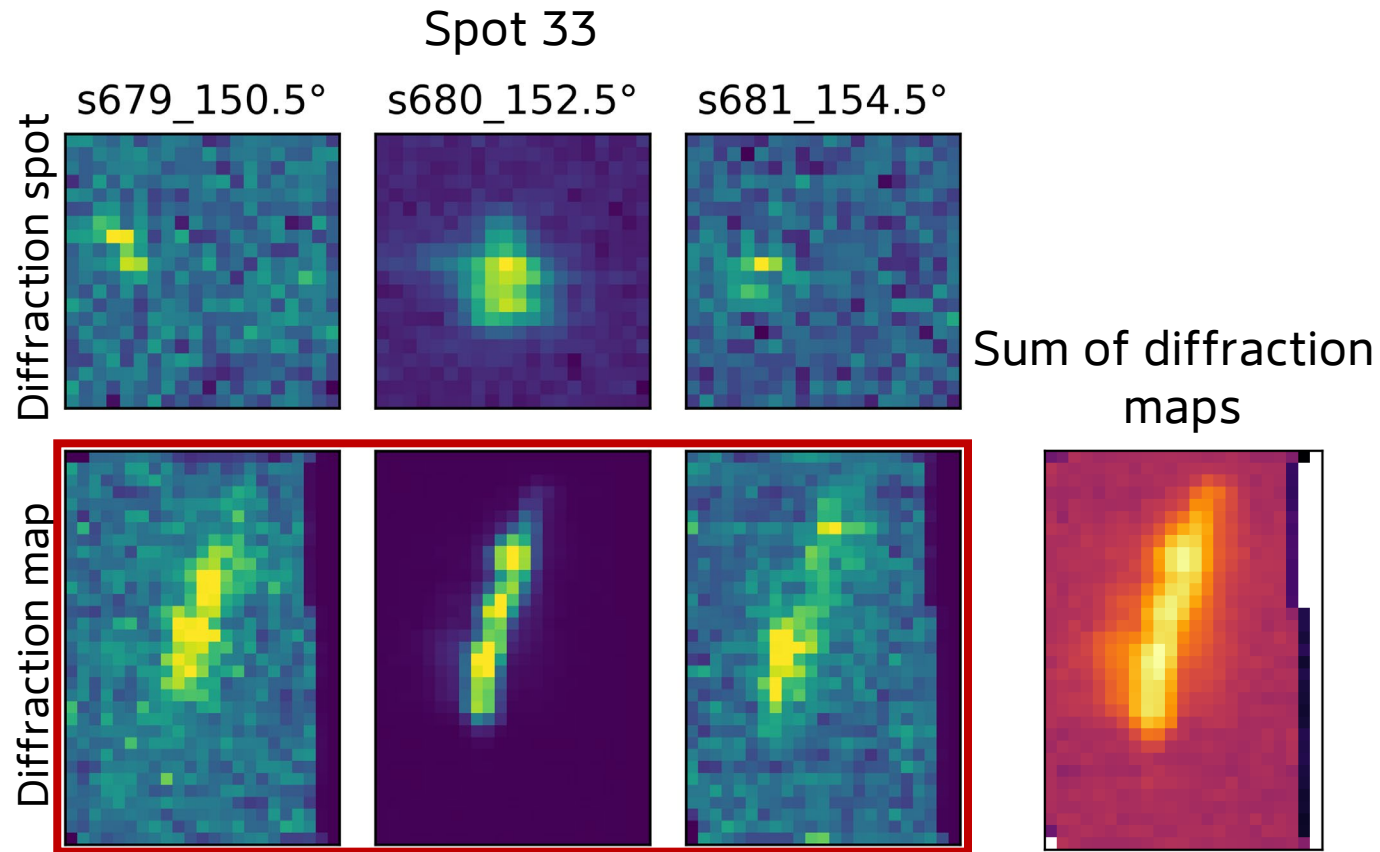
Visualization of Crystals



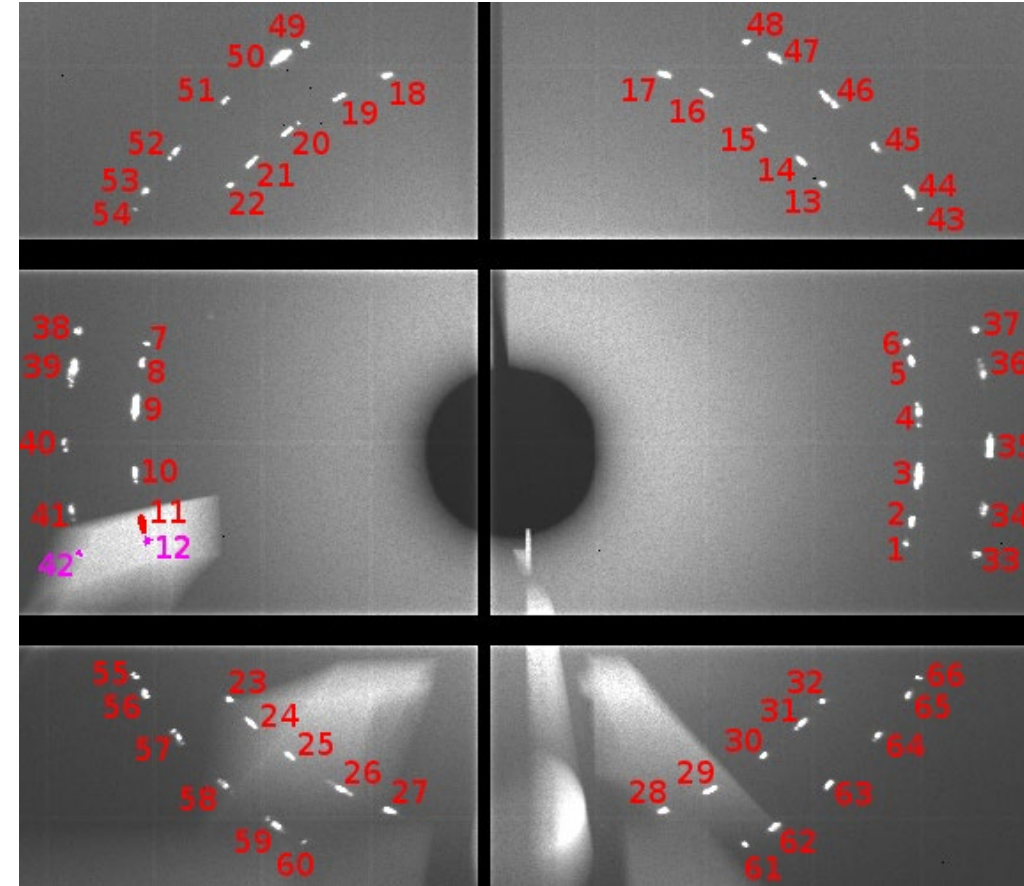
Visualization of Crystals



Visualization of Crystals



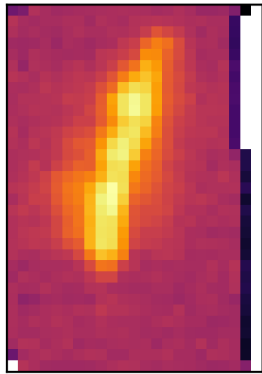
Identify Crystals within Five Crystals



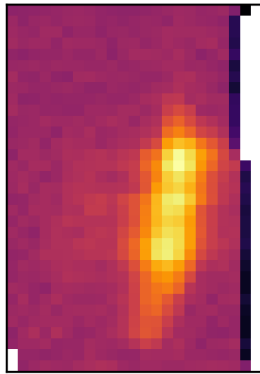
Identify Crystals within Five Crystals

Right side (2nd ring)

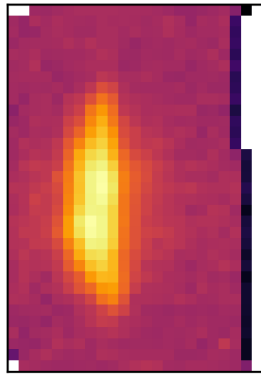
spot 33b



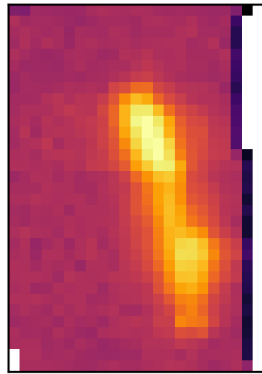
spot 34b



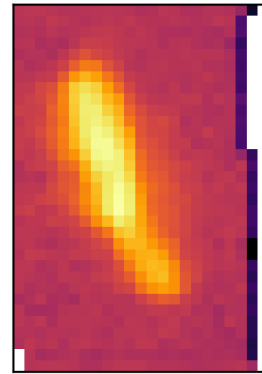
spot 35b



spot 36b

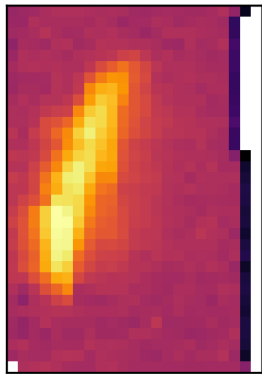


spot 37b

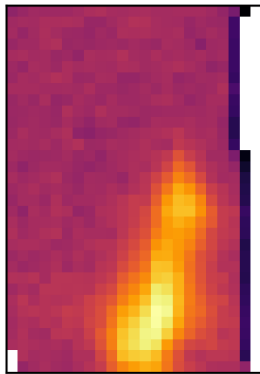


Left side (2nd ring)

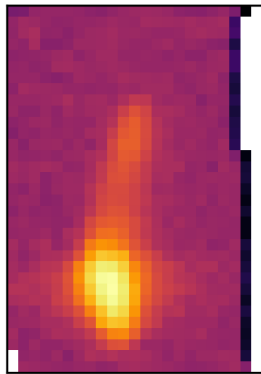
spot 38b



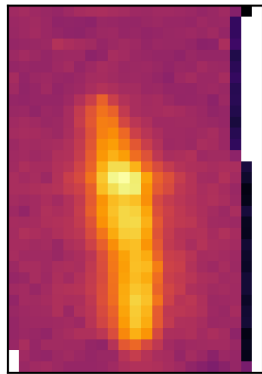
spot 39b



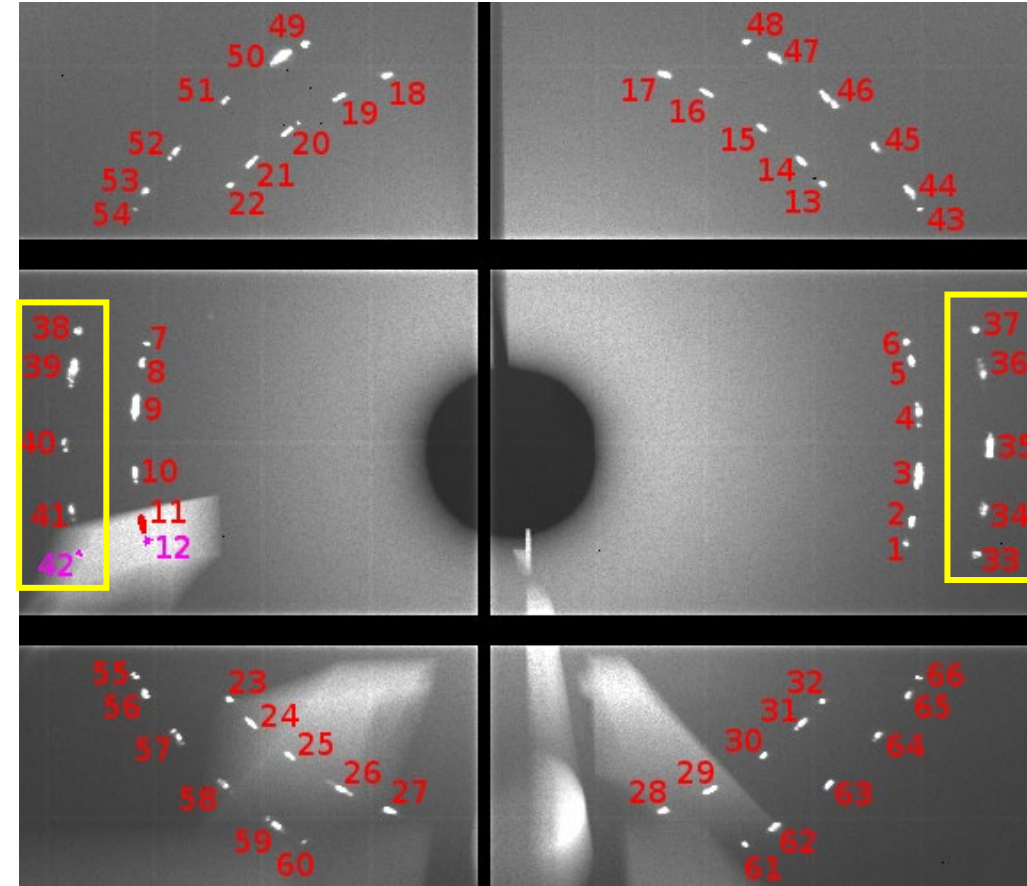
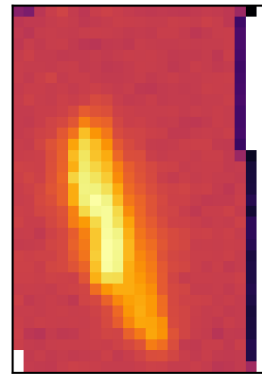
spot 40b



spot 41b



spot 42b

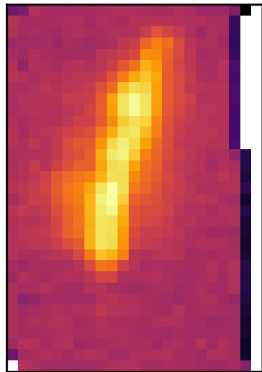


Identify Crystals within Five Crystals

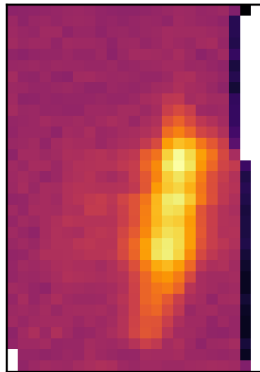
Sum of adjusted diffraction maps
for spots 38-42

Right side (2nd ring)

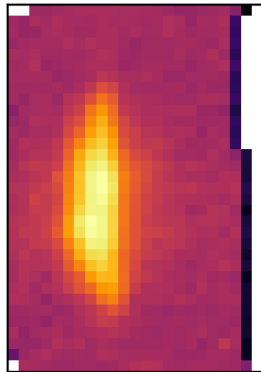
spot 33b



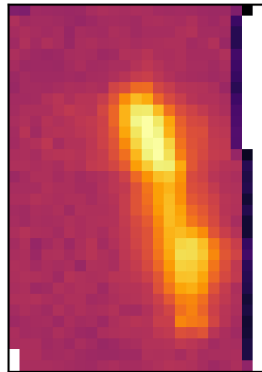
spot 34b



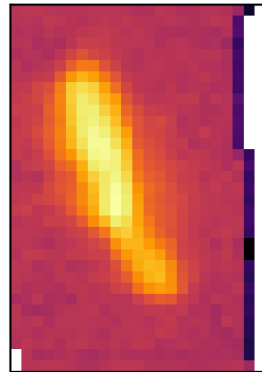
spot 35b



spot 36b

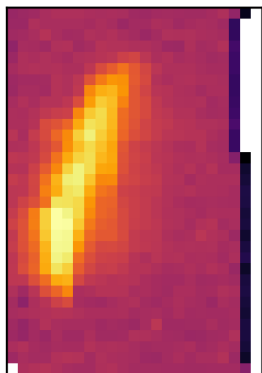


spot 37b

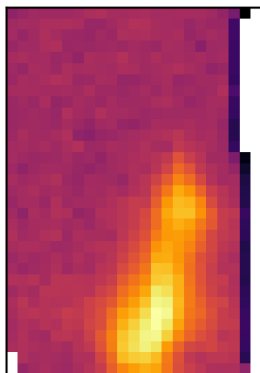


Left side (2nd ring)

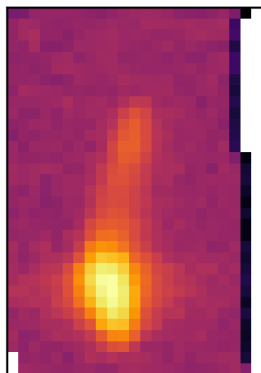
spot 38b



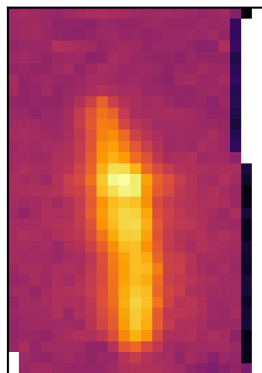
spot 39b



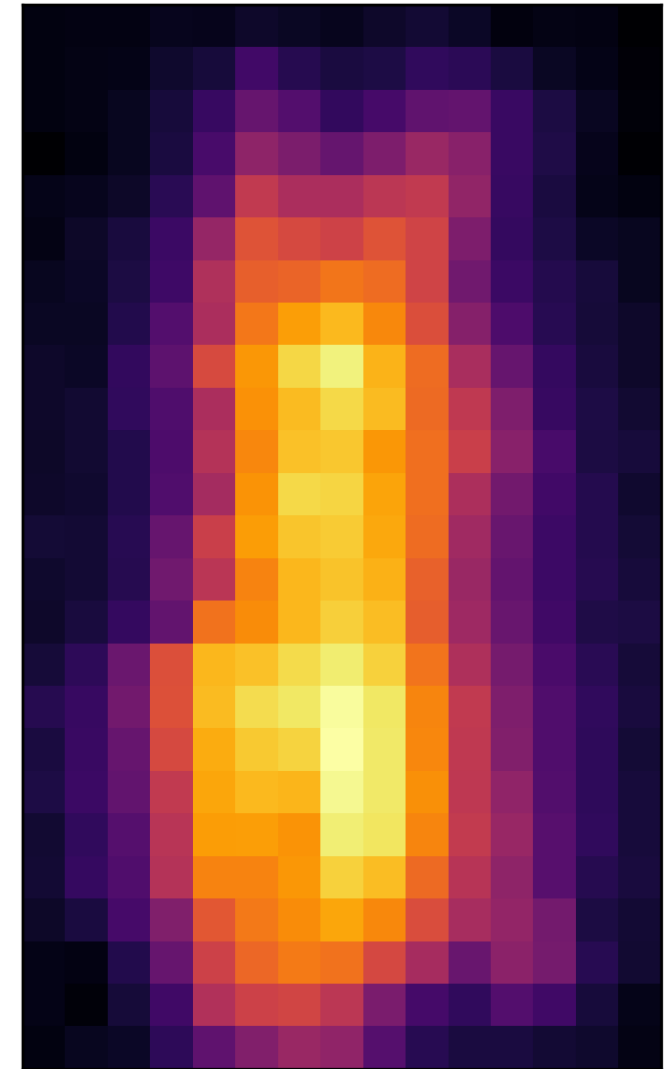
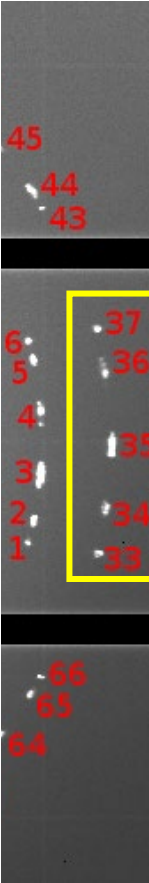
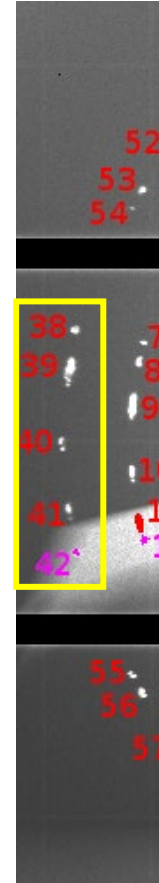
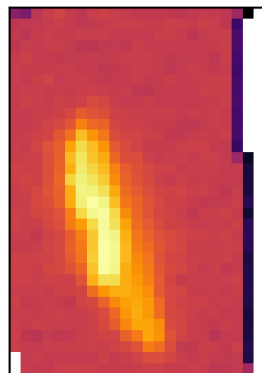
spot 40b



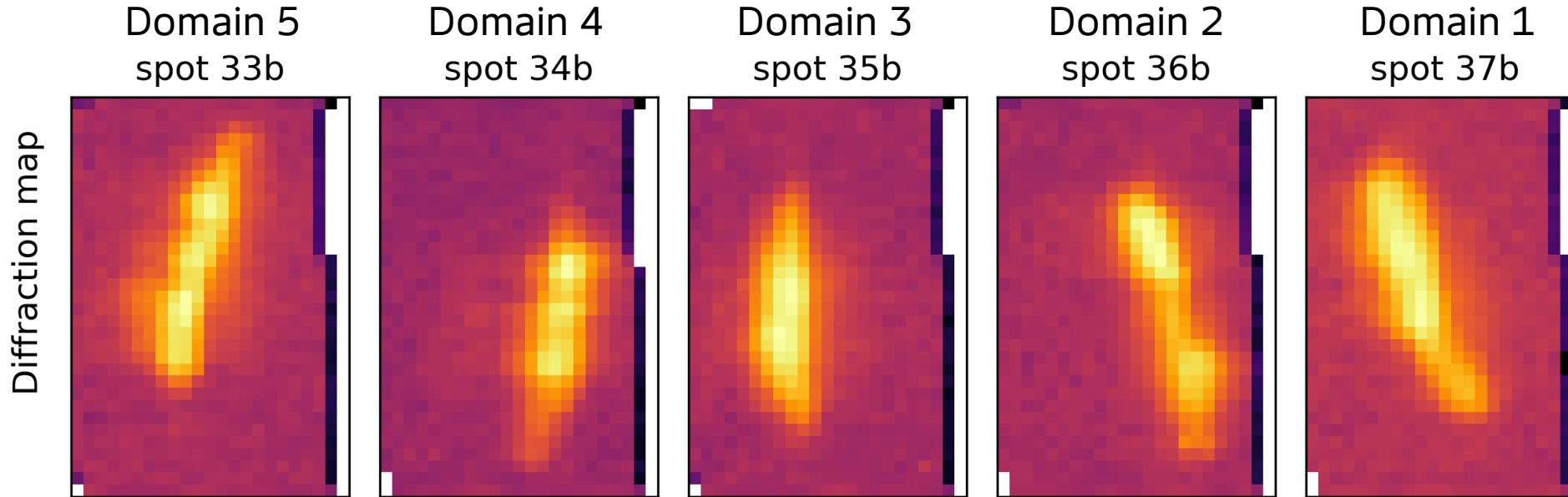
spot 41b



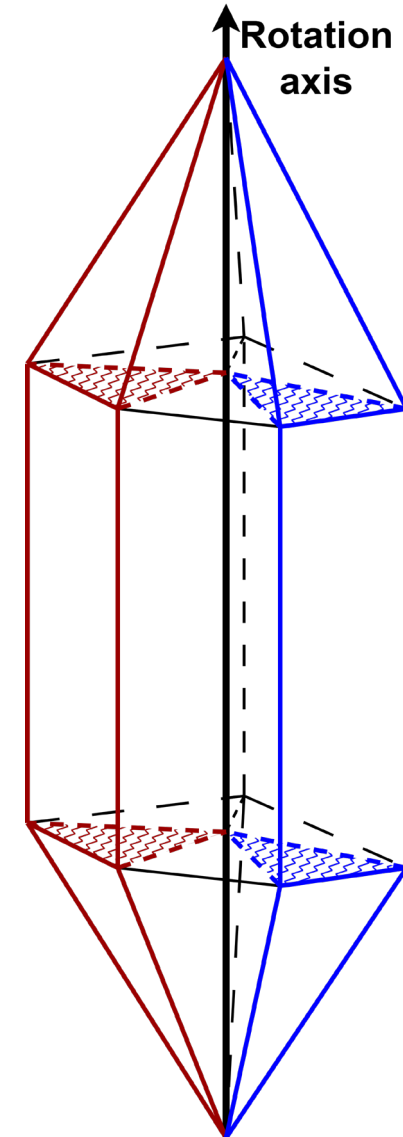
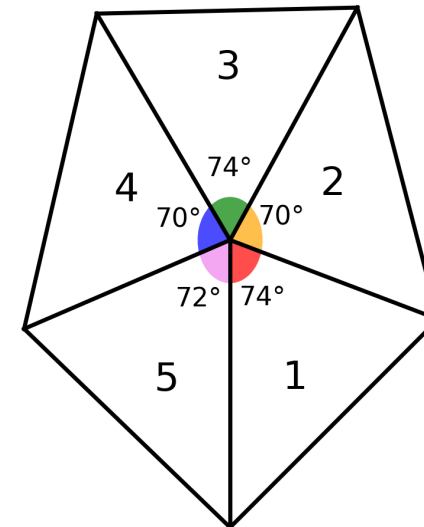
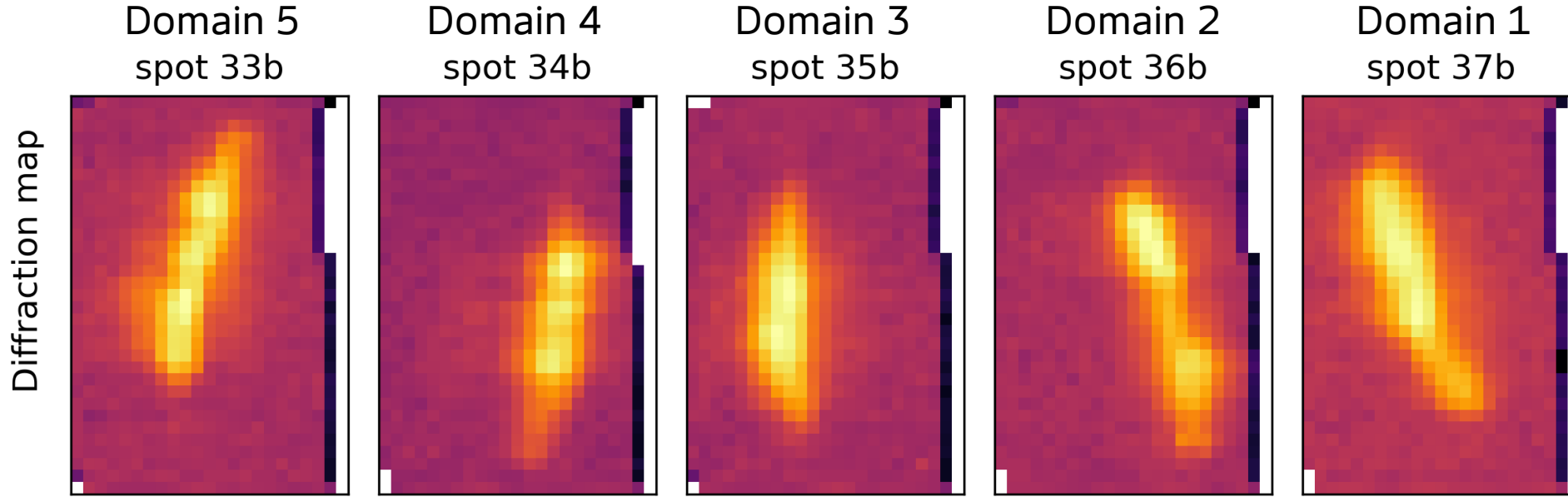
spot 42b



Identify Crystals within Five Crystals



Identify Crystals within Five Crystals

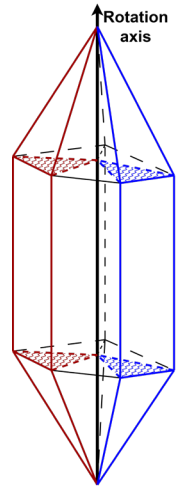
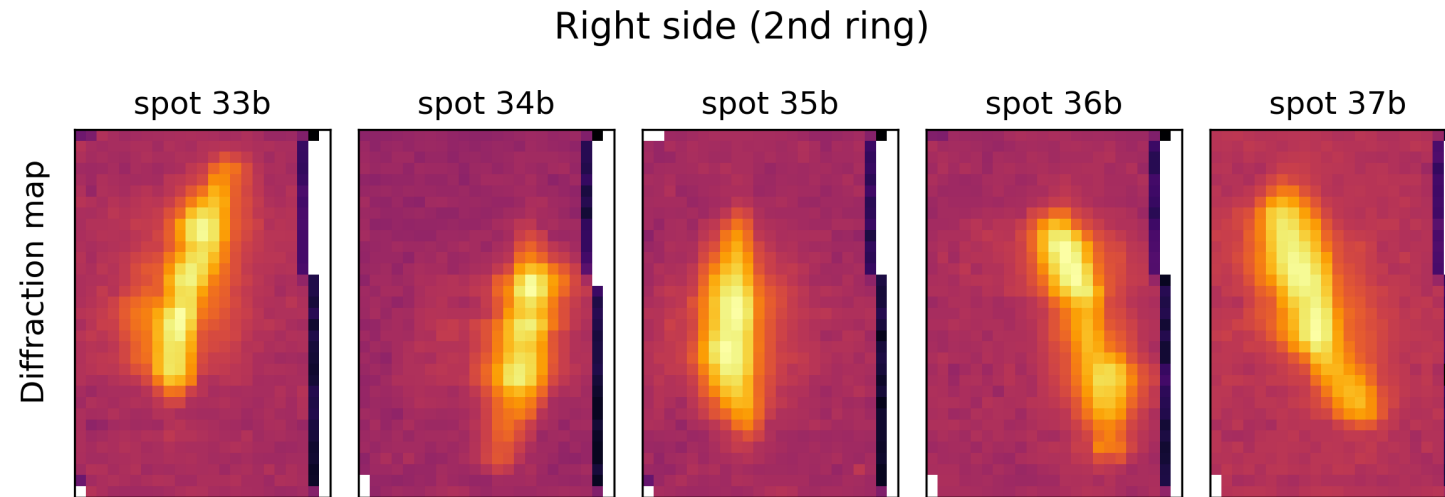
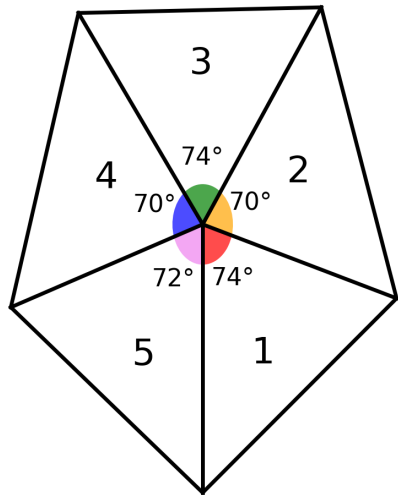


Conclusions

- ✓ Determined twist of $\sim 5\text{-}6^\circ$ along crystallite axis
- ✓ Calculated angular relations between domains
- ✓ Identified crystals within crystallite

TO BE DONE:

- Assign each spot to specific domain
- Calculate crystal strain



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- ✓ A. Kordyuk, V. Bezguba
- ✓ Armed Forces of Ukraine



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Diffraction from 2 lattices

