Moiré Superlattices with Supercrystals of Perovskite Nanocrystals

Final Student Session

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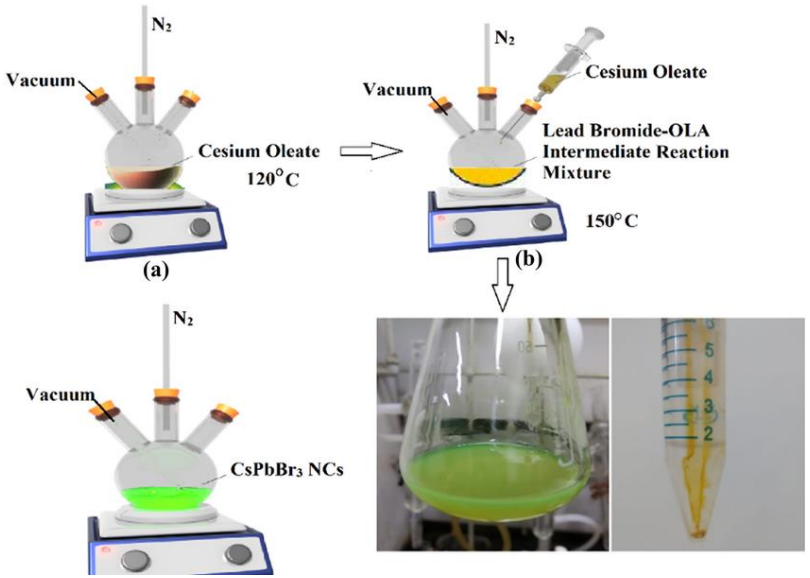
HELMHOLTZ

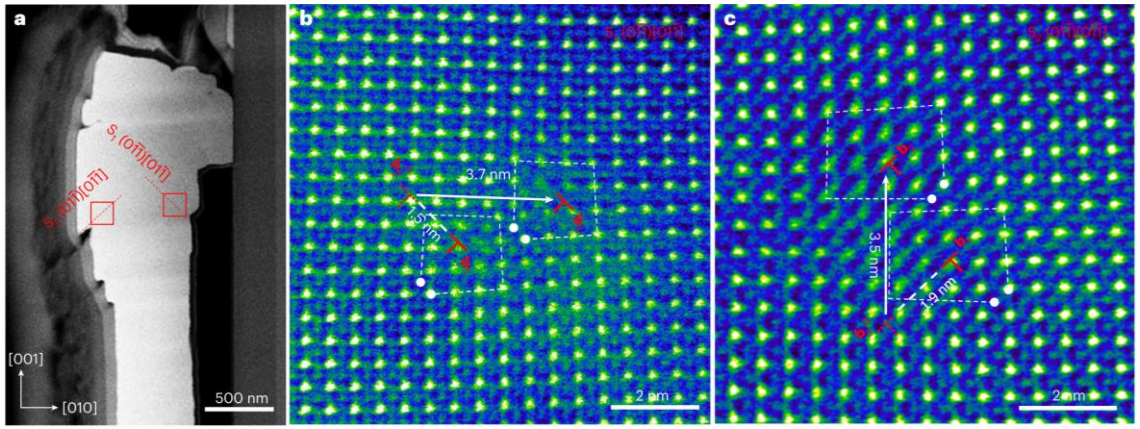
AGH

DESY.

Motivation

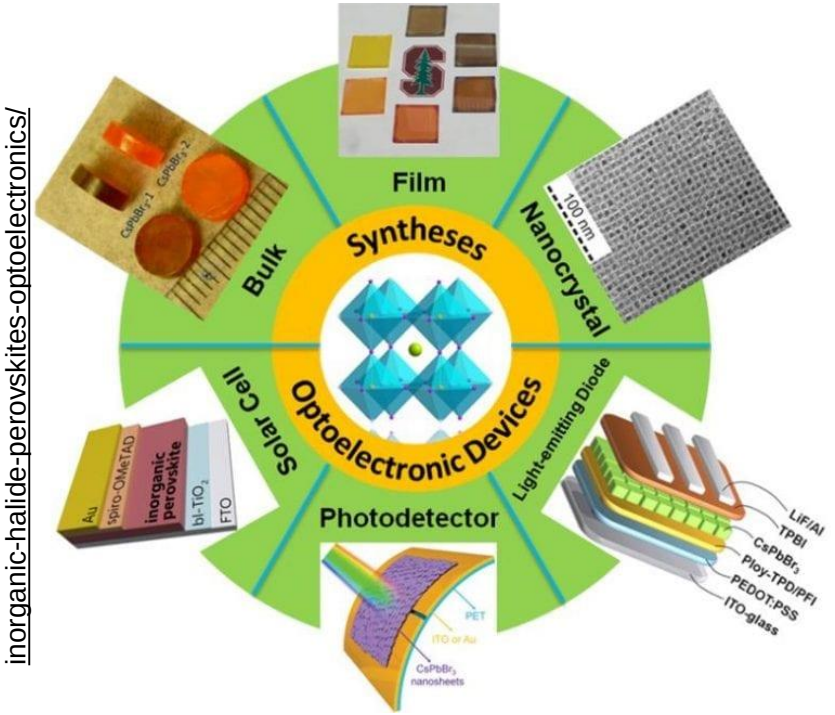


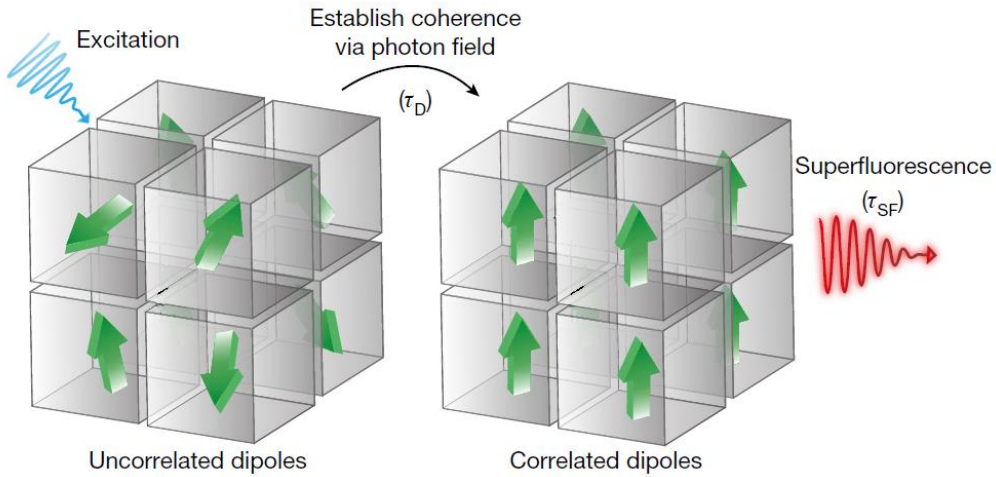
B. Gopal Krishna et al., J Mater Sci: Mater Electron (2022) **33**:1324–1336



X. Li et al., Nature Materials (2023) **22:**1175–1181

https://www.advancedsciencenews.com/evolution-inorganic-halide-perovskites-optoelectronics/



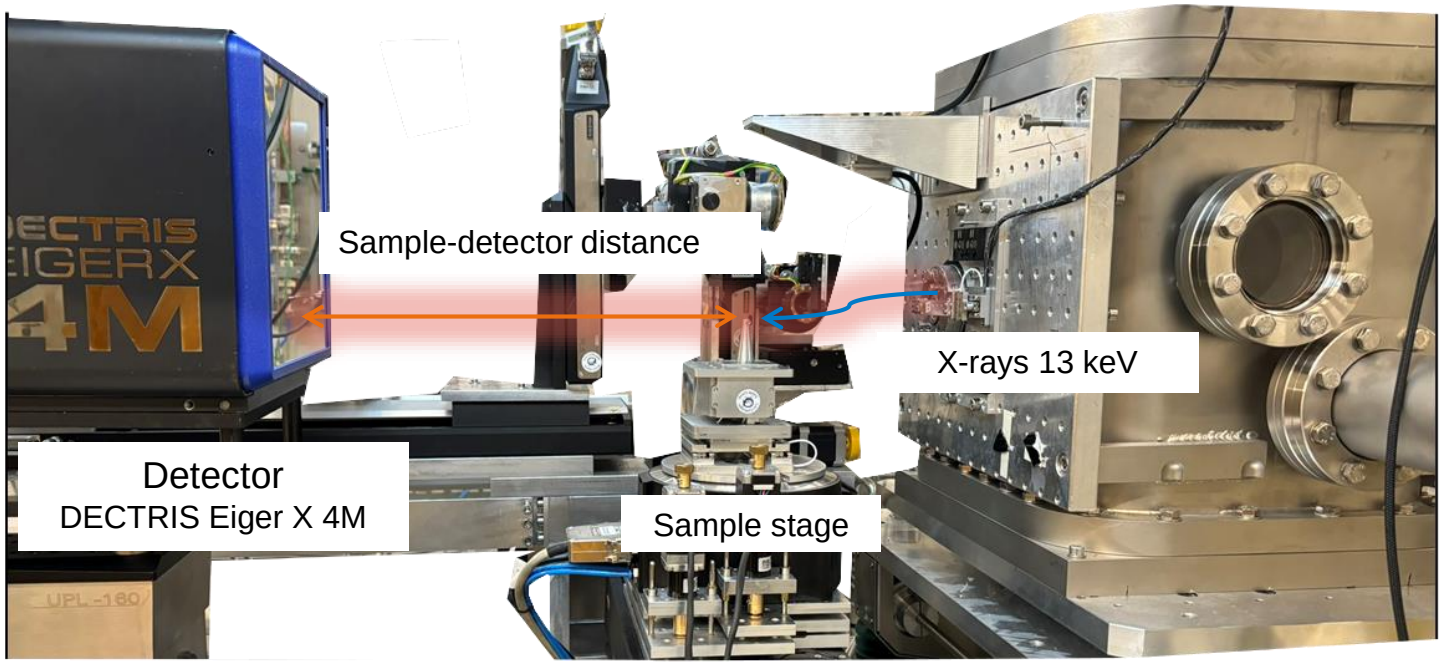


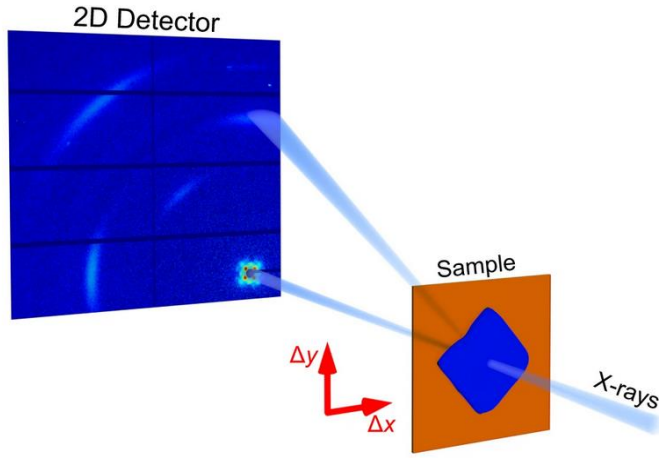
G. Rainò et al. *Nature* (2018) **563**:671-675.

Beamline Parameters

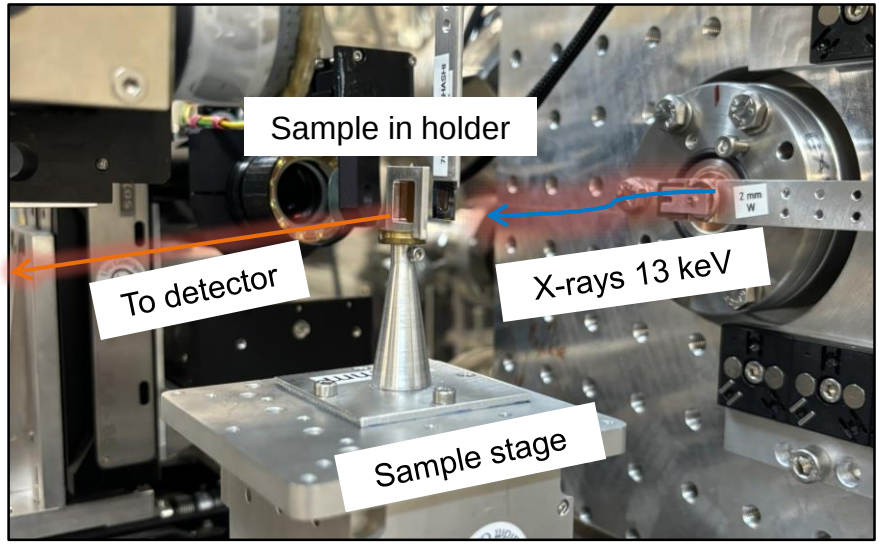
P10 beamline (GINIX setup) at PETRA III

- Energy: **13 keV (λ = 0.954 Å)**
- Beam size (FWHM): **240 (V) x 320 (H) nm²**
- Endstation: **GINIX Nanodiffraction**
- Detector: **DECTRIS Eiger X 4M**
- Exposure time: **1 s**
- Scanning step size (Δx, Δy): **333 - 500 nm**
- Sample-to-detector distance:
  Sample 3-1, 3-2, 3-3, 3-4: **398.5 mm**
  Sample 4-4: **348.5 mm**



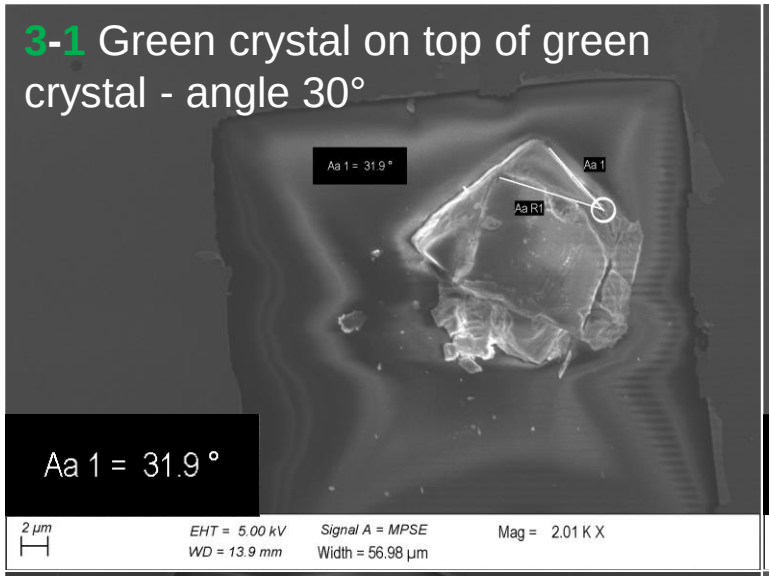


D. Lapkin et al., *Nat. Commun.* **13**, 892 (2022)

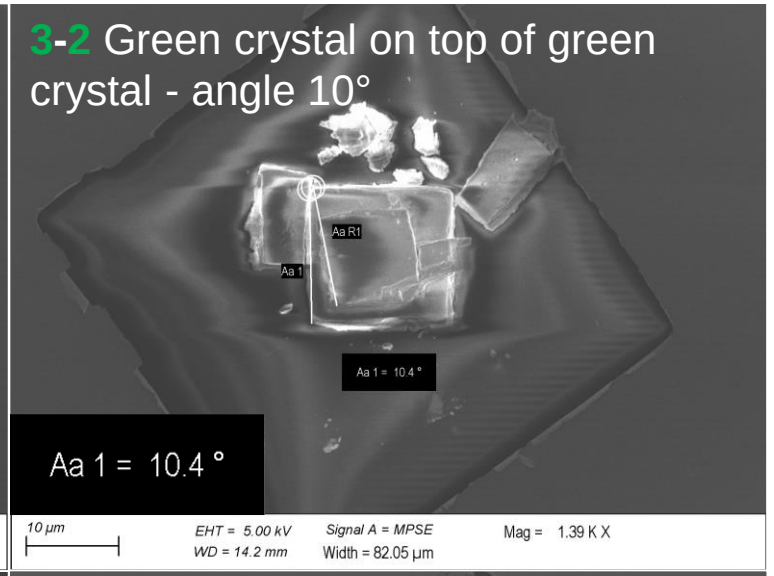


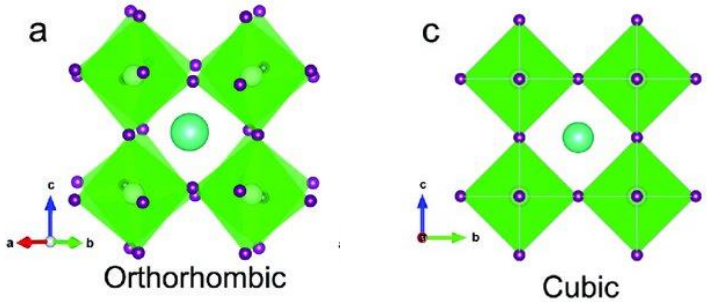
Samples overview

3-1 Green crystal on top of green crystal - angle 30°



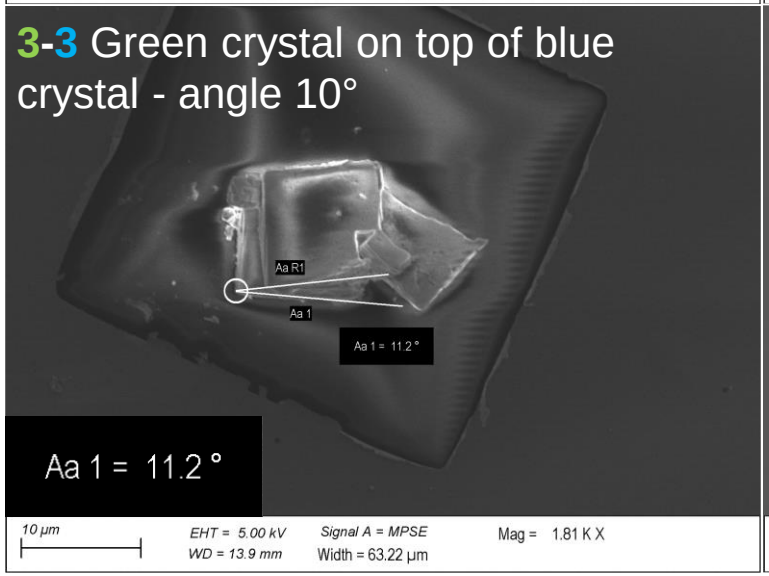
3-2 Green crystal on top of green crystal - angle 10°



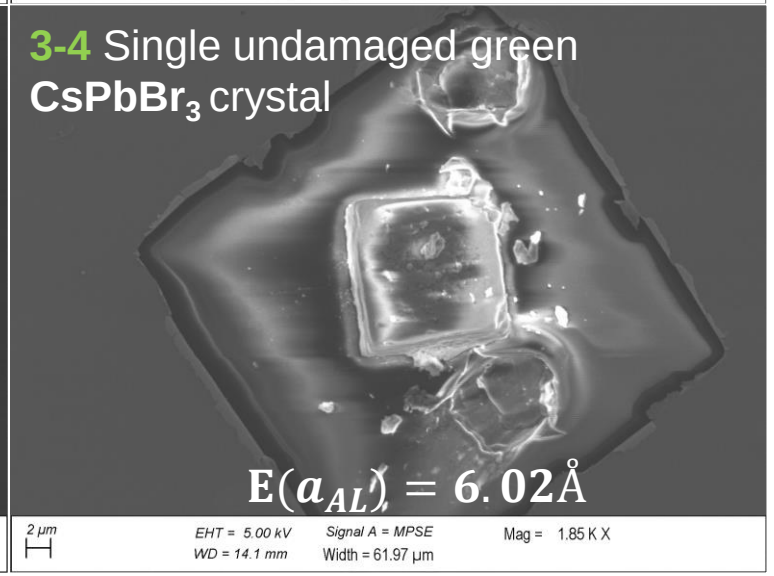


M. Zhang et al., CrystEngComm, **2017**, 6797-6803

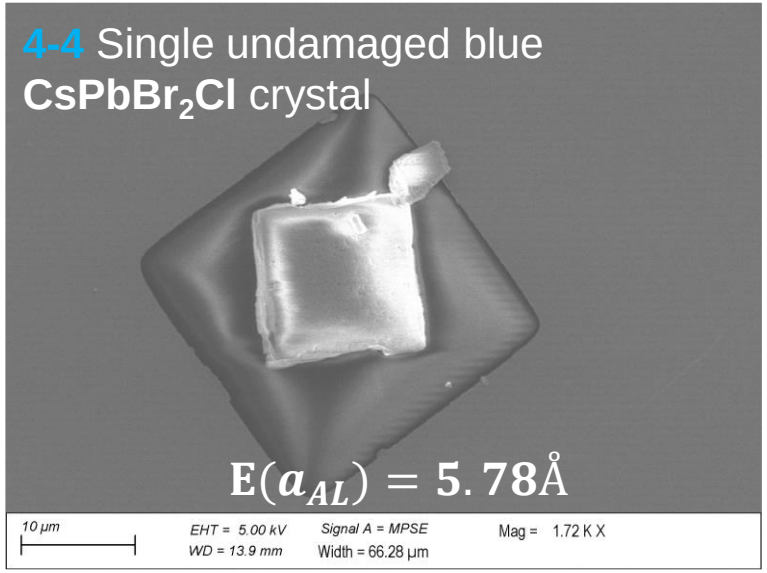
3-3 Green crystal on top of blue crystal - angle 10°



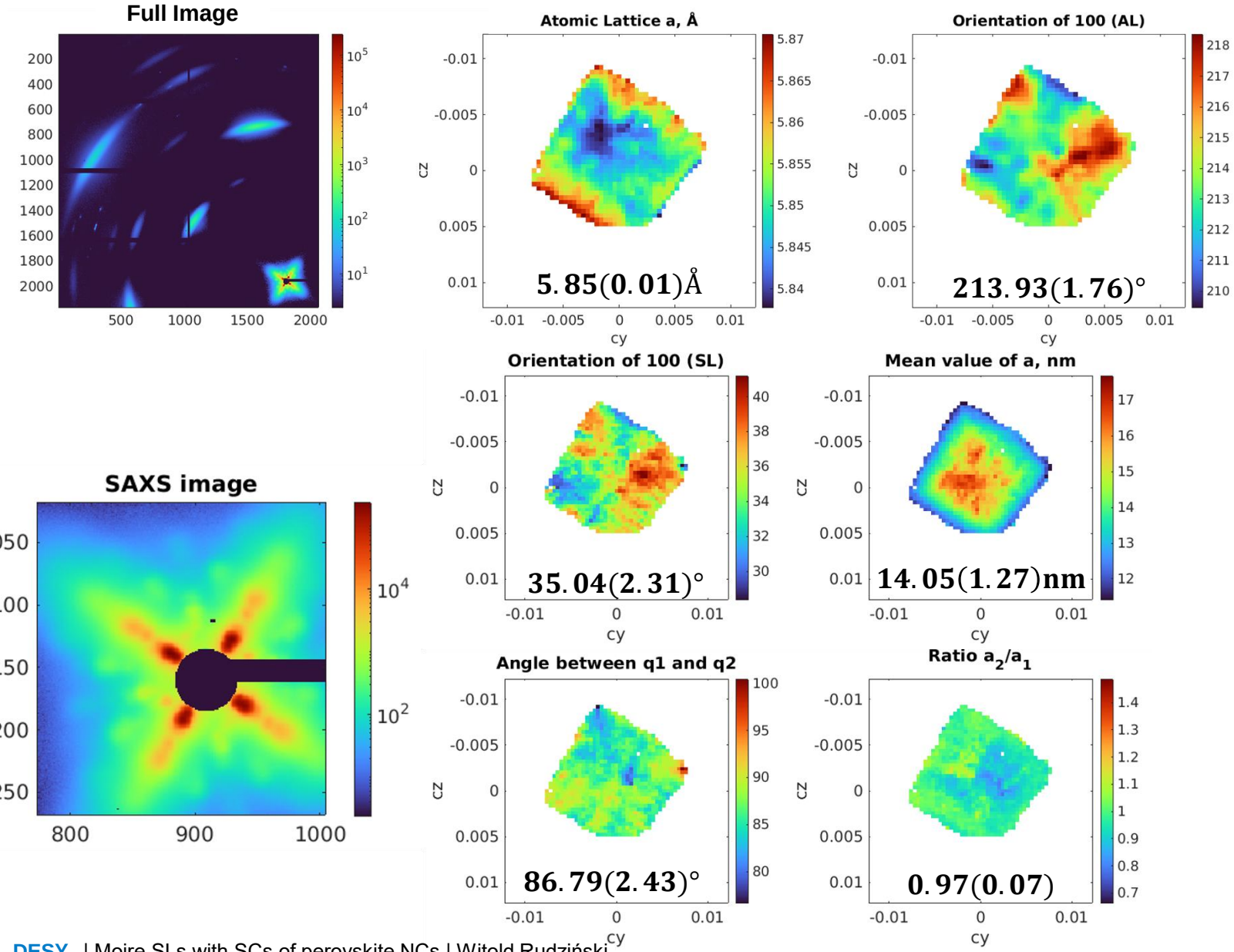
3-4 Single undamaged green **$CsPbBr_3$** crystal

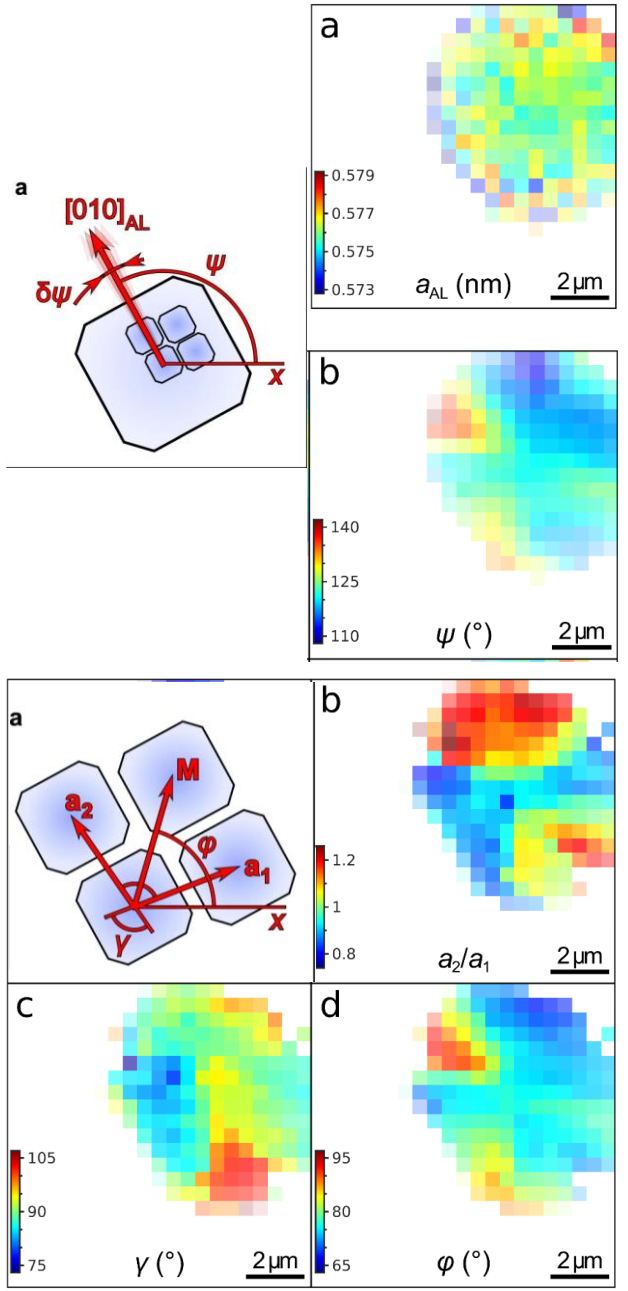


4-4 Single undamaged blue **$CsPbBr_2Cl$** crystal



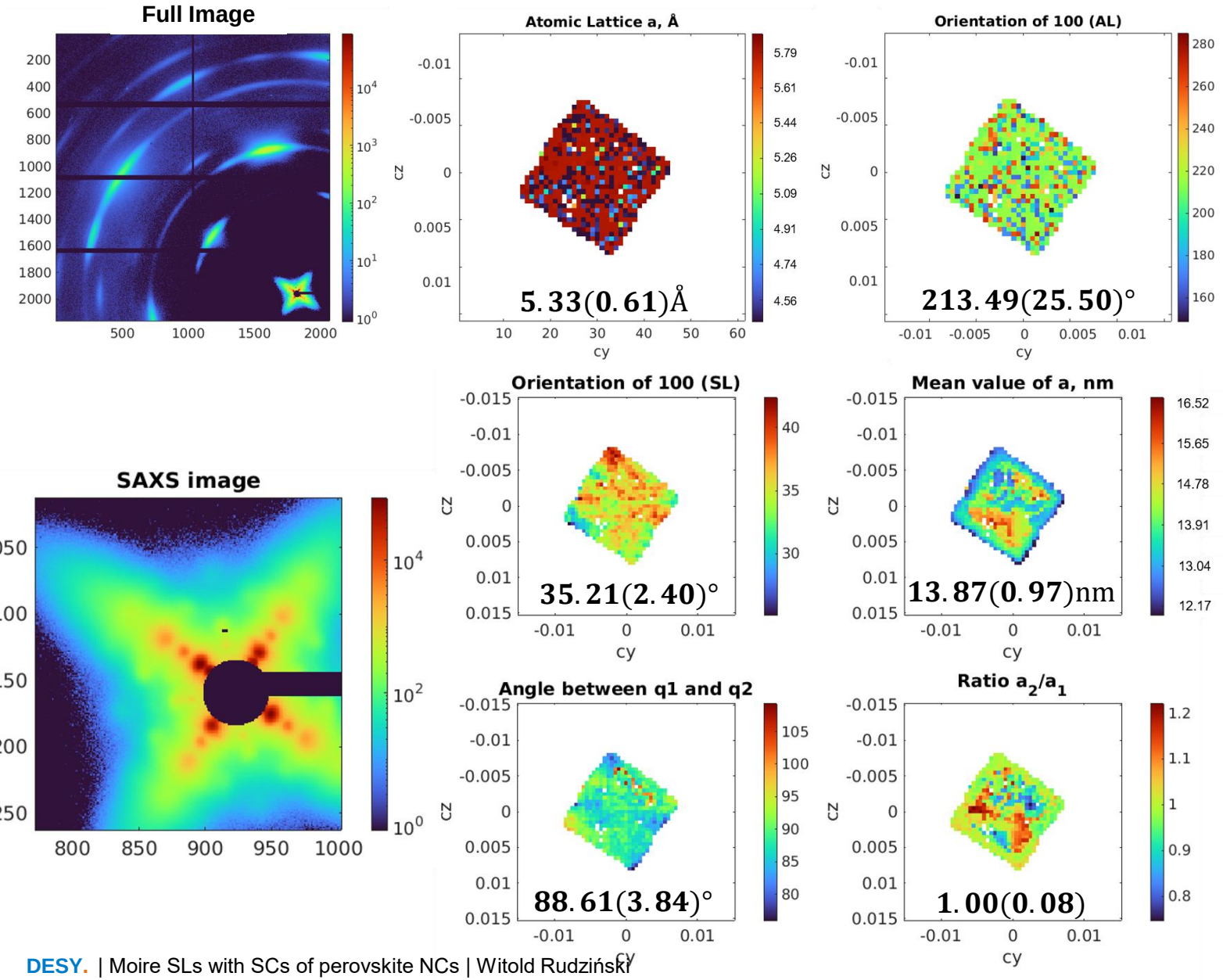
Single green ($PbCsBr_3$) crystals

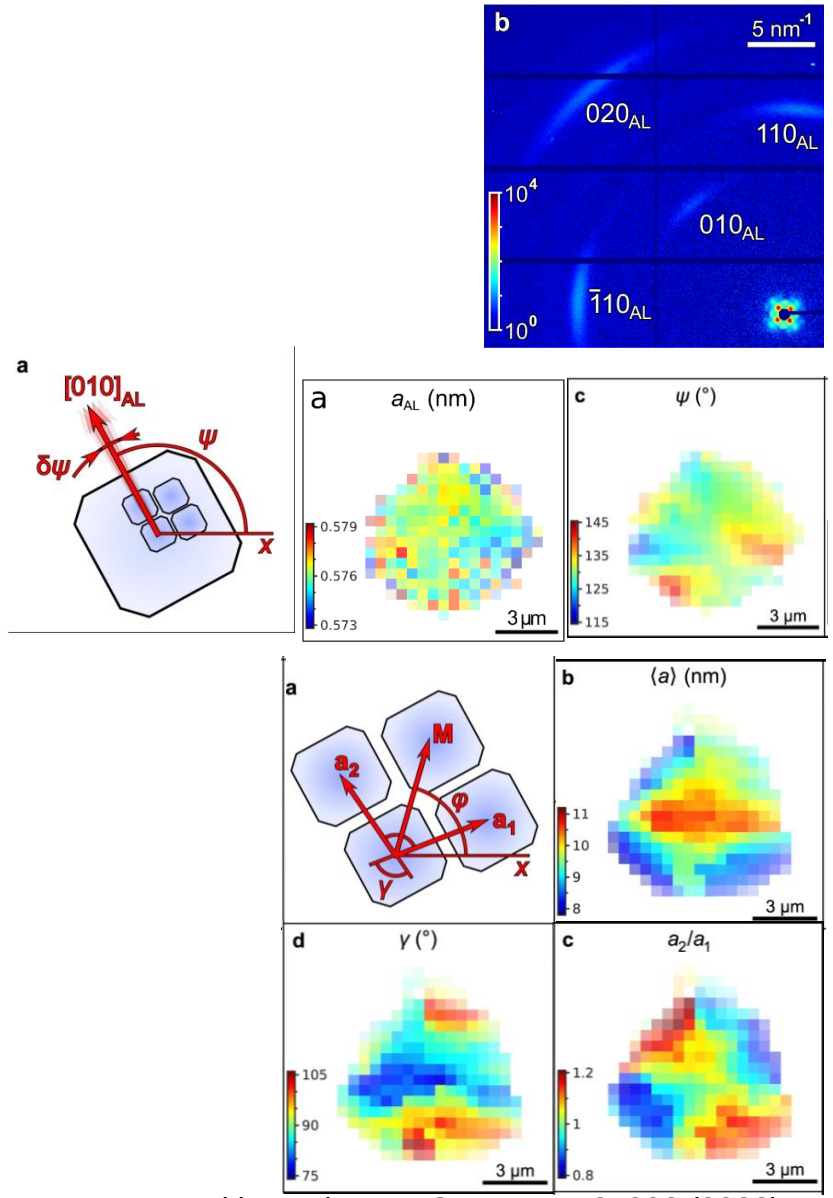




D. Lapkin et al., *Nat. Commun.* **13**, 892 (2022)

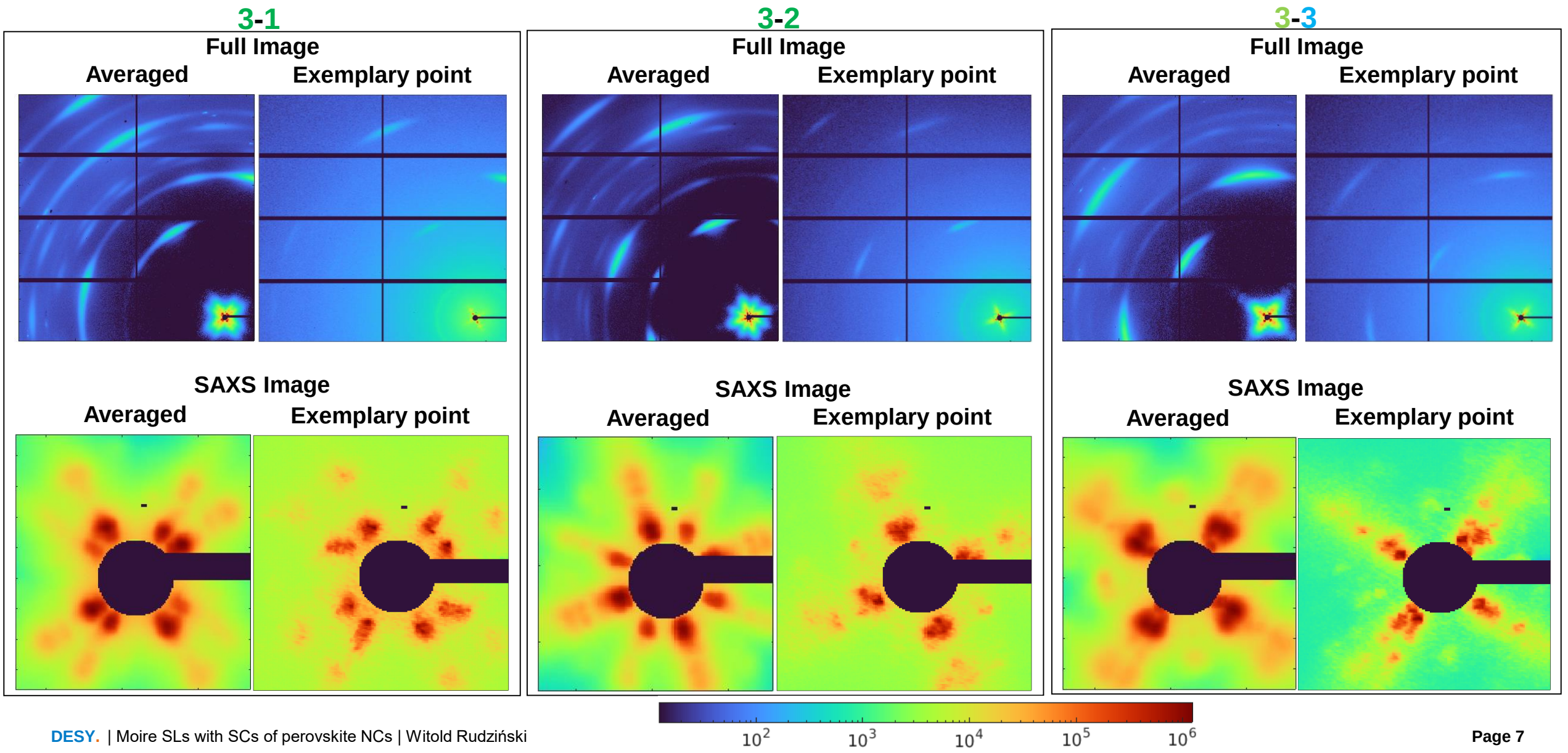
Single blue ($PbCsBr_2Cl$) crystals





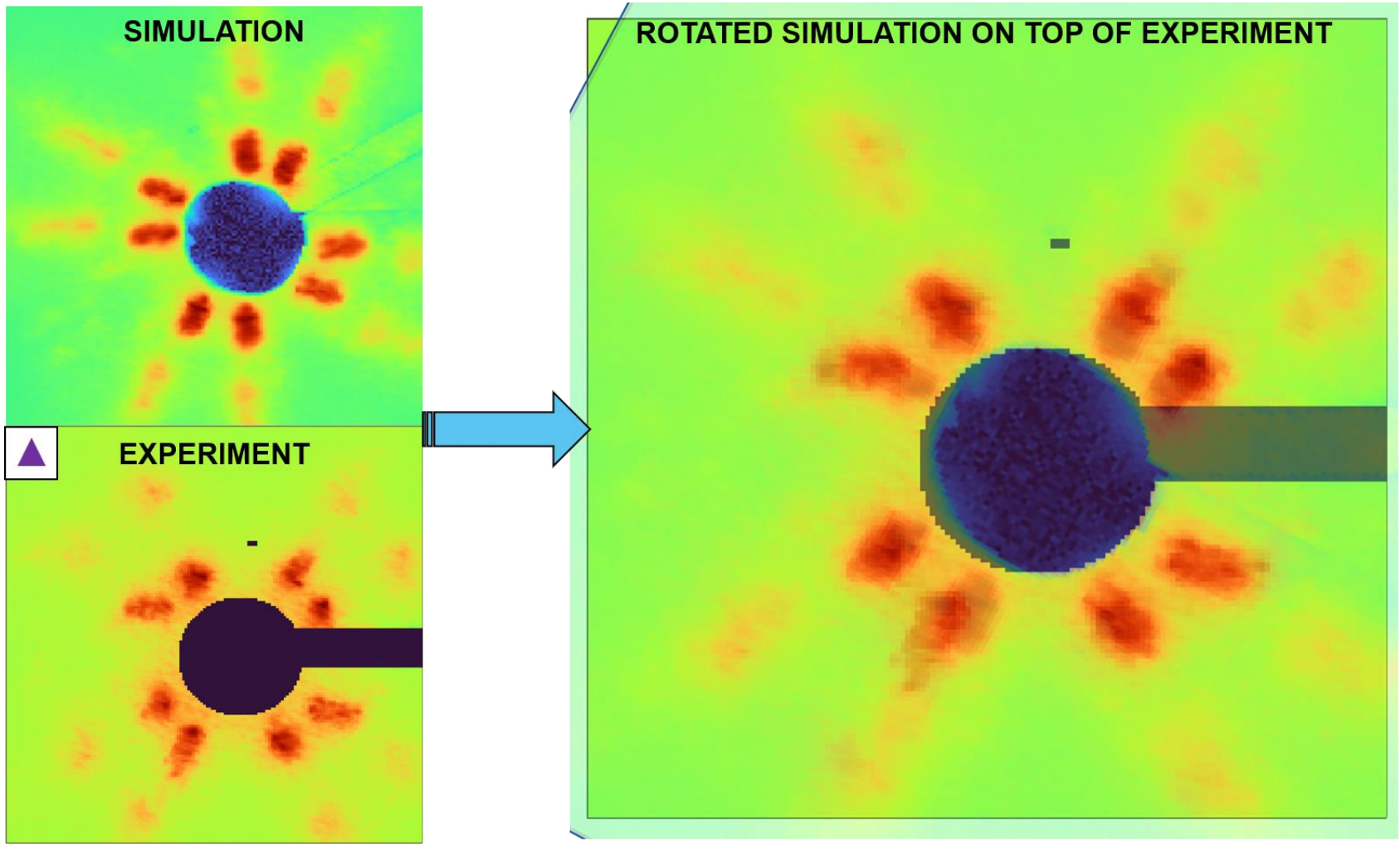
D. Lapkin et al., *Nat. Commun.* **13**, 892 (2022)

Diffraction patterns of samples 3-1, 3-2 and 3-3



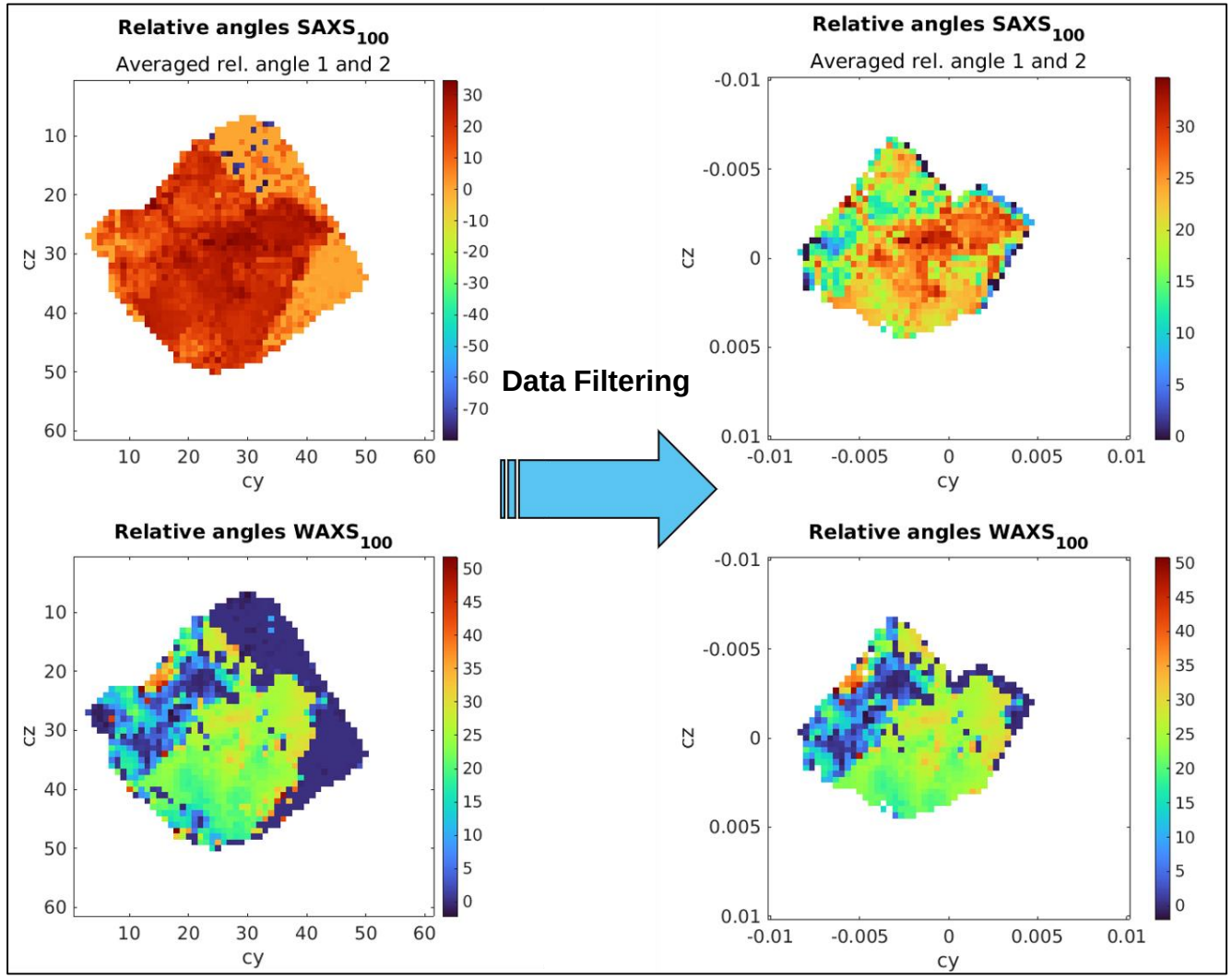
Stacked crystals – easy computational check of intuition

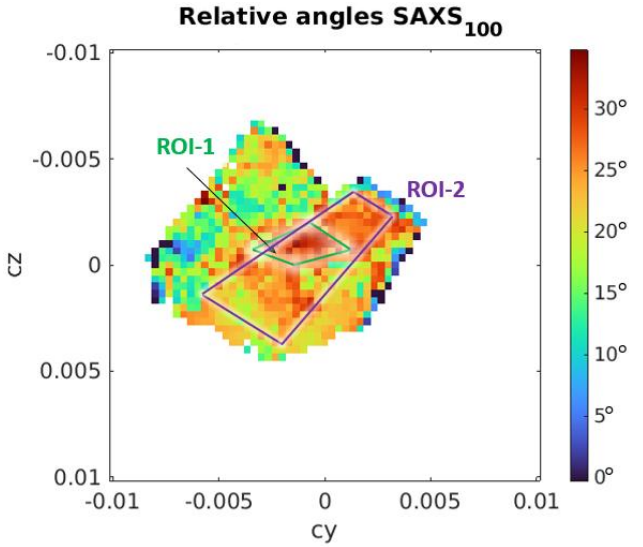
e.g. Case of ‘green on green’ with ~30◦ rotation (sample 3-1)



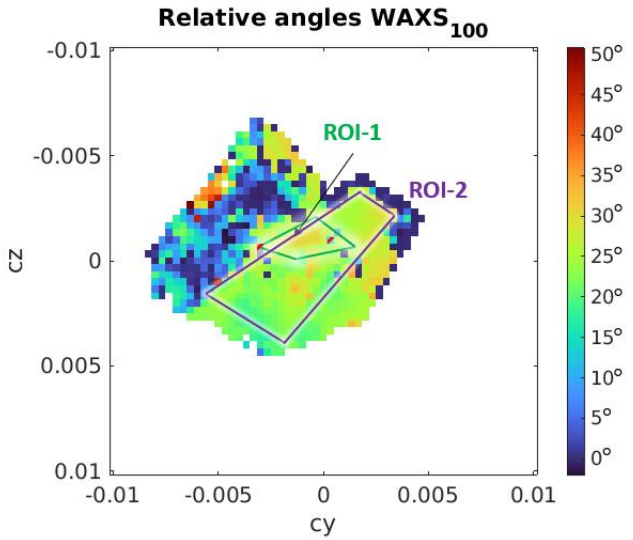
3-1 Green crystal on top of green crystal – angle of 30°

Bragg peak analysis using 2D Gaussian fitting





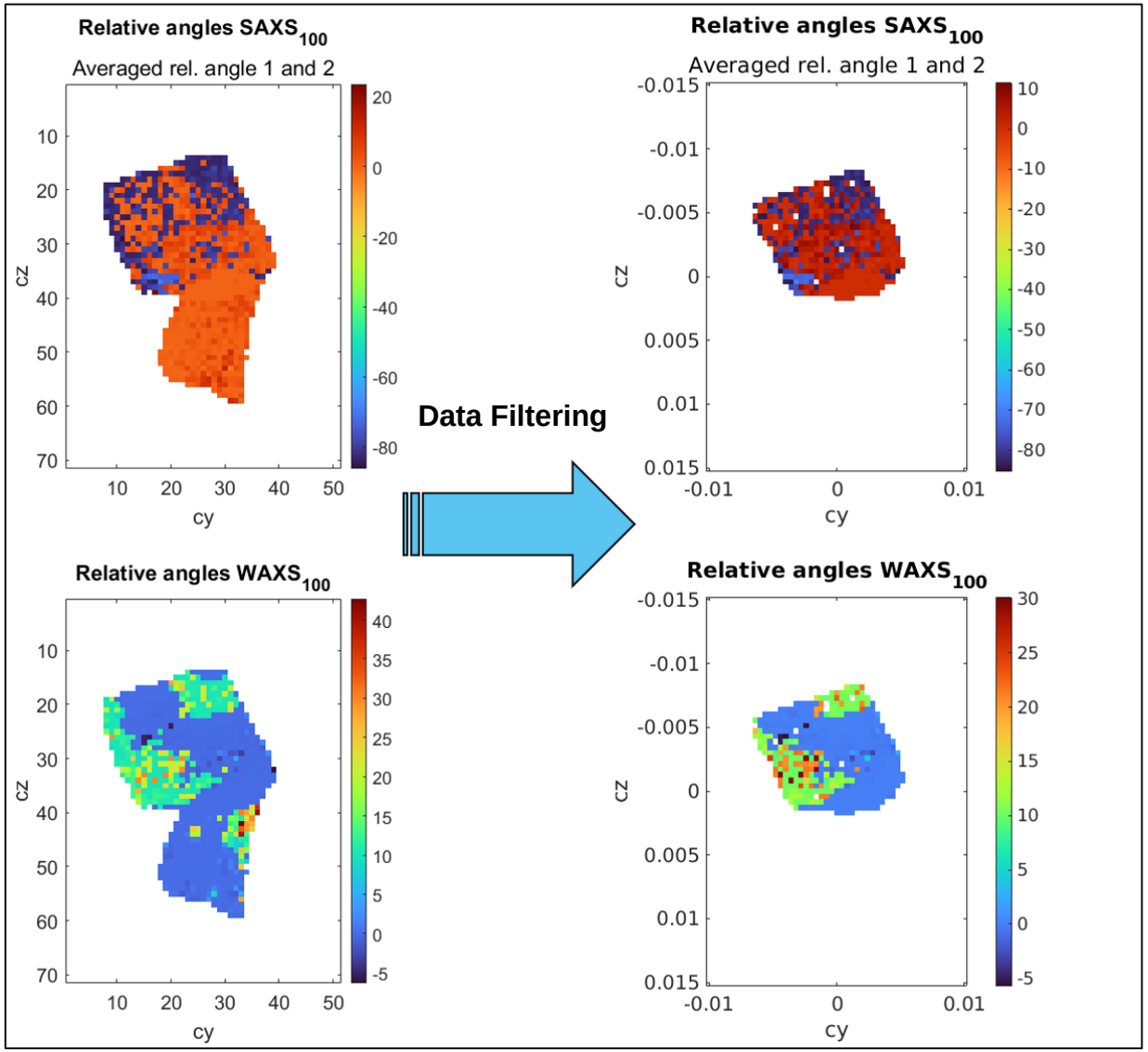
SAXS:
ROI-1 (41 pts):
$28.41(2.74)°$
ROI-2 (228 pts):
$25.05(3.66)°$

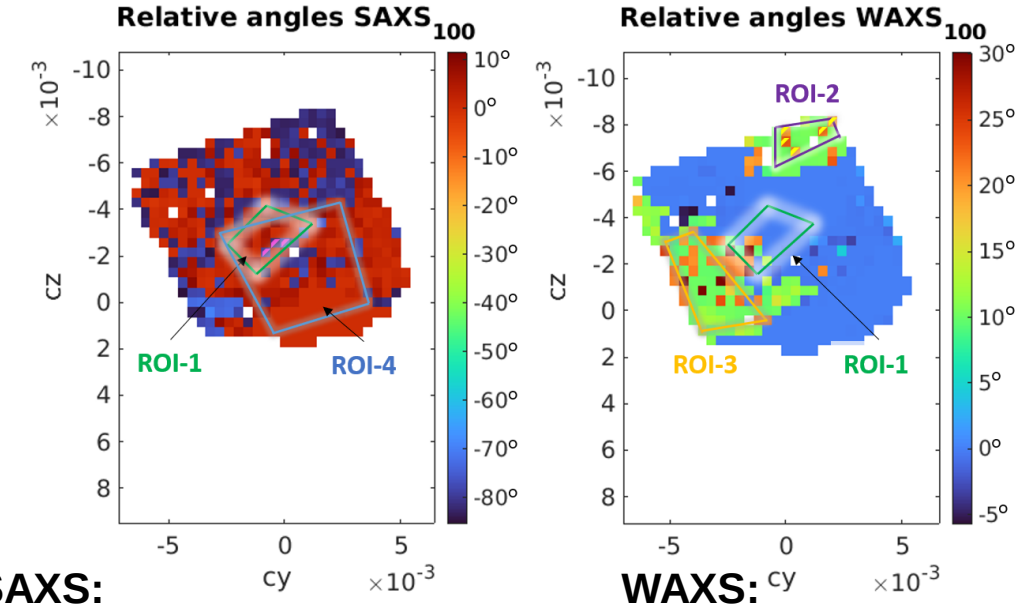


WAXS:
ROI-1* (39 pts):
$27.25(2.11)°$
ROI-2 (228 pts):
$24.01(5.62)°$

3-2 Green crystal on top of green crystal – angle of 10°

Bragg peak analysis using 2D Gaussian fitting





SAXS:

ROI-1 (25 pts): $\mathbf{3.66(2.54)}°$

ROI-4 (132 pts): $\mathbf{-8.74(28.61)}°$

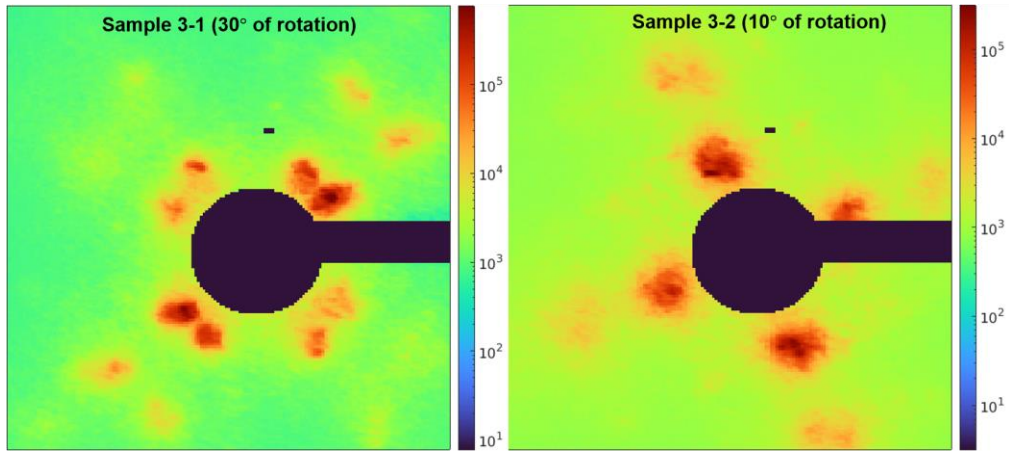
ROI-4* (90 pts): $\mathbf{3.25(2.54)}°$

WAXS:

ROI-1 (28 pts) : $\mathbf{4.81(9.40)}°$

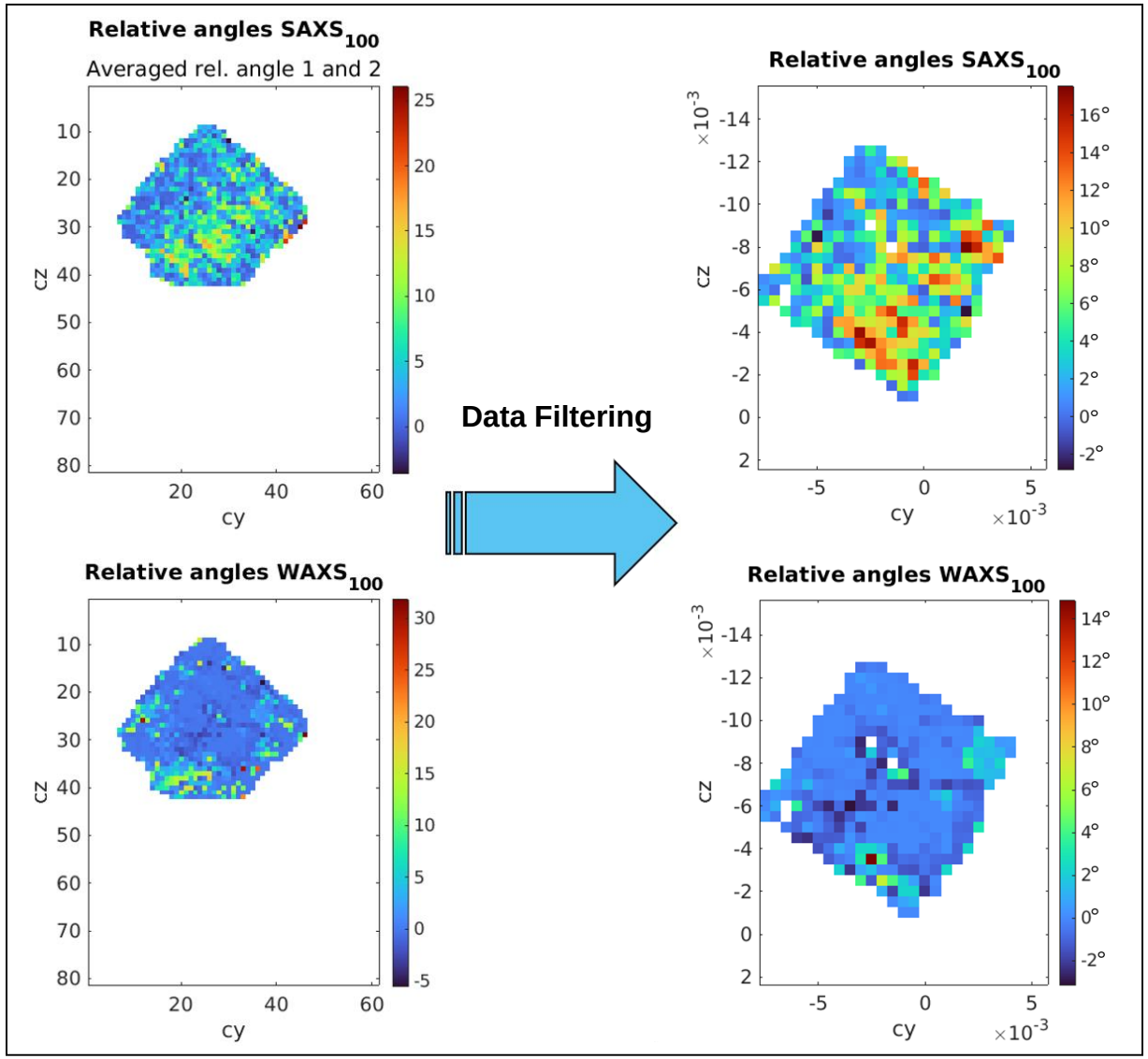
ROI-2* (17 pts): $\mathbf{10.42(0.20)}°$

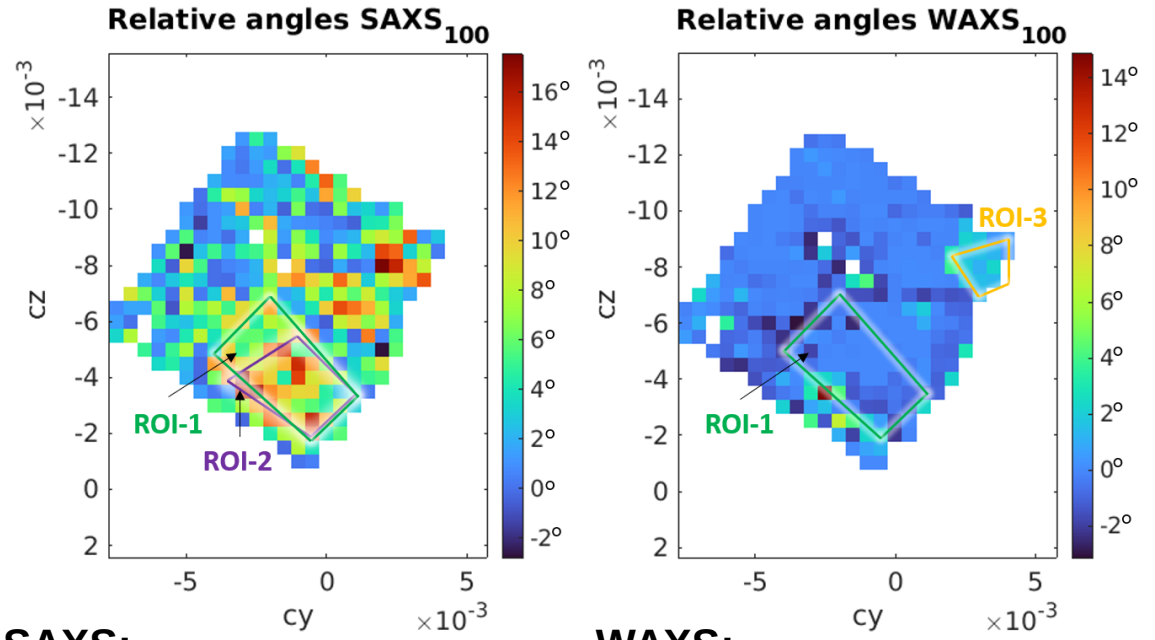
ROI-3 (54 pts): $\mathbf{13.90(6.34)}°$



3-3 Green crystal on top of blue crystal – angle of 10°

Bragg peak analysis using 2D Gaussian fitting





SAXS:

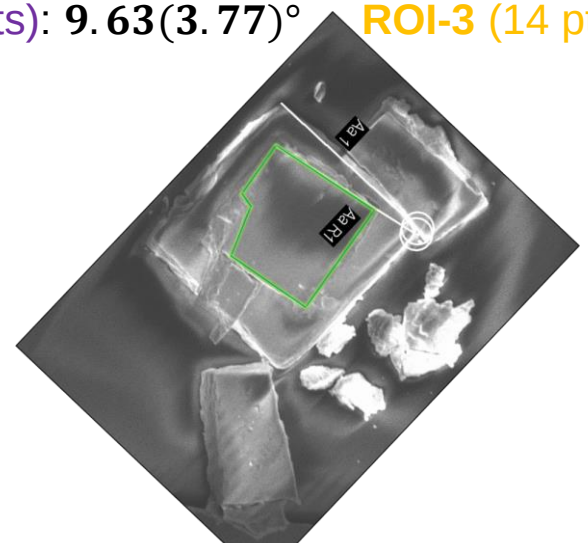
ROI-1 (48 pts): $\mathbf{8.60(3.29)}°$

ROI-2 (36 pts): $\mathbf{9.63(3.77)}°$

WAXS:

ROI-1 (48 pts): $\mathbf{-0.21(1.18)}°$

ROI-3 (14 pts): $\mathbf{2.19(1.99)}°$



Conclusions and outlook

1. **Samples of single crystals were analyzed:**
    - Sample 3-4 (single undamaged green crystal) shows high degree of structural homogeneity, which cannot be said about sample 4-4 (single undamaged blue crystal)
        - Bragg peak analysis technique for blue crystals should be reviewed as clearly something has changed.
        - Resolution still is a problem – the variability in orientation of (100) SL in 3-4 crystal is ~6 degrees coming from inside the crystal to its edges. This may cause problem in analysis of stacks of SCs.

What is left to do?

1. Look for possible analysis improvements
2. Check of correctness of my analysis (I am still just an undergradute)
3. Analyze and compare the rest of the samples s(different angles, possible halide migration, surface defects…)

2. **Samples of stacked crystals were analyzed:**
    - Sample 3-1 gave promising results for distinguishing between top and bottom crystals despite the resolution problem mentioned above - due to the angle of rotation being ~30 degrees
    - Samples 3-2 and 3-3 did not show a good distinction between top and bottom crystal – due to angle of ~10 degrees being to close to resolution problem mentioned above. Also code for Bragg peak analysis has its own resolution limitations (fitting had to be performed for values with certain upper and lower boundaries).
        - New approach for Bragg peak analysis is needed, tough the biggest problem is still the resolution.
3. **Code has been checked:**
    - Unfortunately parts of code that take the longest time to compute are built-in MatLAB functions – we cannot change them.

Acknowledgements

- **FS-PS Fachgruppe CXI** (Ivan Vartaniants, Kuan Hoon Ngoi, Bihan Wang, Gerard Hinsley, Shweta Singh), for letting me work with them and for all their insightful thoughts and ideas
- **Ivan Zaluzhnyy,** for providing MatLAB scripts used in the analysis
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Thank you

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