THE UNIVERSITY of TENNESSEE KNOXVILLE

Quantification of TEM/STEM Data

Lecture 5 : Machine Learning in STEM

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Machine Learning in STEM
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Why Quantification?

- Comparison with Theory
- Comparison of Different Methods
- Comparison of Different Materials
- Comparison of Different Instruments
- Comparison of Different Days
- Comparison of Different Parts of Datasets

- Additional Information

GOOD TRAINING DATASETS and WIDE APPLICABILITY

What is the problem?

Problem

- Electrons interact strongly with matter

Advantage

- Electrons interact strongly with matter

Opportunity for Machine Learning

- Electrons interact strongly with matter

How Precise Can EELS and Imaging in TEM/STEM Be?

- How well can we determine absolute atom positions and strain
  - Relative positions are well determined
  - Strain is a tensor

- How well can we quantify electron energy-loss data
  - Composition
  - Bonding
  - Optical Response

Images – Z-contrast Images

Artefacts

- Sample drift
- Noise
  - Uncertainty in atom position
- Scan distortions
  - Uncertainty in absolute position determination
  - Prevents strain determination

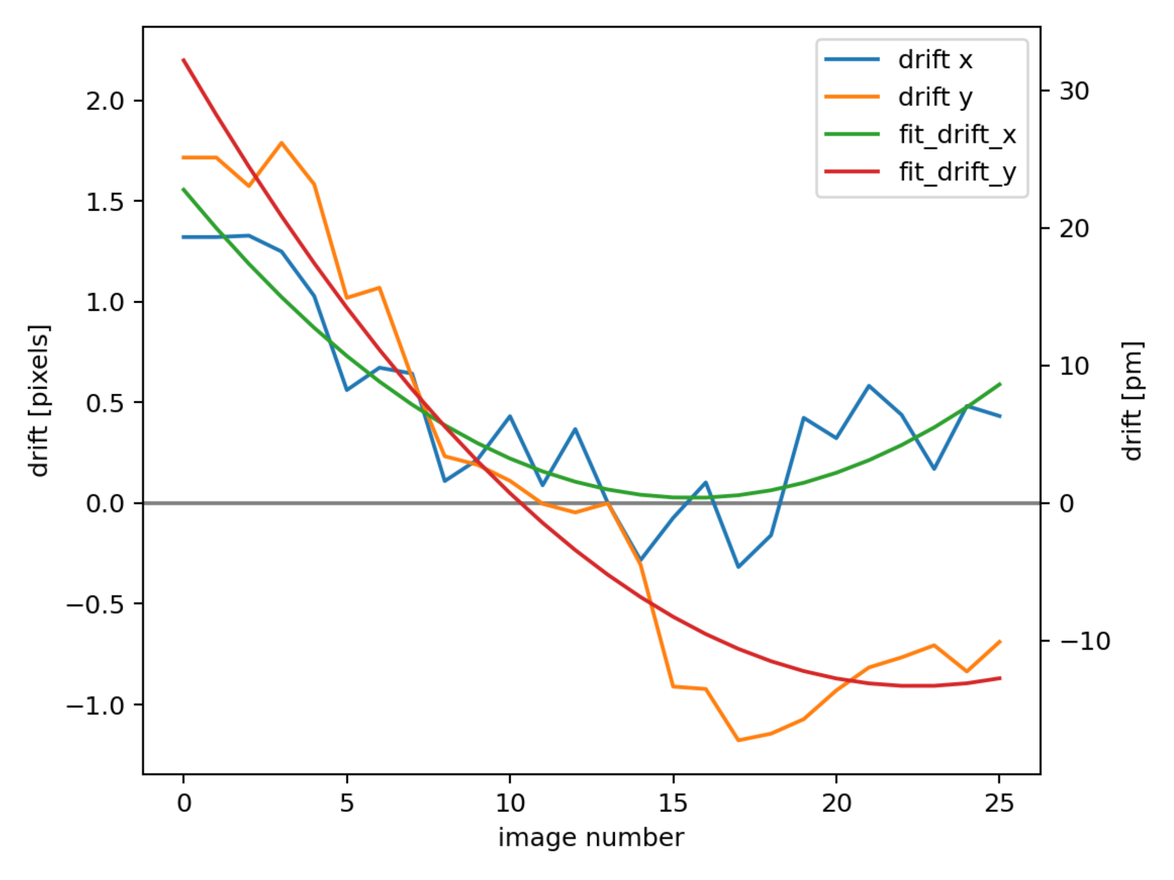
Data Analysis

- All data analysis is done with jupyter notebooks
- Data are represented as **sidpy datasets**
- Data and results are stored in **pynsid format**

- Most routines are made publicly available through **pycroscopy at github page**

- **Notebooks will explain the basics.**

Sub-Pixel Accuracy in Drift Correction



Removal of all the random drift from dataset is essential.
rigid registration

If drift from frame to frame is small no additional correction is necessary.

We need:

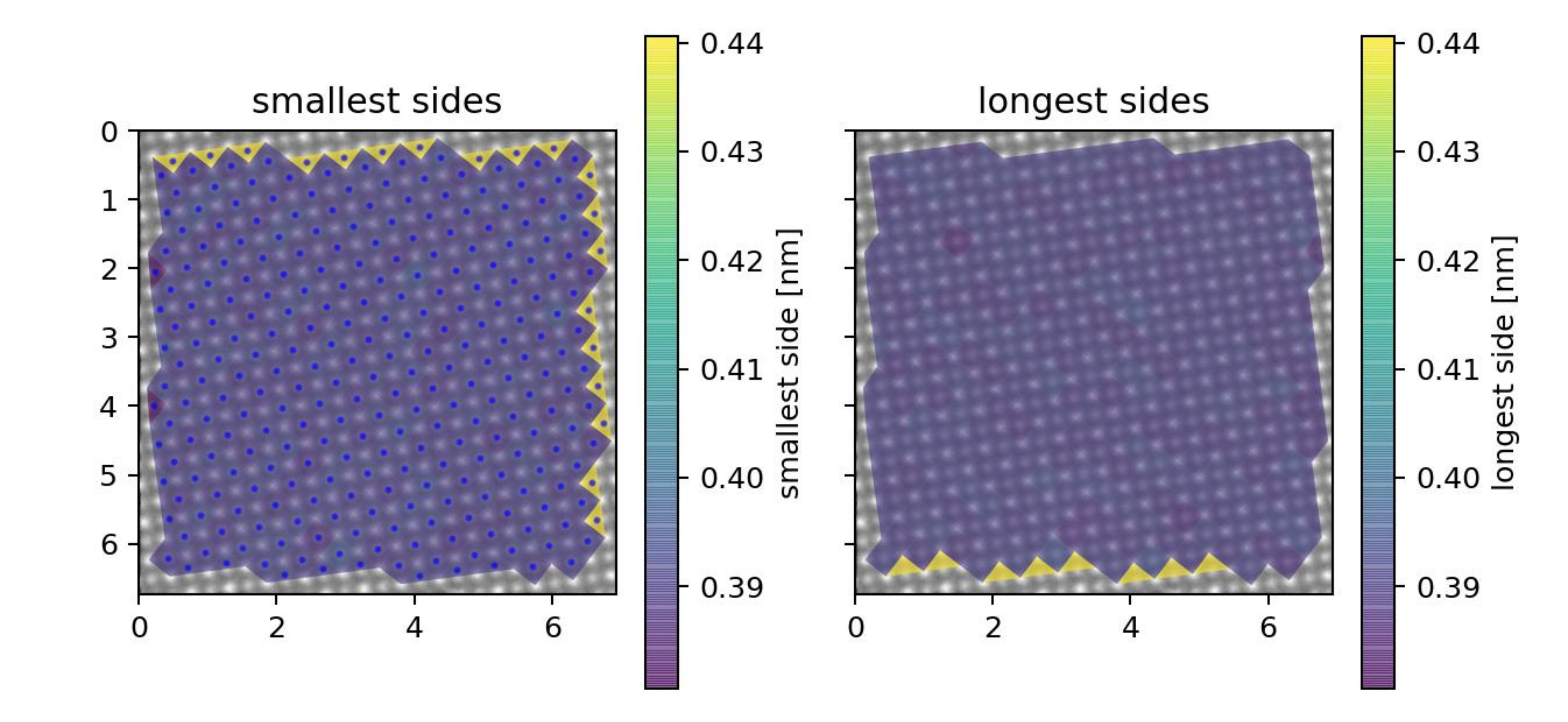
stacks of images with low sample drift.

Question: Is the jitter true or should we use smooth fit?

standard deviation of jitter in x direction: 2.98 pm
standard deviation of jitter in y direction: 3.62 pm

Median of smalles side: 0.3894 nm with standard deviation: 2.4 pm

Tetragonal Distortion



After:

distortion correction
(same dataset)
rigid registration
non-rigid registration
atom finding
atom position refinement
unit cell finding

Evaluation of Squares Only
(not of triangles at rim)

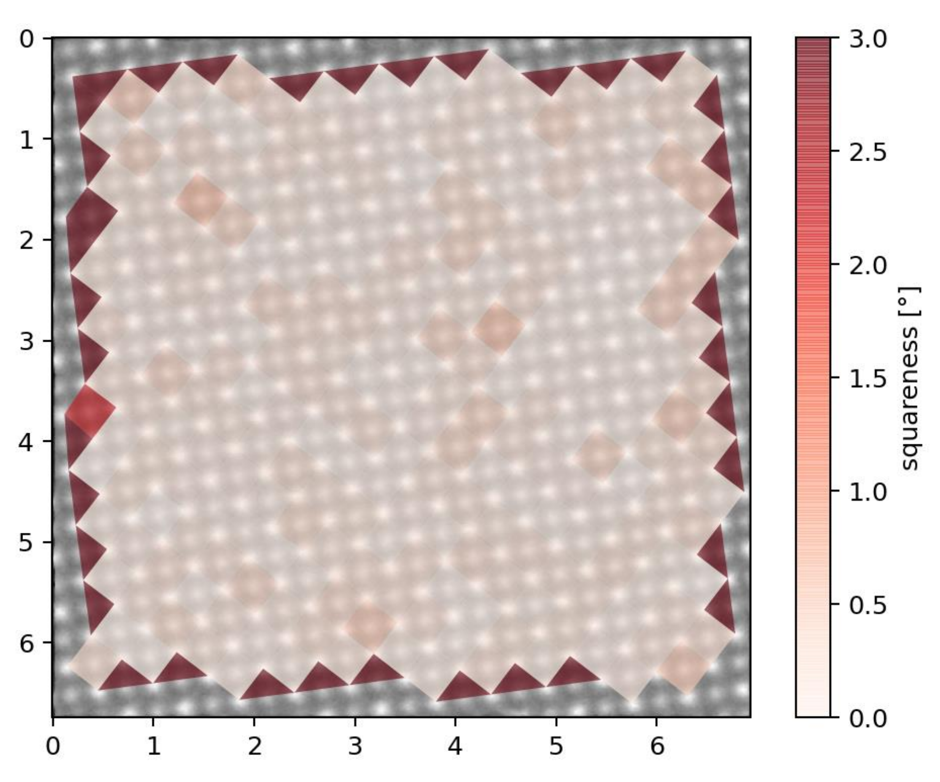
Median of smallest side: 0.3894 nm
with standard deviation: 2.4 pm

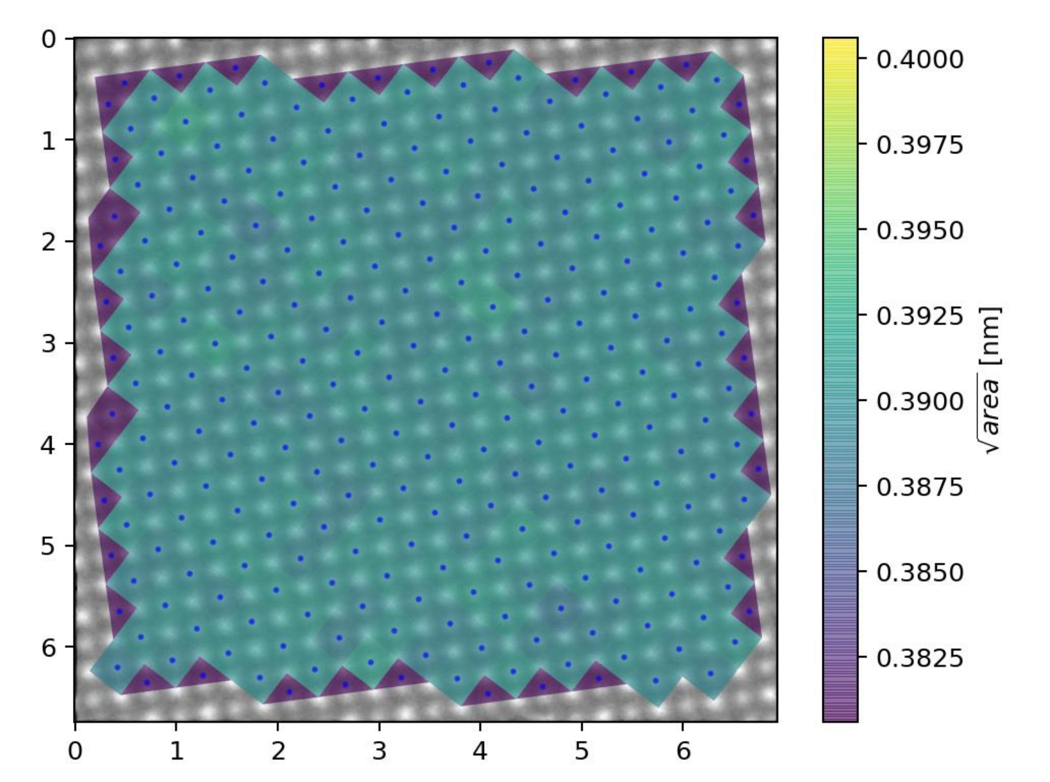
Median of longest side: 0.3915 nm
with standard deviation: 0.8 pm

pixel size is 14.6 pm

Unit Cell Scale

Evaluation of Squares Only
(not of triangles at rim)
pixel size is 14.6 pm

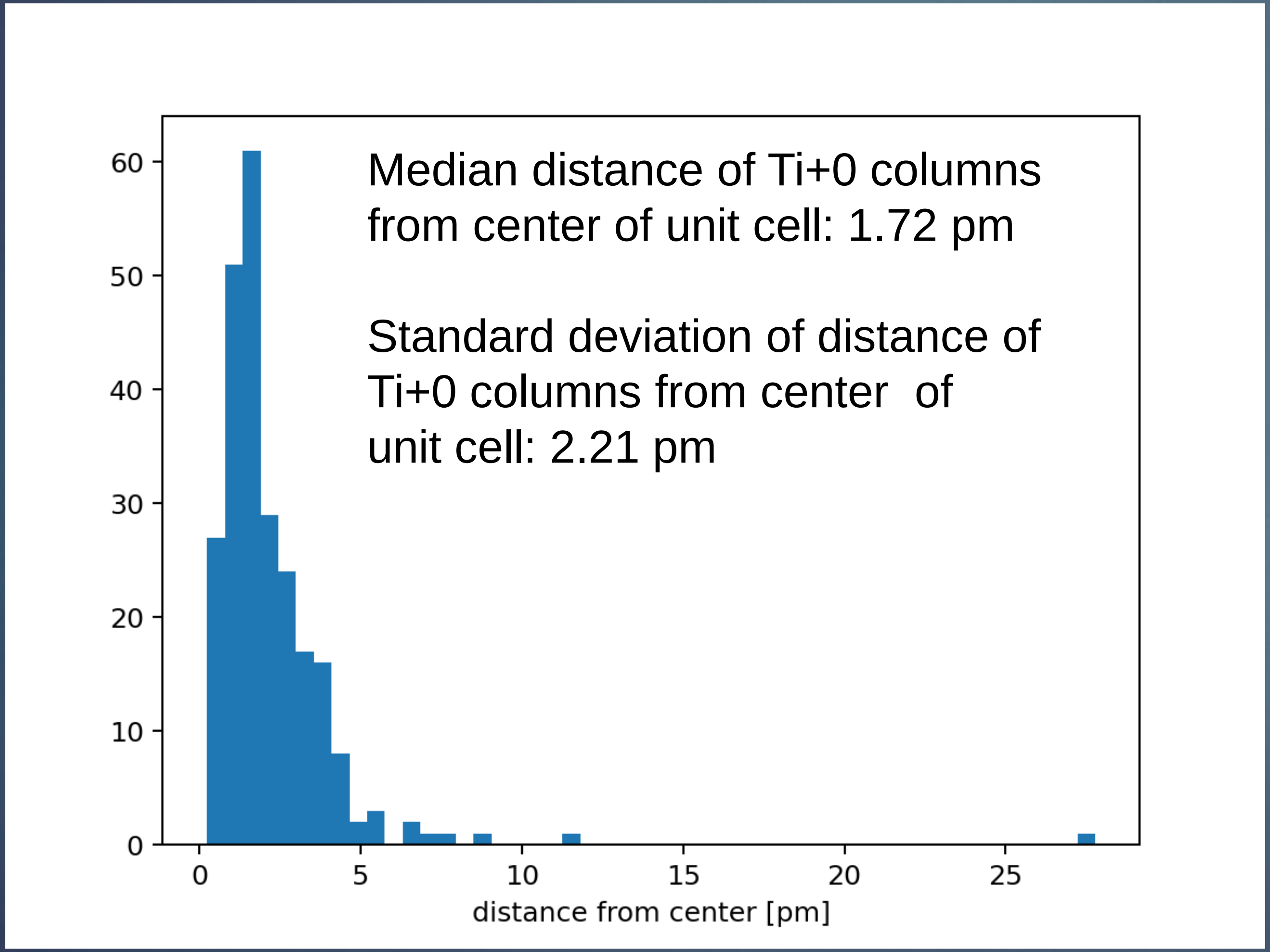




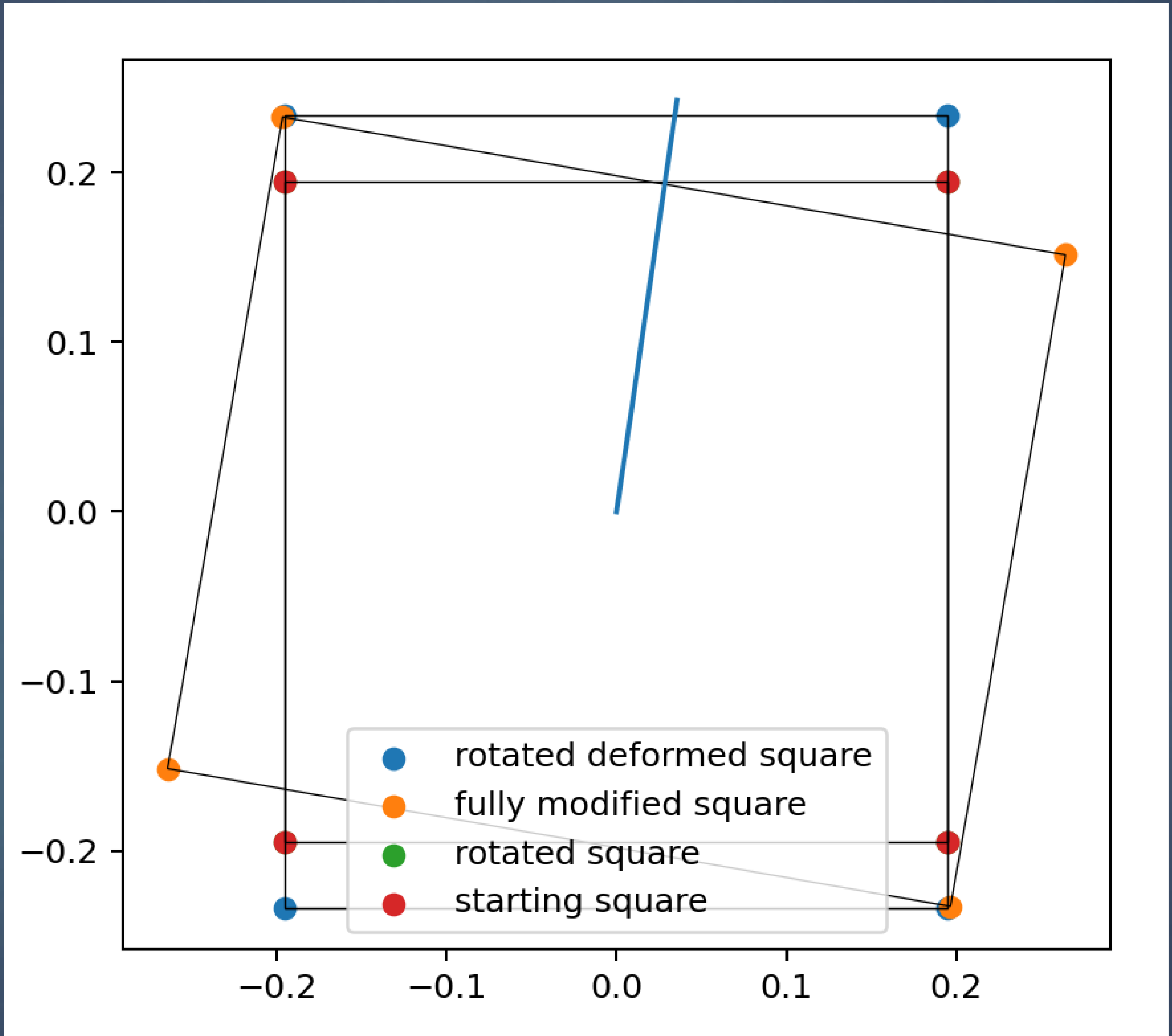
Evaluation of squares only
Median angle deviation from square: 0.24 deg
with standard deviation: 0.25 deg

Median area: 0.1525 nm^2
which is 0.3905 nm squared
with standard deviation: 0.0009 nm^2
which is 1.0 pm squared

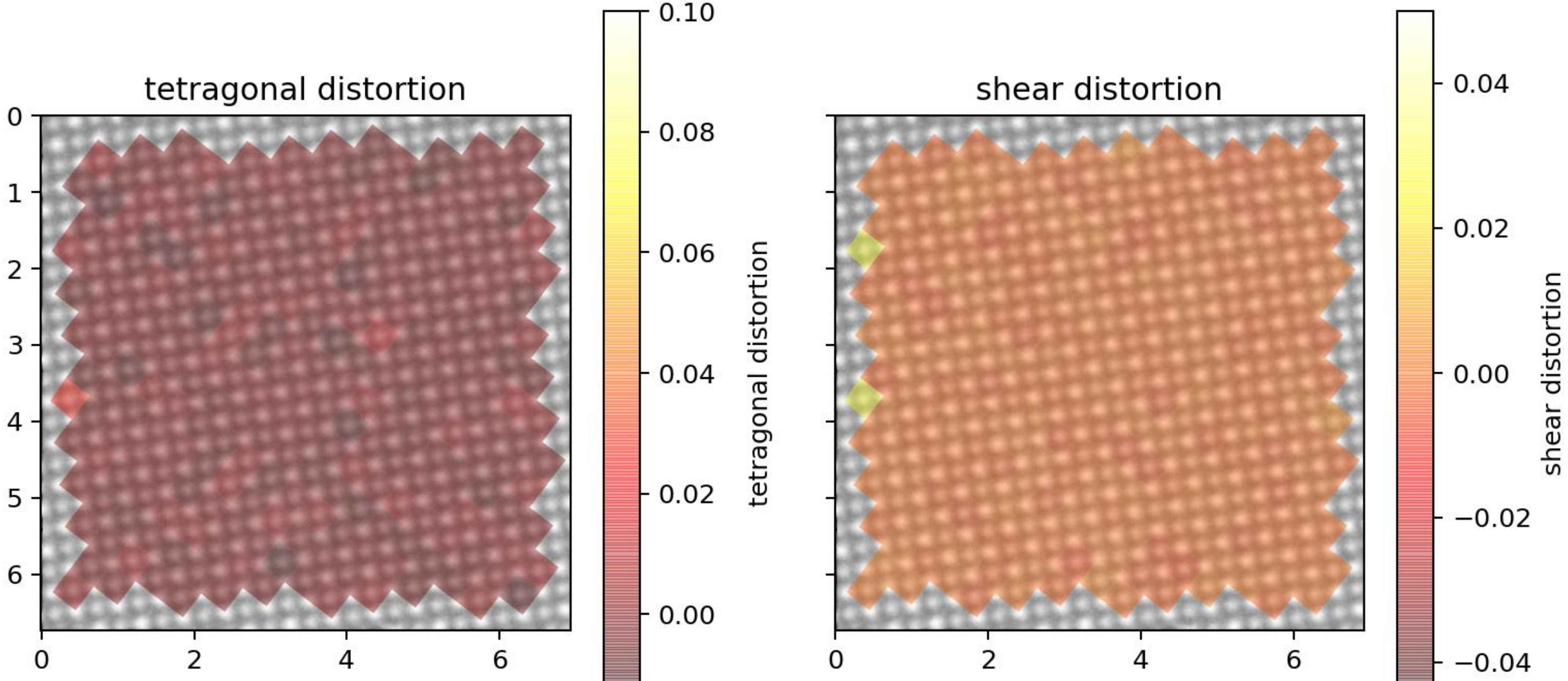
Distance of Ti-O columns from center



Strain


0.2
0.1
0.0
−0.1
−0.2
−0.2
−0.1
0.0
0.1
0.2
rotated deformed square
fully modified square
rotated square
starting square

Strain in Image



median tetragonal distortion -0.00008 with std. deviation 0.0035

median shear distortion 0.00028 with std. deviation 0.0029

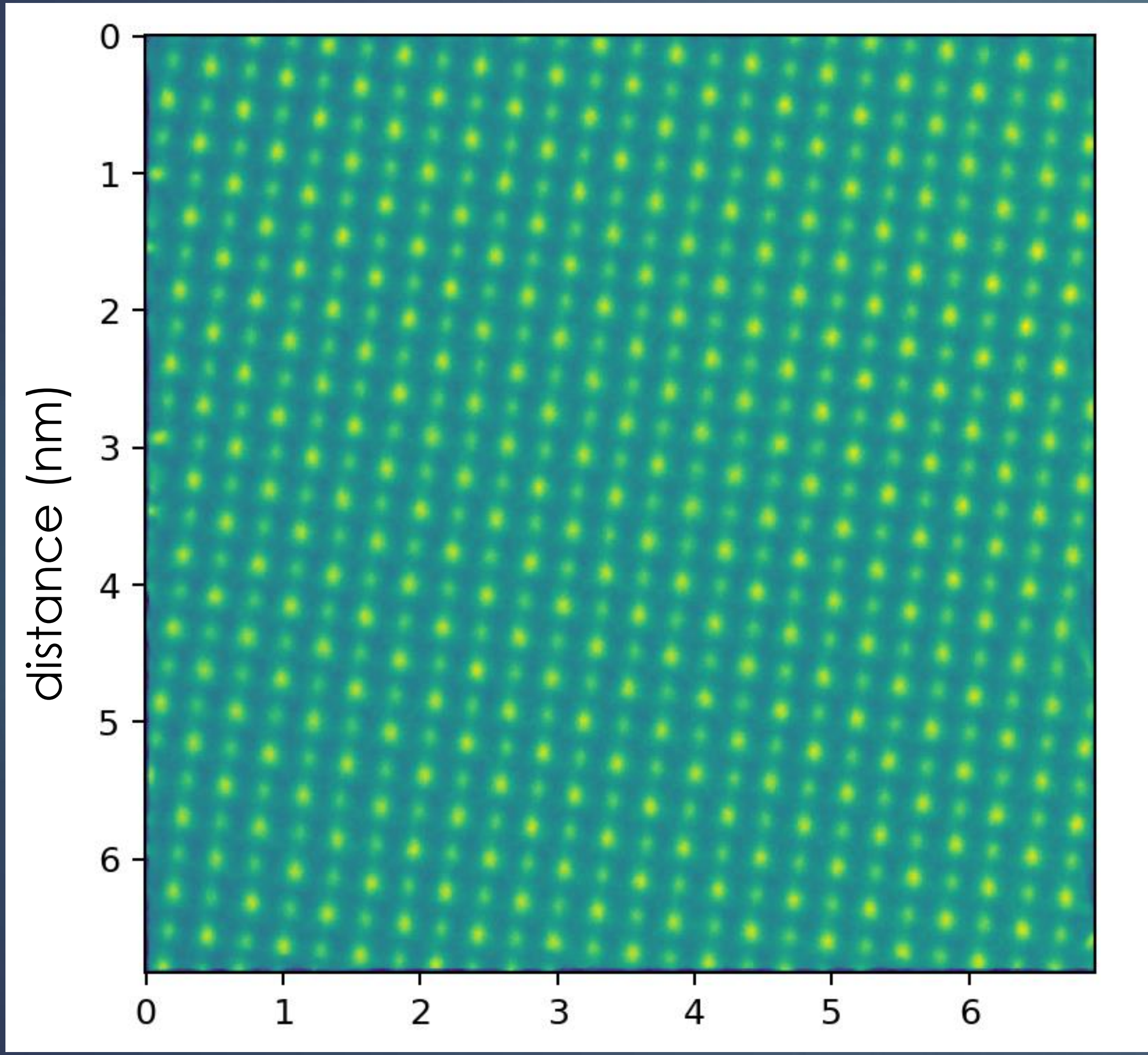
Up to now

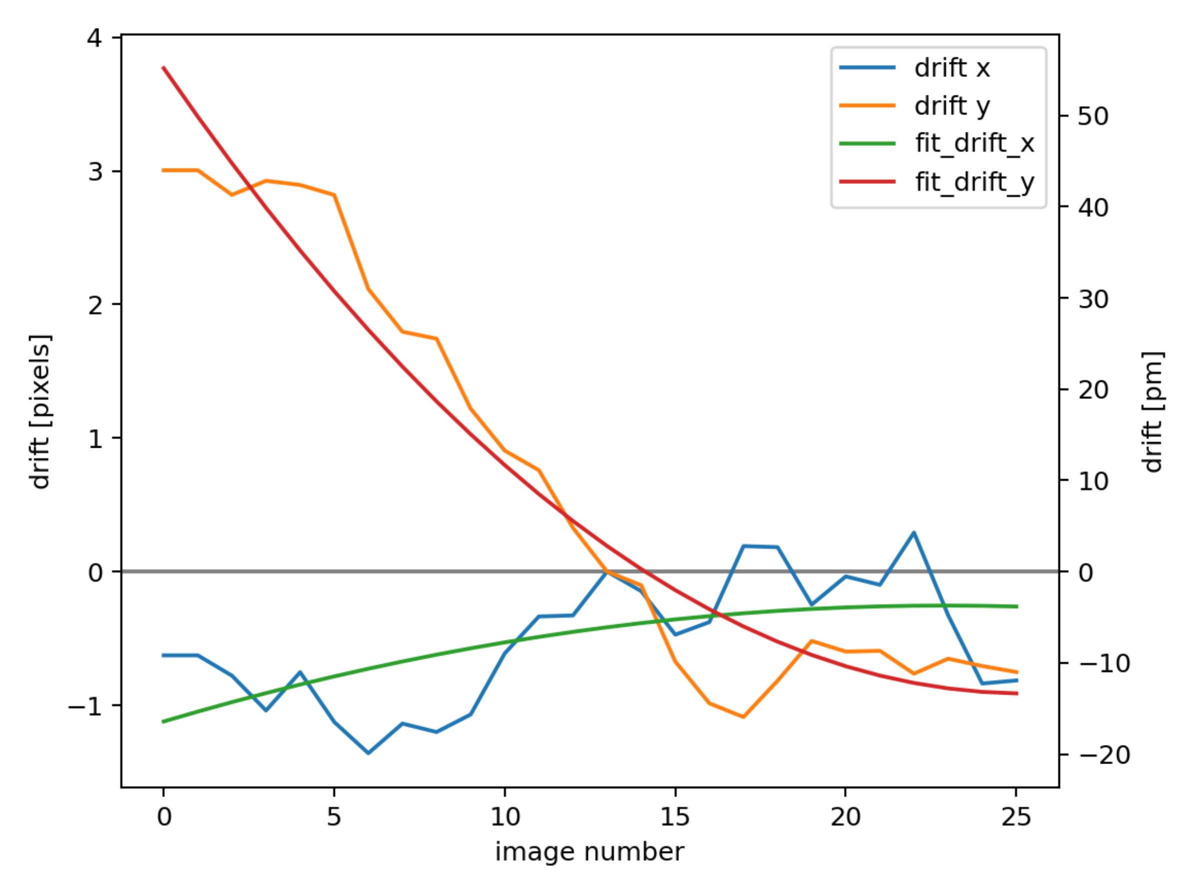
- Determination of minimal error
- Reached precision of relative positions almost to the level of Voyles group with similar method.

Next

- Determine distortion matrix from reference dataset to correct another dataset.
  - Ideally, same sample
  - same rotation
  - same magnification
  - collection of both datasets within a short time frame

Another Dataset



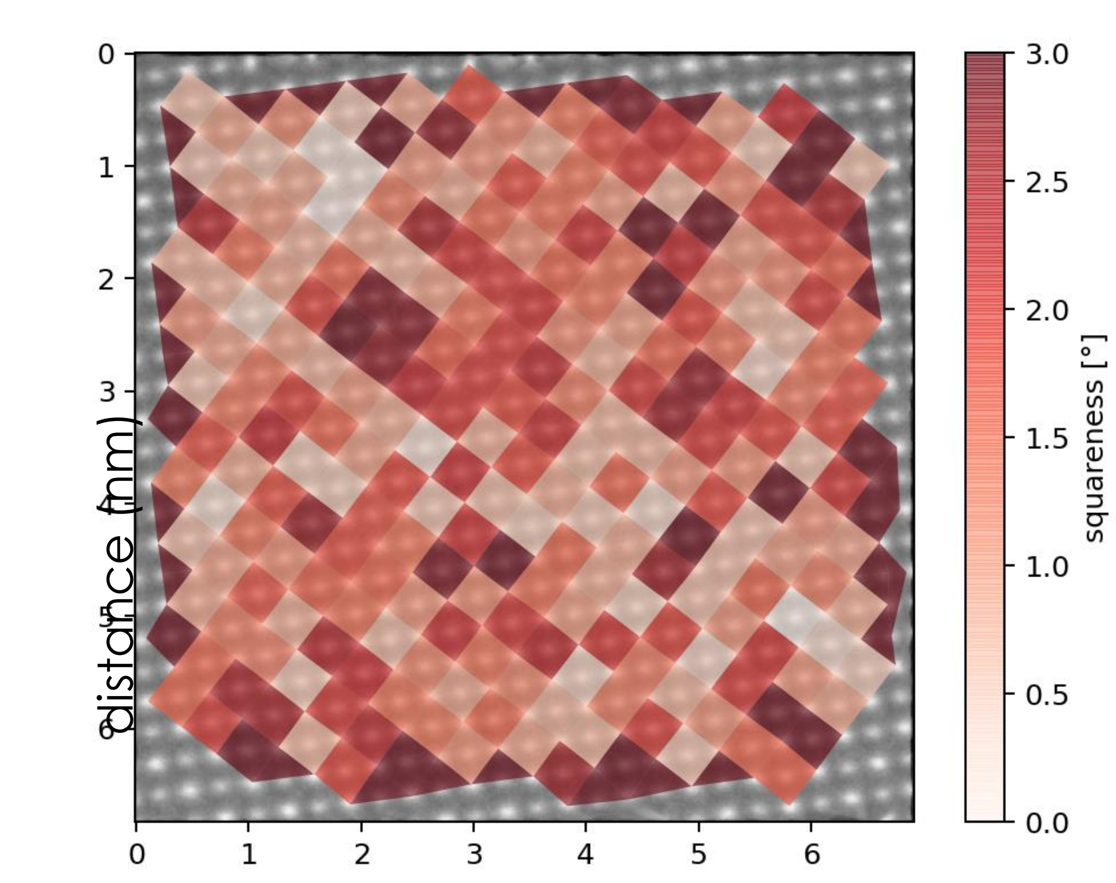


standard deviation of jitter in x direction: 5.45 pm
standard deviation of jitter in y direction: 5.46 pm

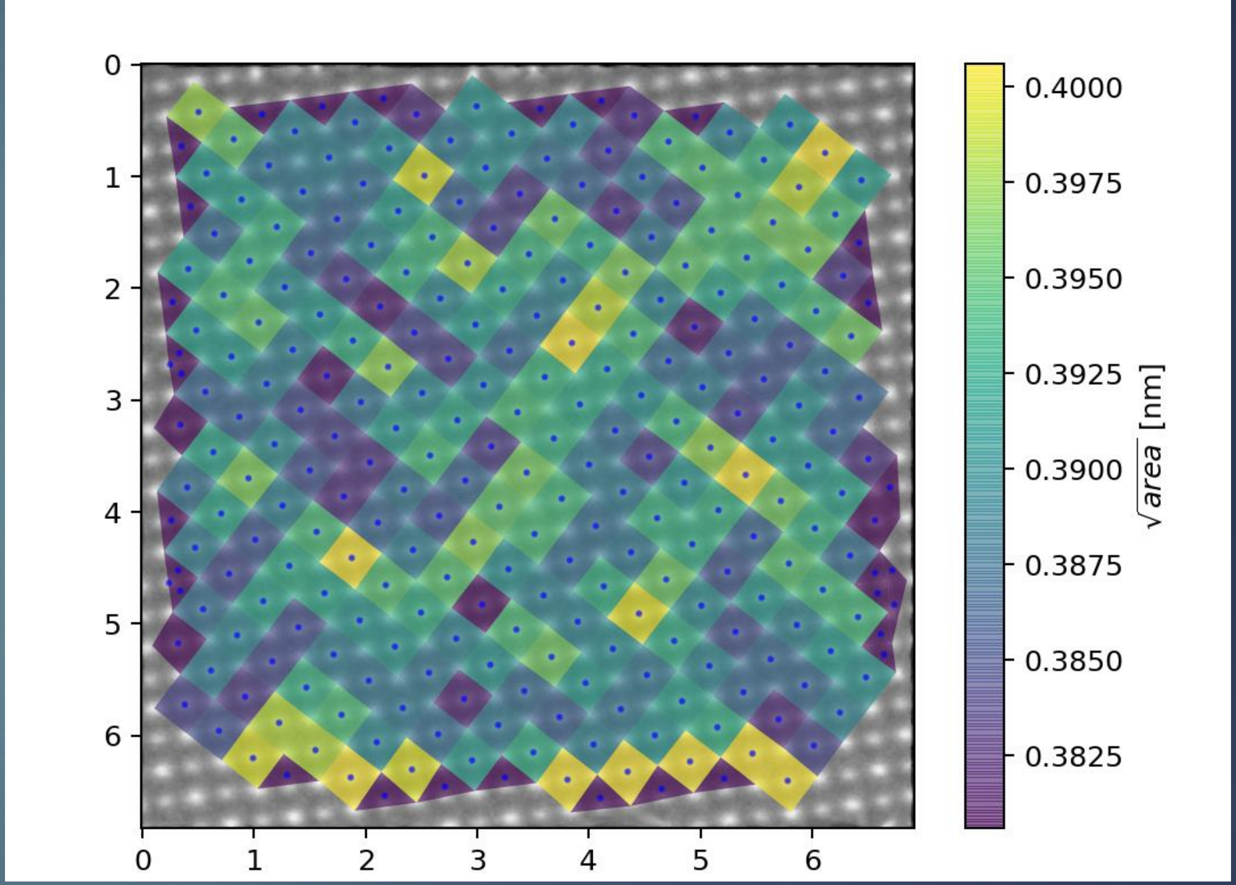
Median area: 0.1523 nm² which is 0.3903 nm squared with standard deviation: 0.0076 nm² which is 2.8 pm squared pixel size is 14.6 pm

Unit Cell

pixel size is 14.6 pm



median angle deviation from square: 1.45 deg
with standard deviation: 4.09 deg



median area: 0.1523 nm²
which is 0.3903 nm squared
with standard deviation: 0.0076 nm²
which is 2.8 pm squared

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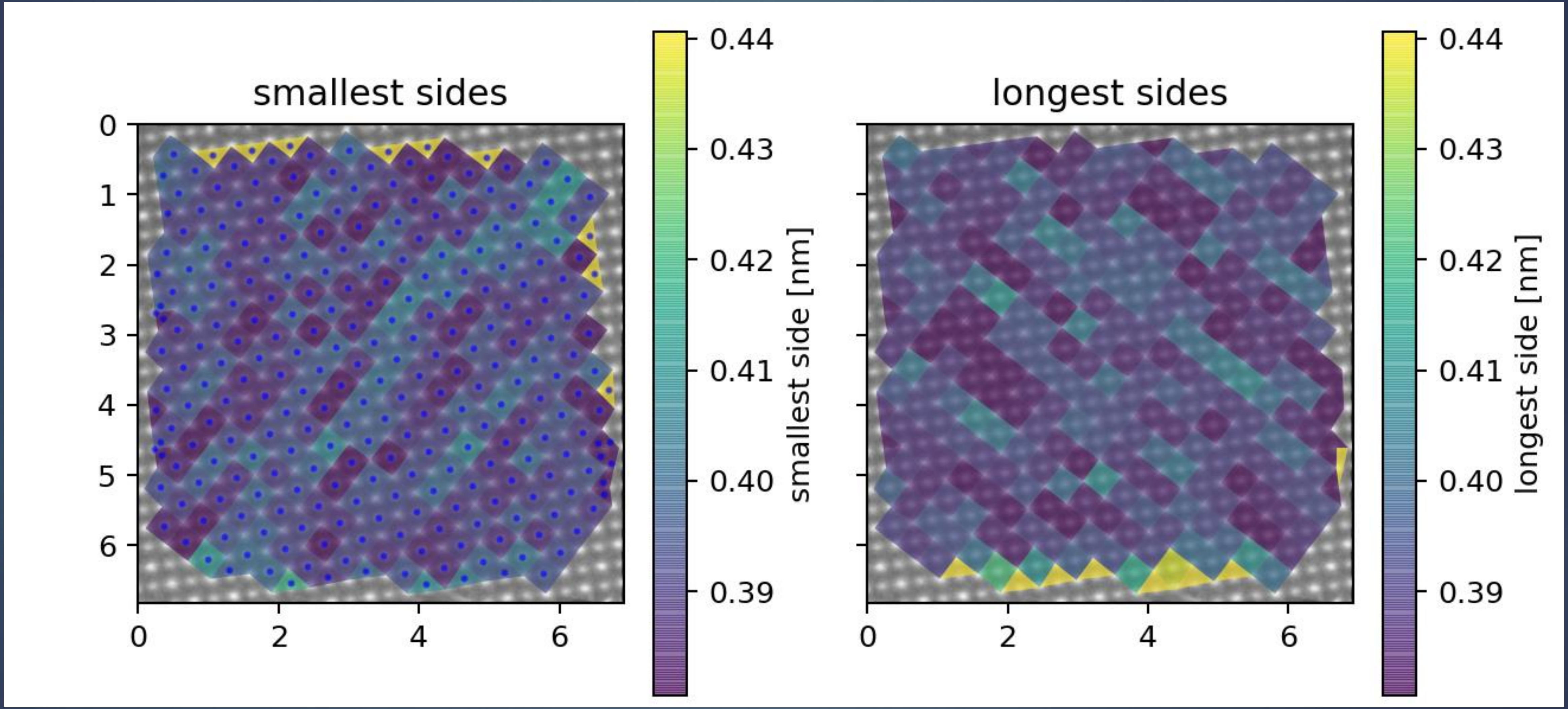
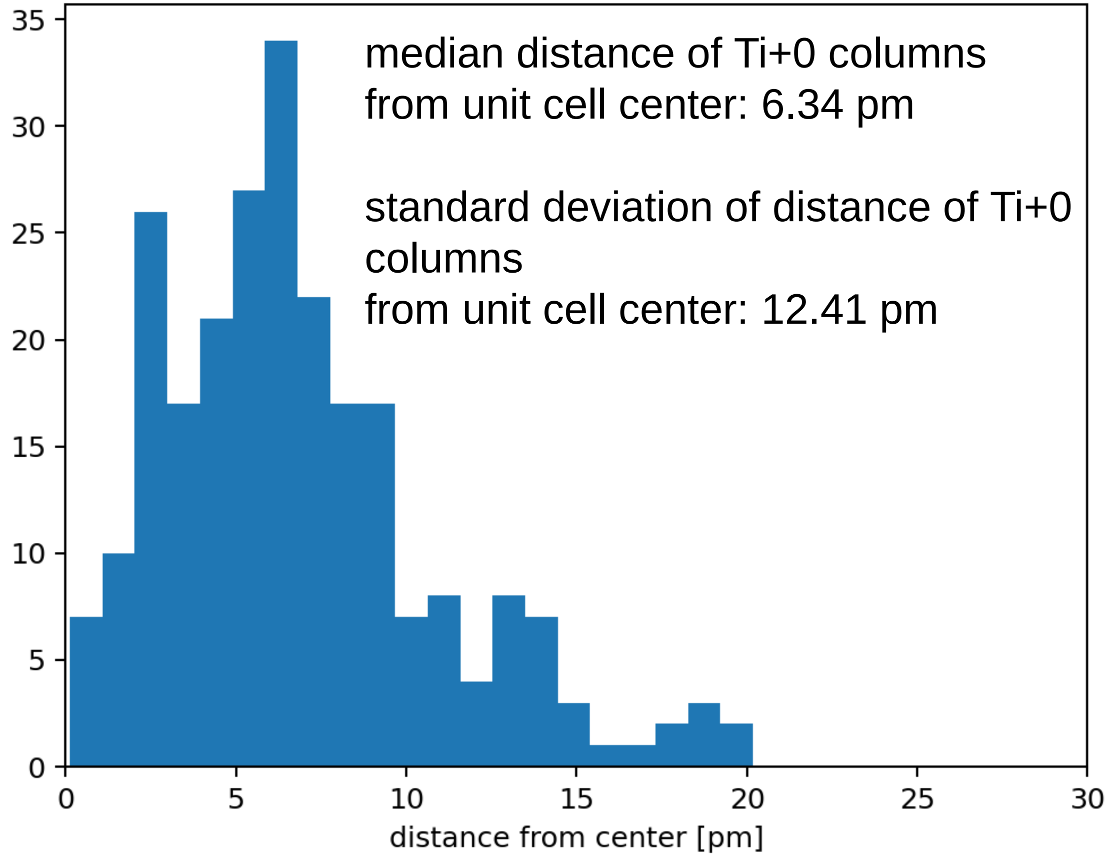
Sides

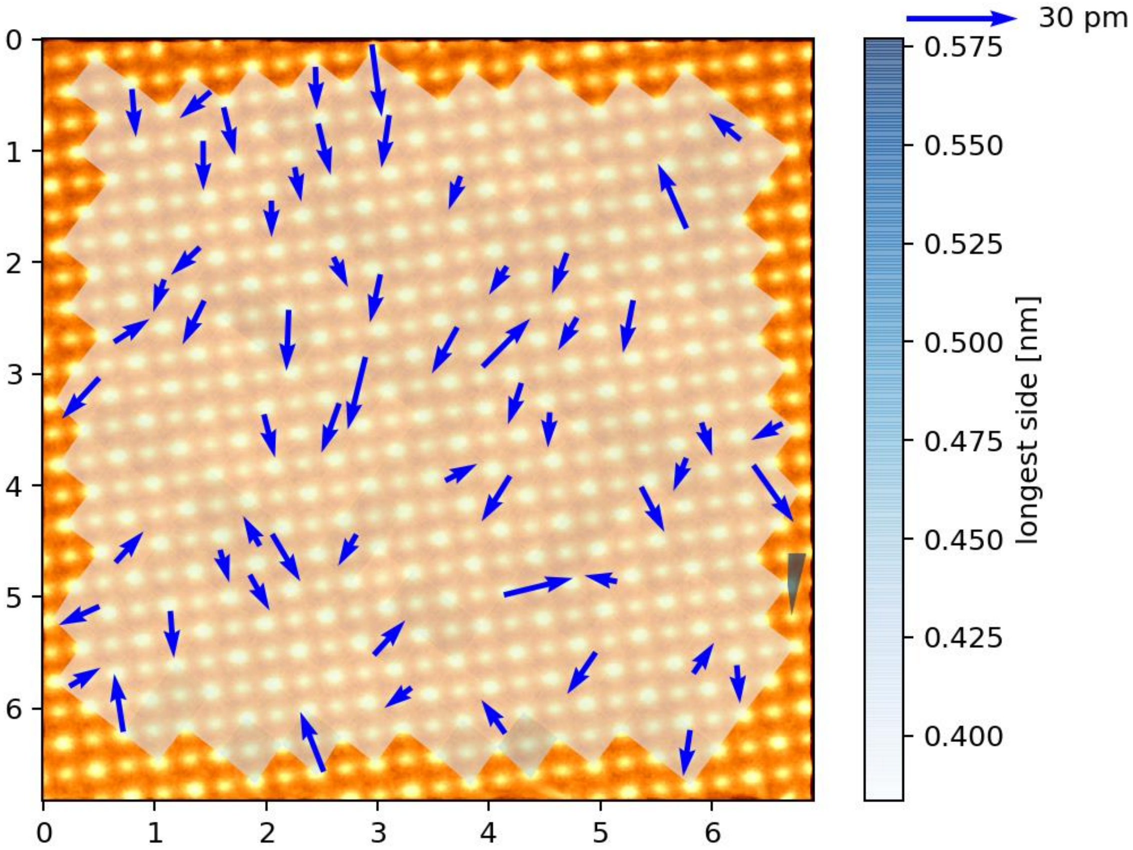


Median of smalles side: 0.3843 nm
with standard deviation: 15.7 pm

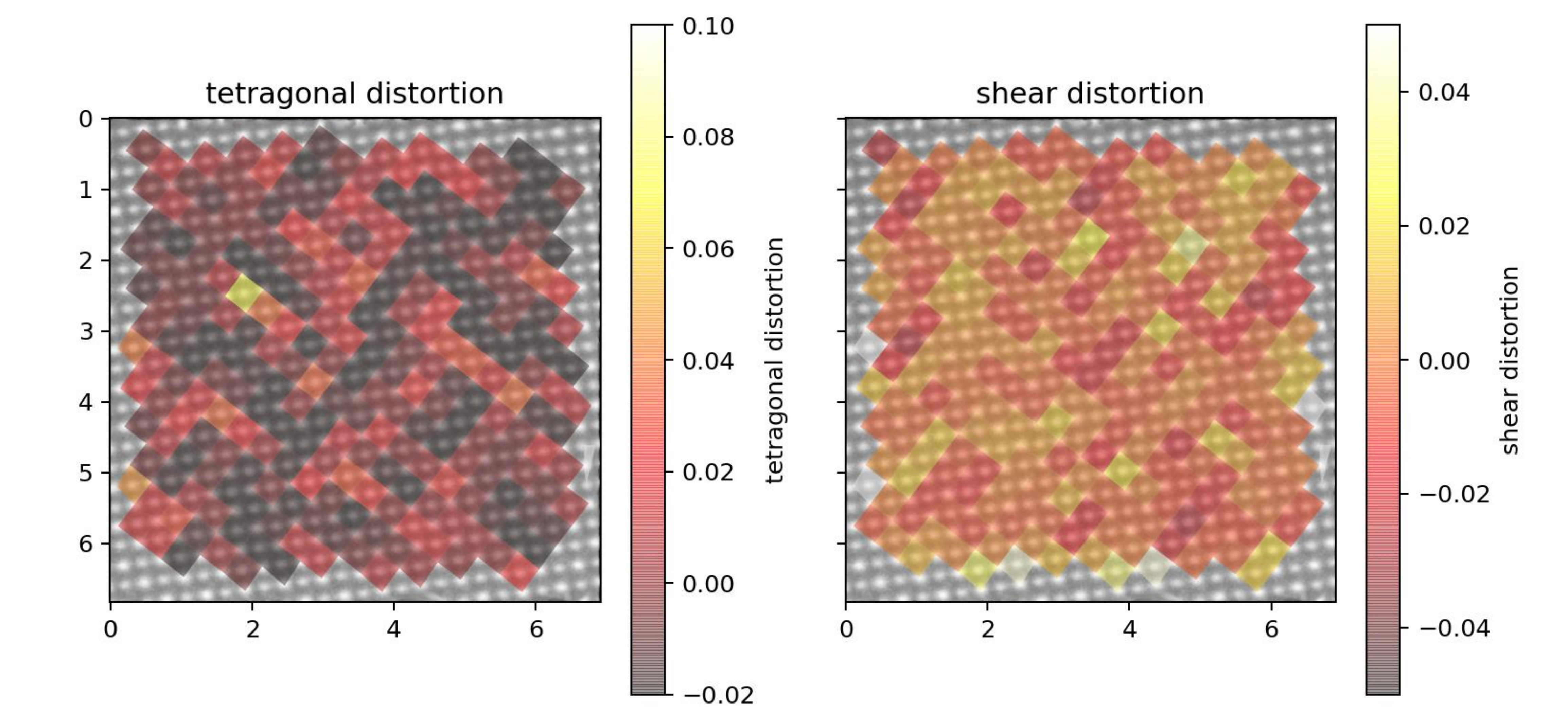
Median of longest side: 0.3967 nm
with standard deviation: 13.4 pm

Distance of Ti-O columns from center



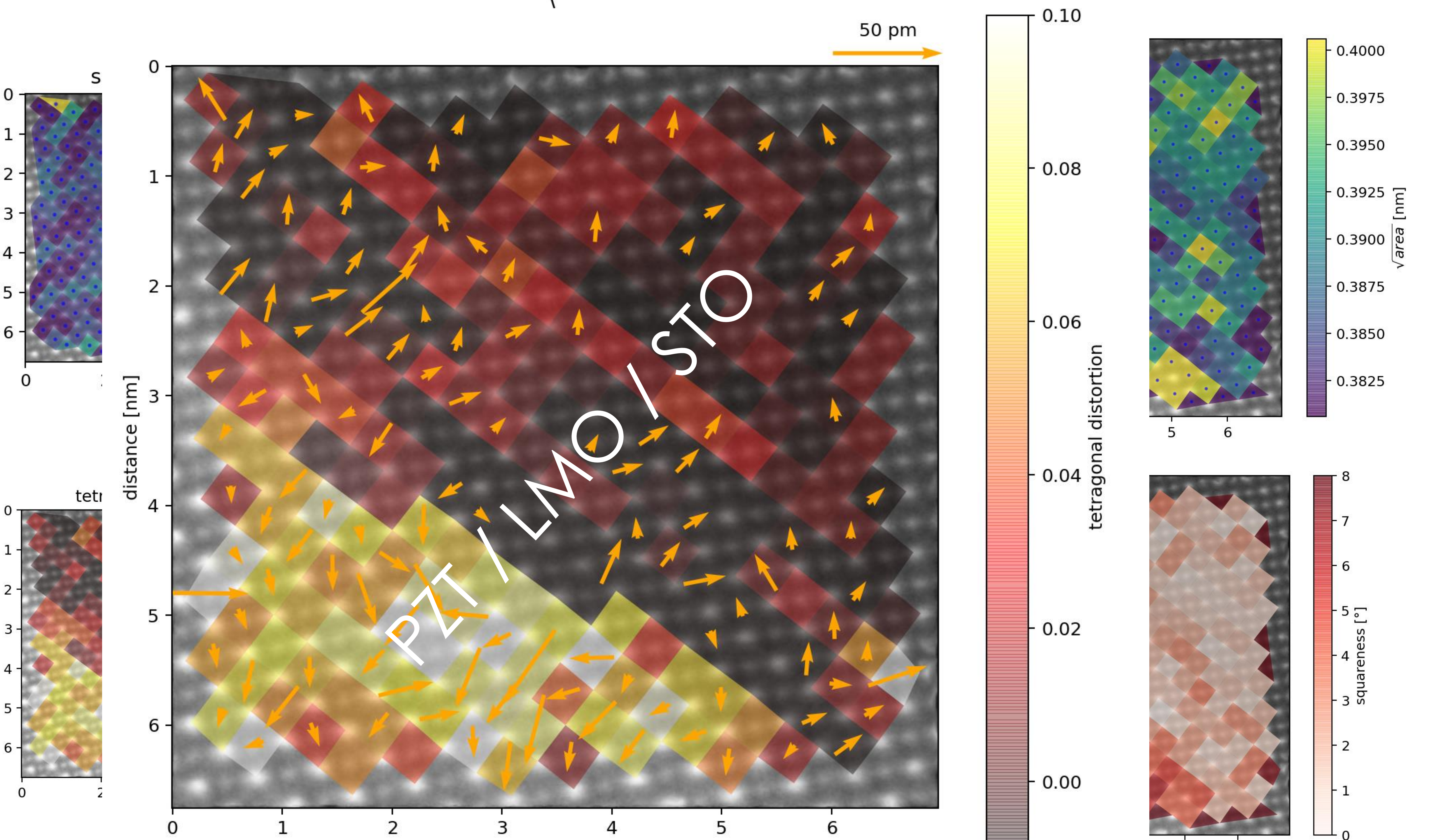


Strain



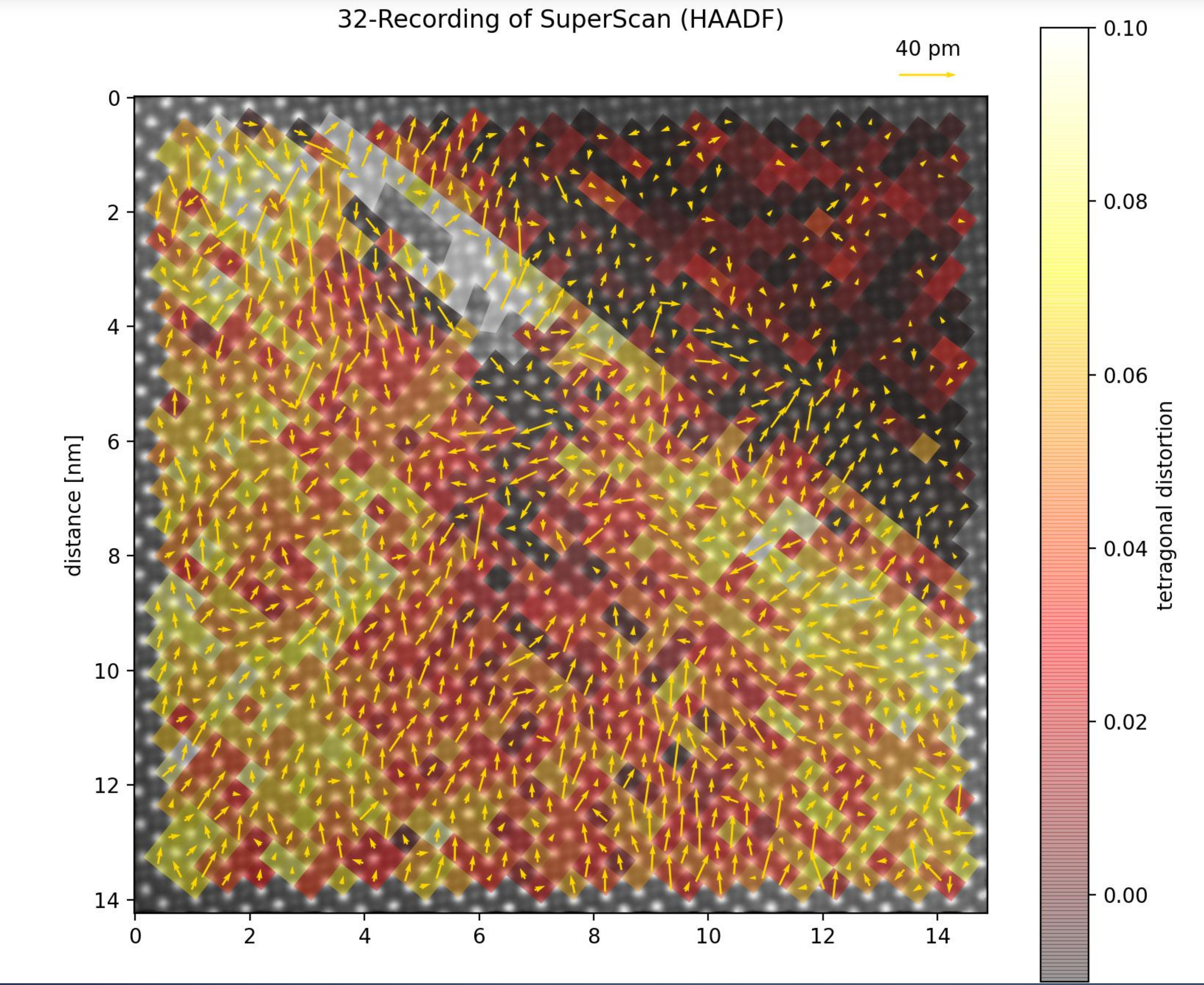
median tetragonal distortion: -0.00300
with std. deviation: 0.0502

median shear distortion: -0.00025
with std. deviation: 0.0208



50 pm
PZT / LMO / STO
distance [nm]
tetragonal distortion
$\sqrt{area}$ [nm]
squareness [°]
tetr
s

STO/LMO/PZT



- Tetragonal distortion in PZT
- Compression in LMO
- Complicated polarization induced by interfacial dislocation

We see, that we need a larger view.

Summary

- We showed how error bars for quantification can be determined
- Variation in scan distortion from dataset to dataset are limiting strain determination to less than a pixel.
- Strain determination benefitted from high brightness of cold field emitter and super stable sample stage in Nion.

Outlook

- Demand good datasets, that can be quantified.

- Include noise in analysis.
- Use artificial intelligence algorithms for quantitative analysis.

- Good datasets for machine learning that are universally usable.
- Use machine learning on datasets from different sources.