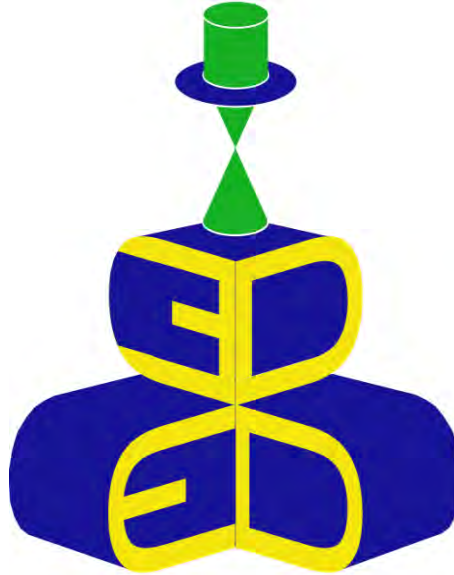
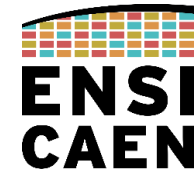




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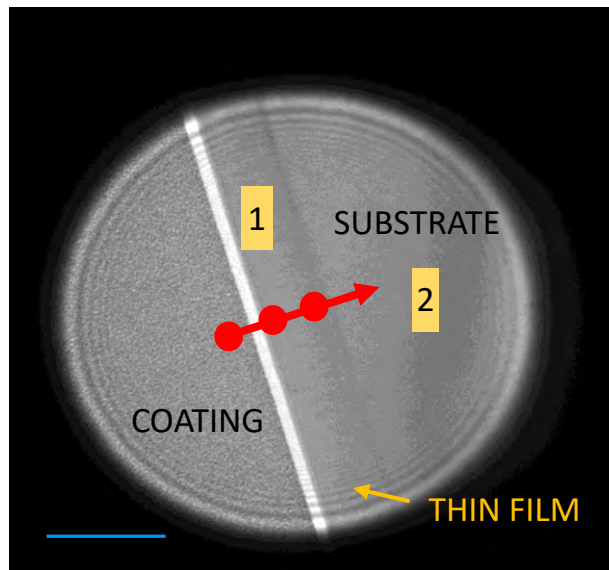


Nan ED



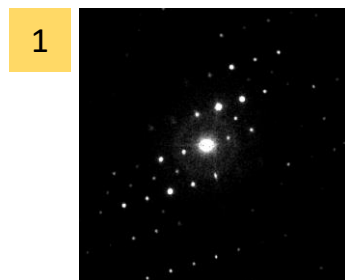
ESR 12 – Sara Passuti

Electron crystallography of nanodomains in functional materials

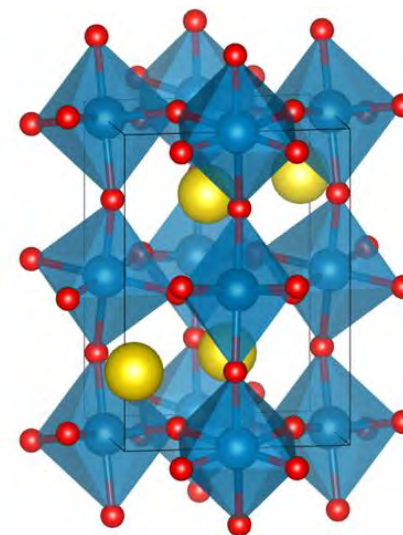
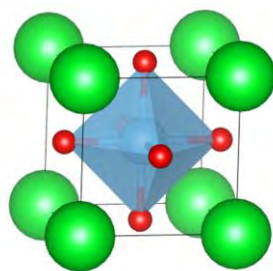
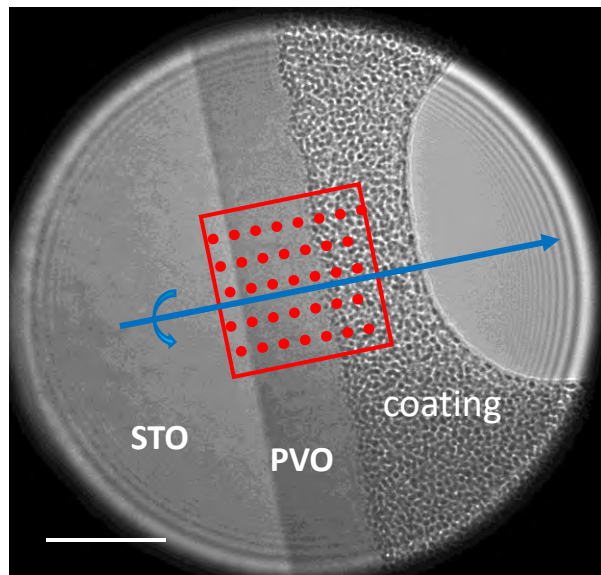


➔ Diffraction pattern sorting

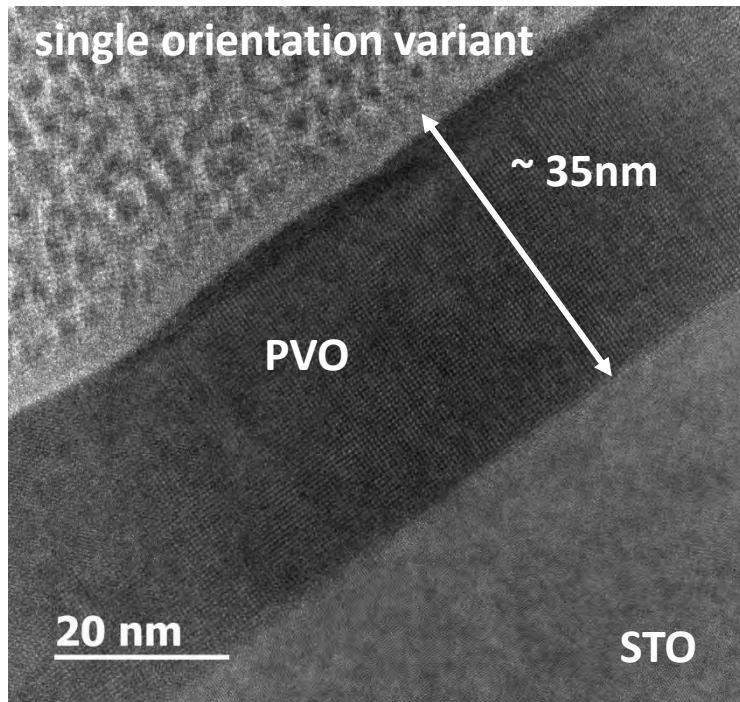
➔ Diffraction dataset reconstruction



➔ Structure solution and refinement

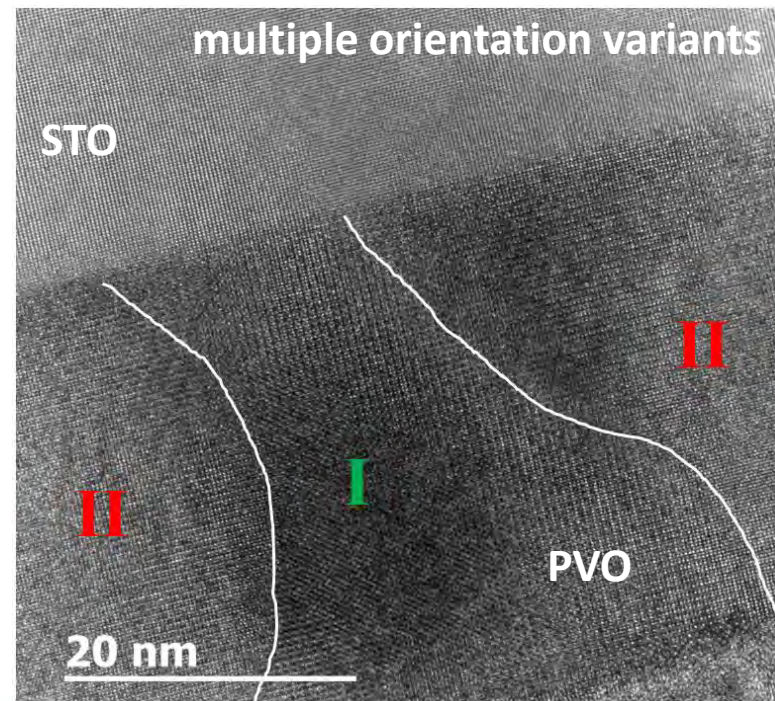


PVO / STO[110]

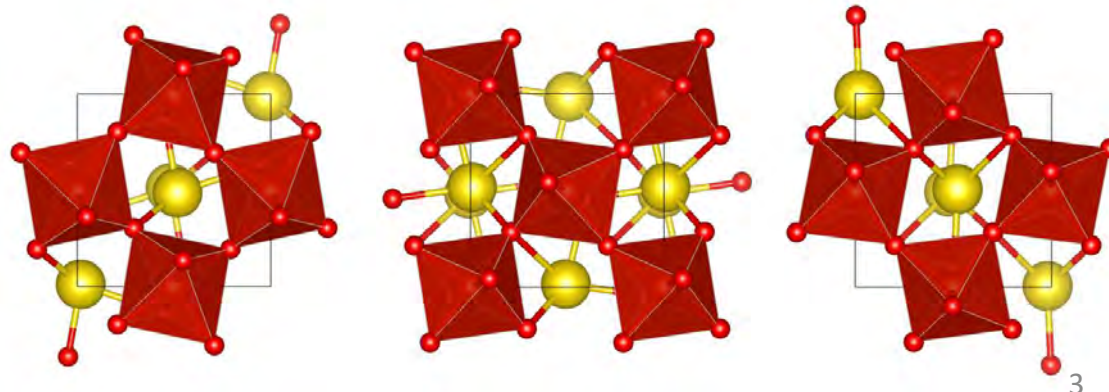
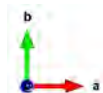


vs.

PVO/STO[111]



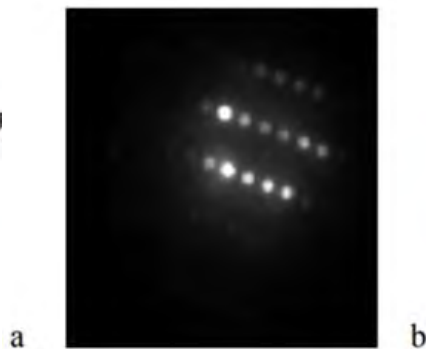
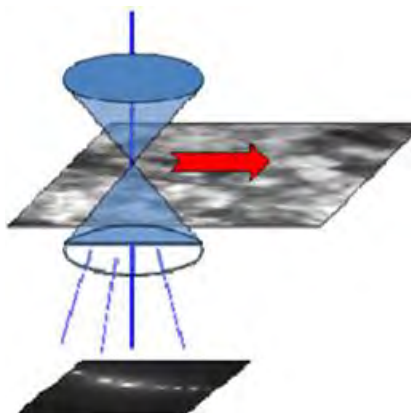
Different tilting systems in the domains



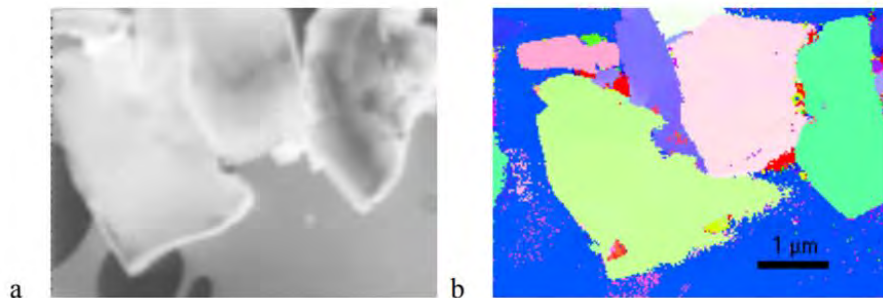
SPEDT - Scanning Precession-assisted Electron Diffraction Tomography

Scan of an area of the sample ► similar to ACOM and 4D STEM

1. identification of domains (via cross-correlation)
2. Integrate diffracted intensity for a given domain and use it for structure refinement

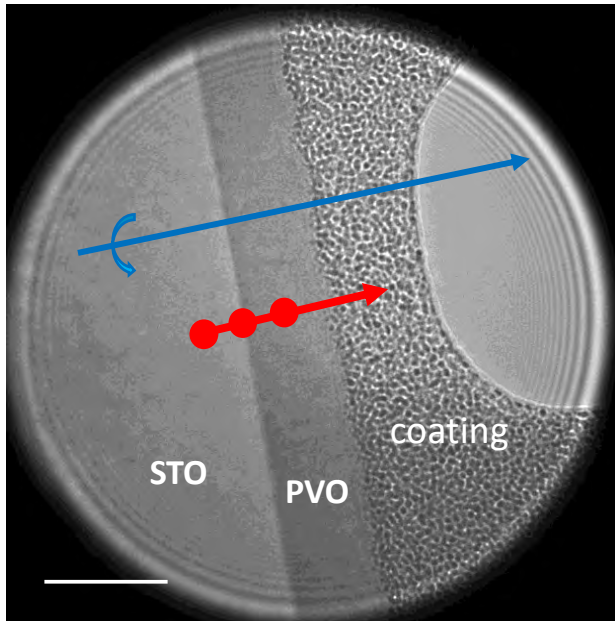


(a) experimental PED pattern and (b) superposition with the matching template



(a) bright field image and (b) reconstructed domain map

- ✗ Sync. scanning / detector
- ✗ Data sorting
- ✓ Analyze multiple ROI (known or not)
- ✓ No need for domain tracking
- ✓ Applicable to other materials

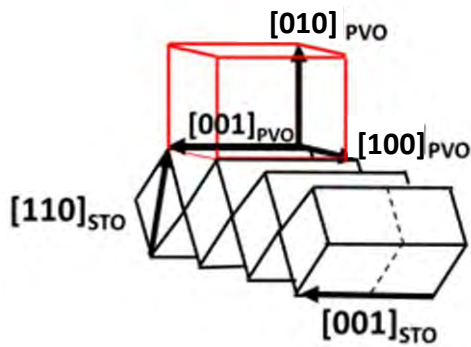
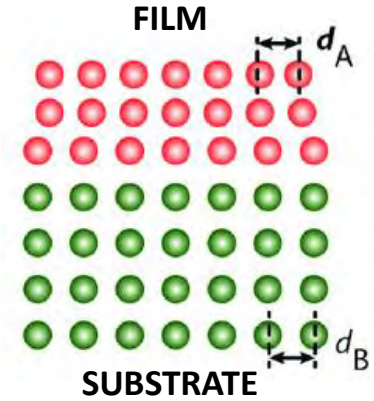


PrVO₃ thin film on SrTiO₃[110] (Beam size 10 nm)

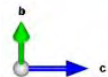
Aim:

Observe **evolution along the thickness of the film in**

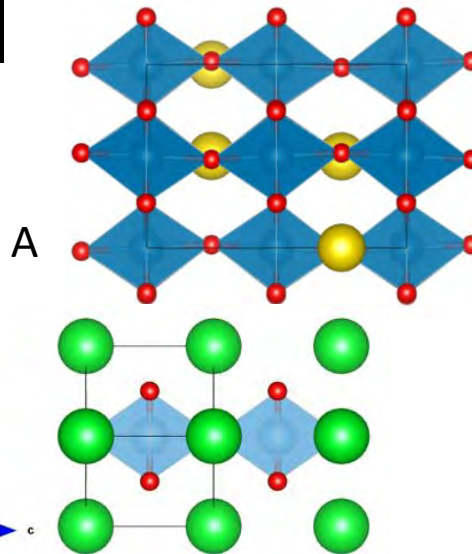
- ➔ unit cell parameters
- ➔ VO₆ octahedra tilting



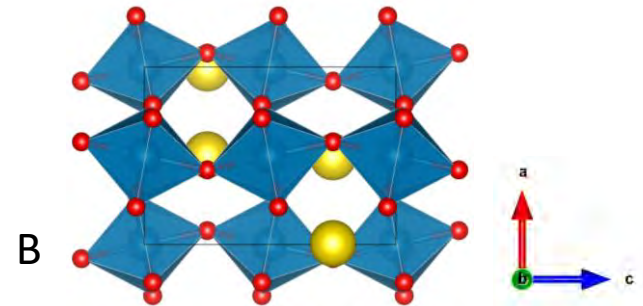
$c \text{ (PVO)} \approx 2x \text{ a (STO)}$



NEAR SUBSTRATE



BULK PVO



- A. V-O₁-V ≈ 180°
V-O₂-V ≈ 180°
- B. V-O₁-V ≈ 153°
V-O₂-V ≈ 152°

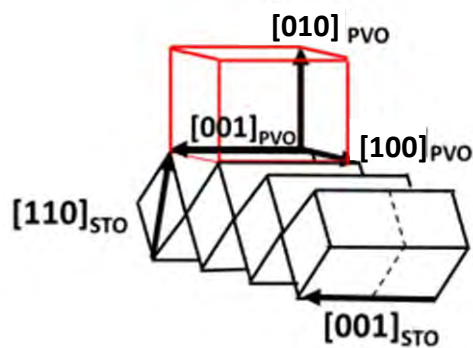
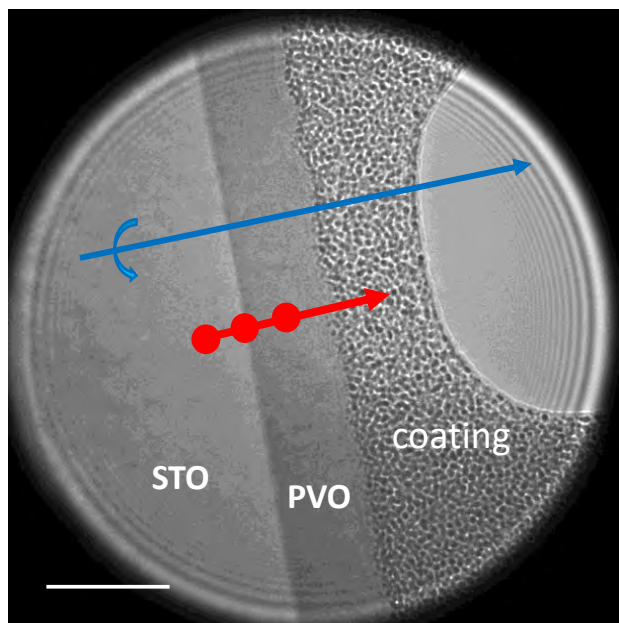
PrVO₃ thin film on SrTiO₃[110] (Beam size 10 nm)

Pets2.0

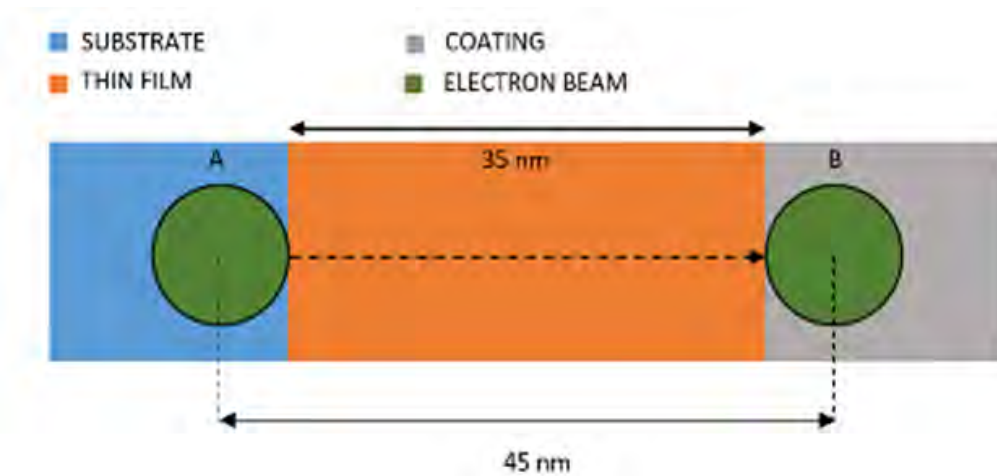
- ✓ Calibration constant adjusted wrt STO
- ✓ Distortion parameters refined for STO
- ✓ Imposed distortion parameters to PVO

Jana2020

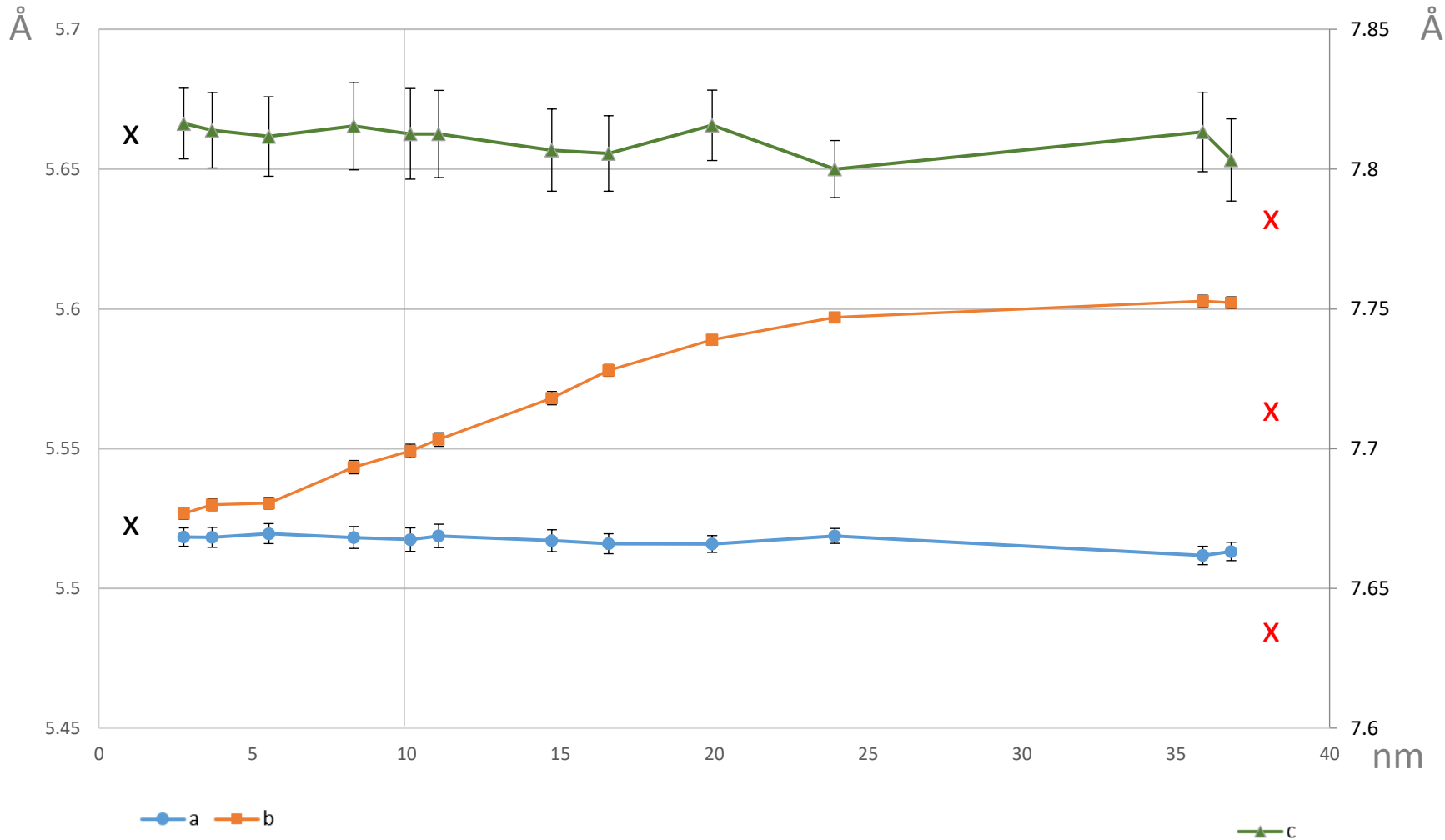
- ✓ Imported model from ref .cif file



$c(\text{PVO}) \approx 2x a(\text{STO})$

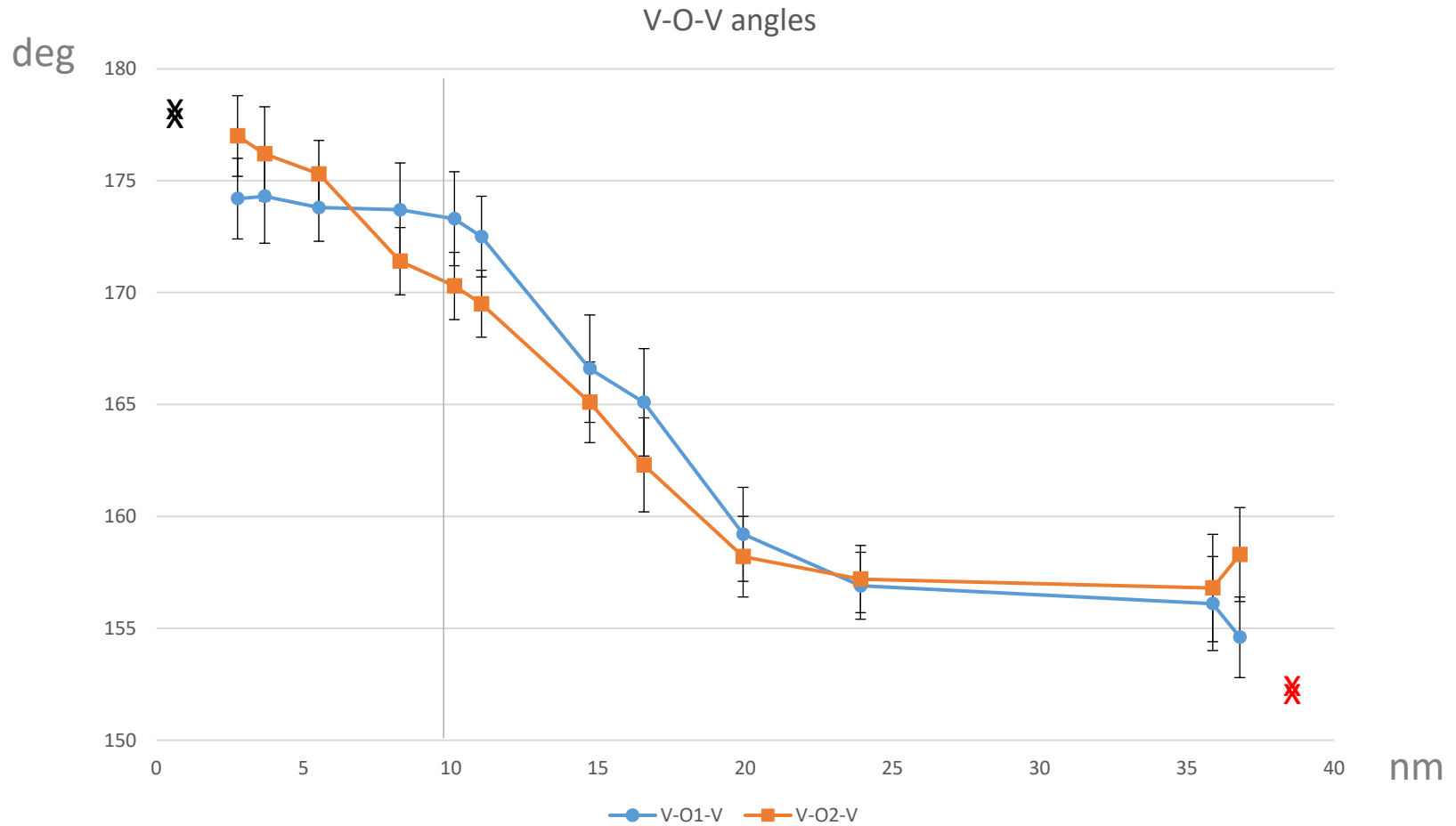


PVO unit cell parameters



x = substrate as ortho

x = bulk PVO parameters



x = substrate as ortho

x = bulk PVO parameters

CONCLUSIONS

- ✓ SPEDT on 35 nm PVO thin film
- ✓ Reconstructed reciprocal space for different layers
- ✓ Performed dynamical refinements
- ✓ Evolution in cell parameters and tilt angles observed
- ✓ Observations in agreement with expected results

Open questions:

- Impact of the substrate in the analysis of the first layers
- Cell parameters
- Calibration parameter (0.00708 vs 0.007084)

