TWEET - Towards ferroelectricity in 2D (TWEET) and beyond

Growth of HZO/LSMO films on vicinal substrates

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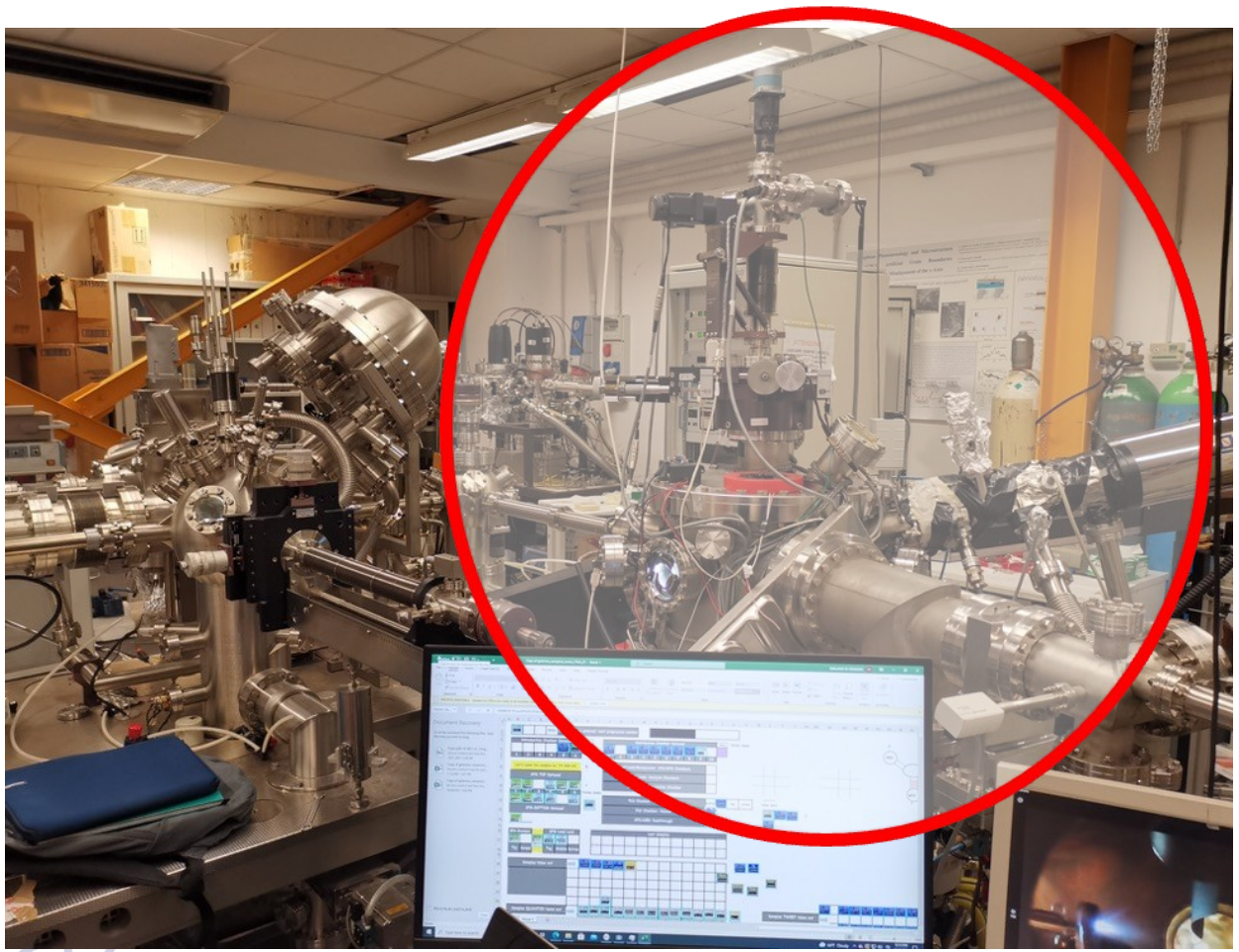
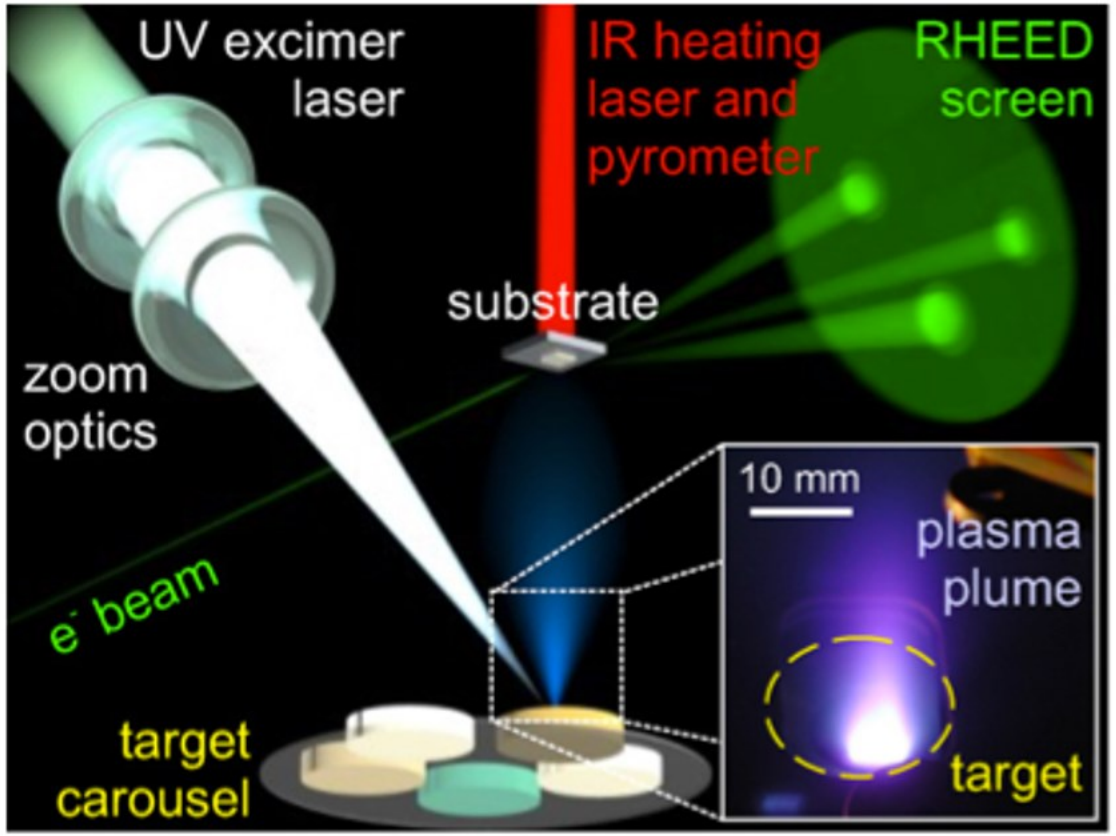
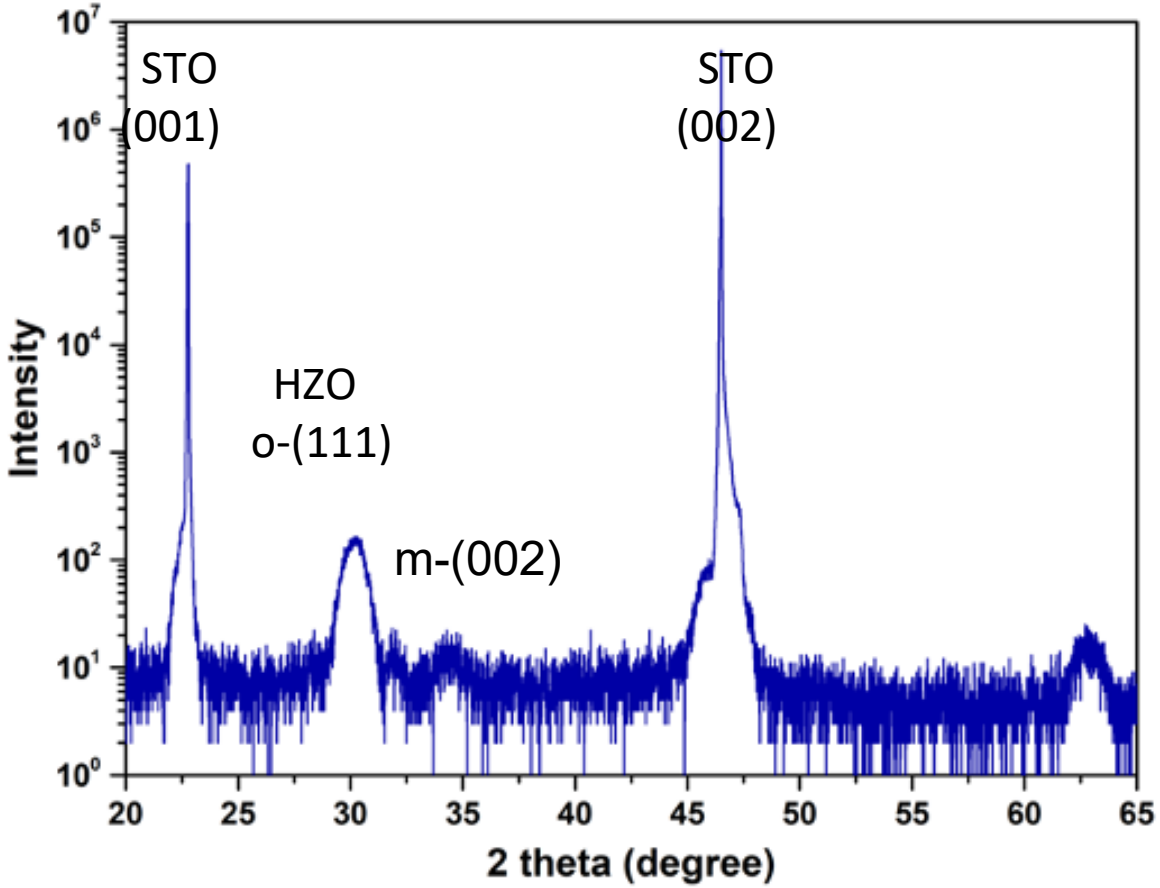
Istituto SPIN - Genova, L'Aquila, Napoli, Roma, Salerno

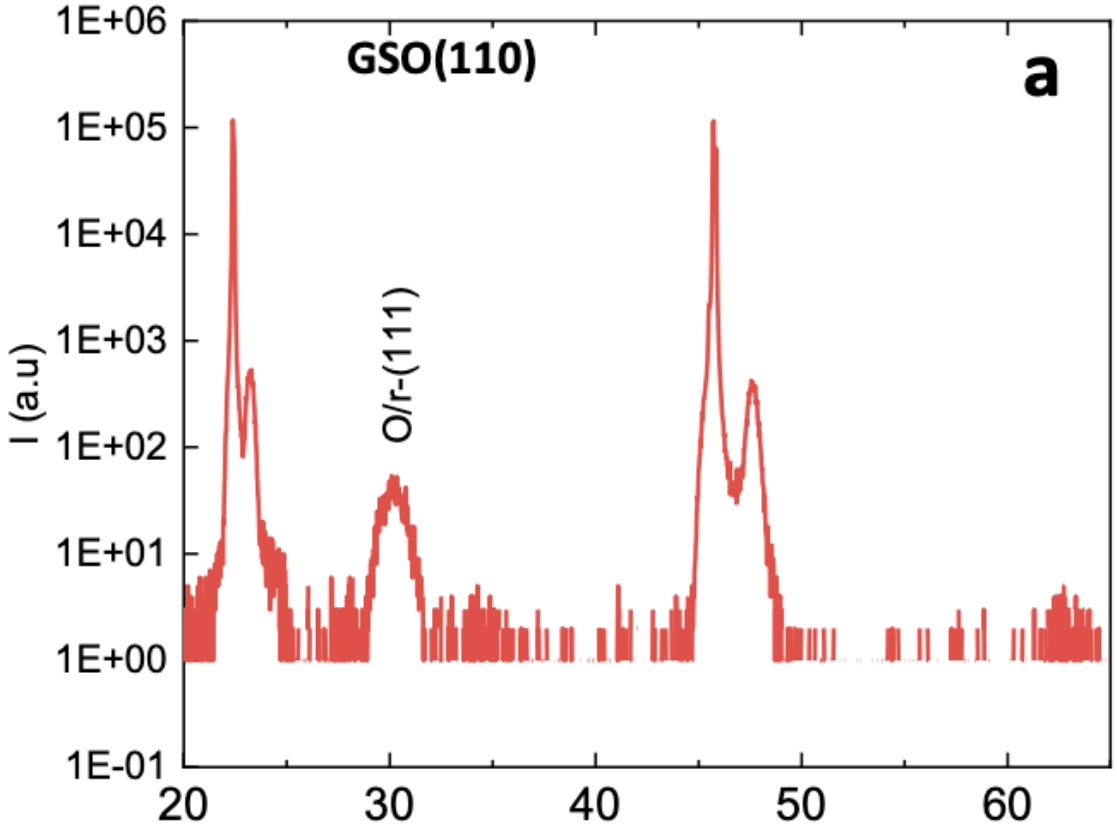
MODA set up at CNR-SPIN of Naples



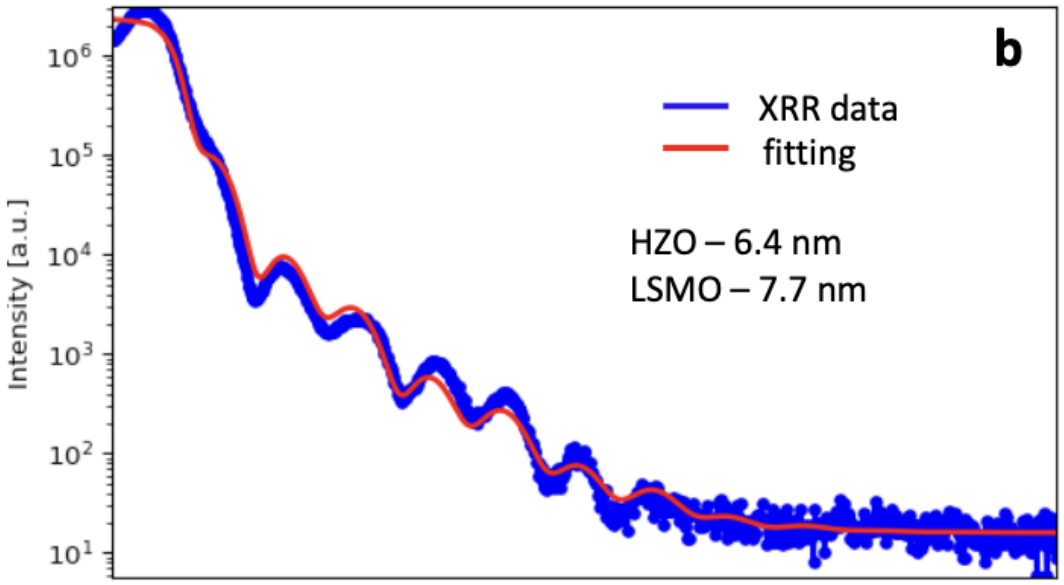


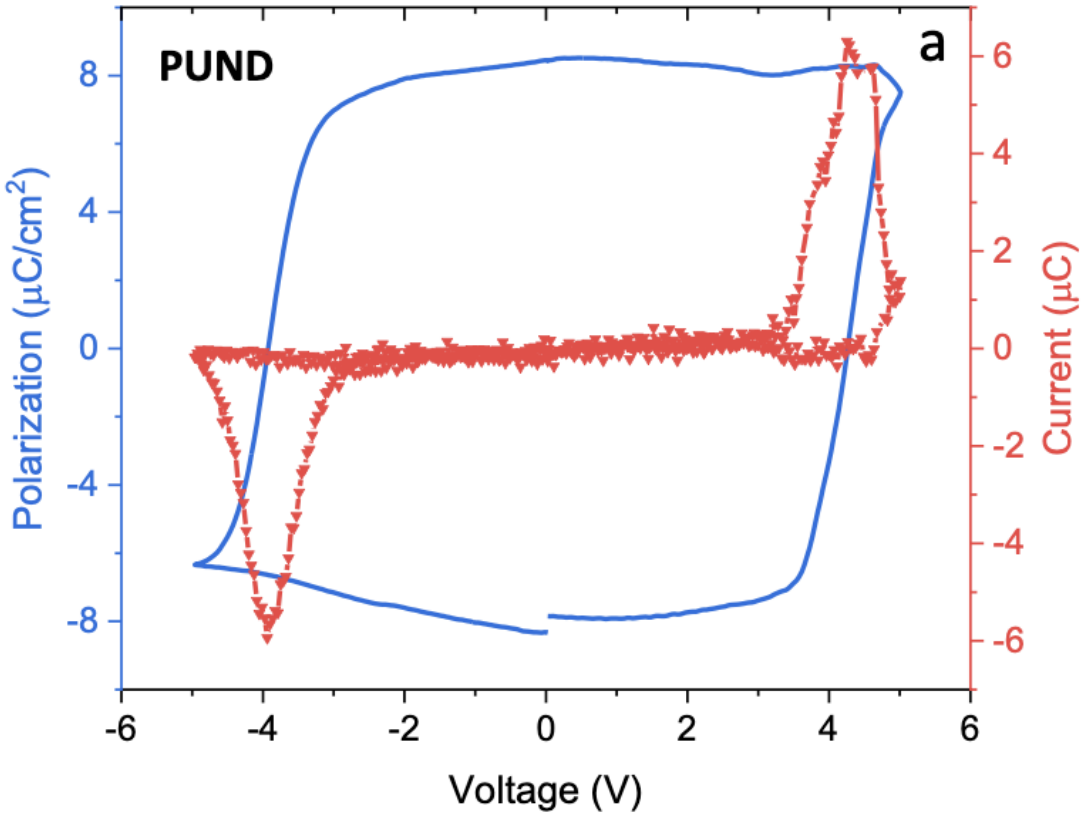
HZO on LSMO buffered- 001 STO and 110-GSO substrates



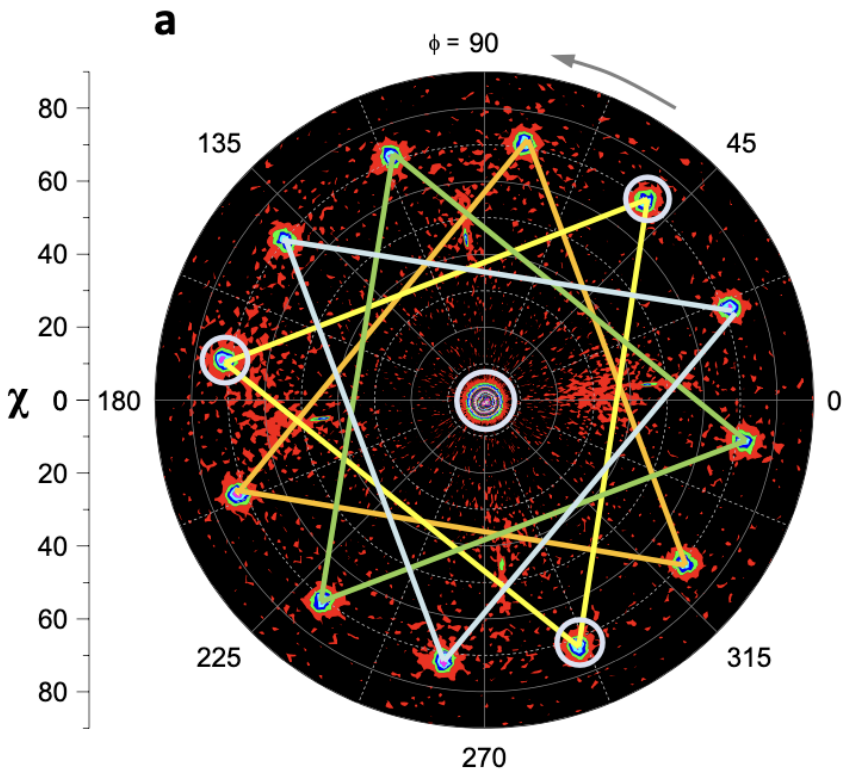


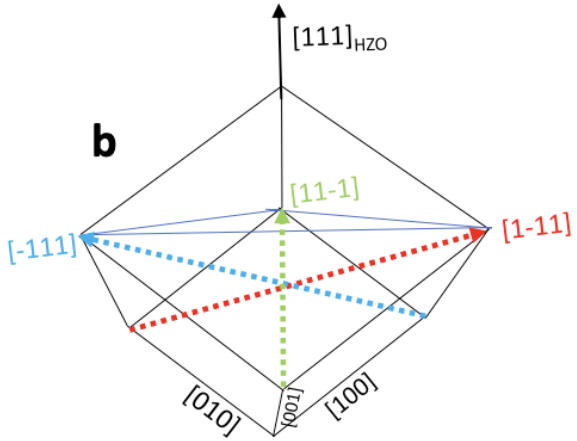
FE measurements

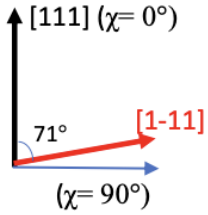


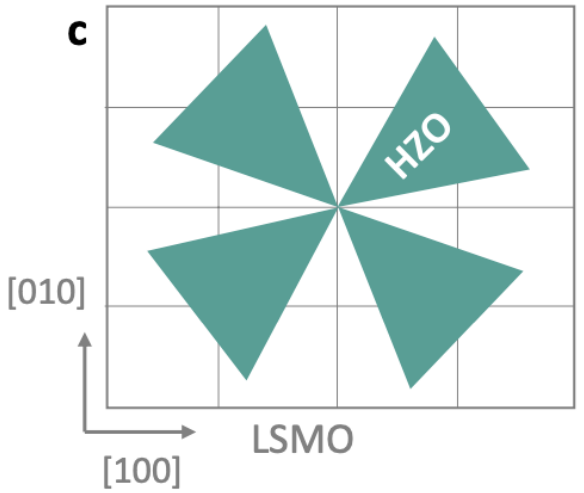


o-HZO: pole figure @Groningen University









Crystal variants in o-HZO(111)/LSMO/STO 001

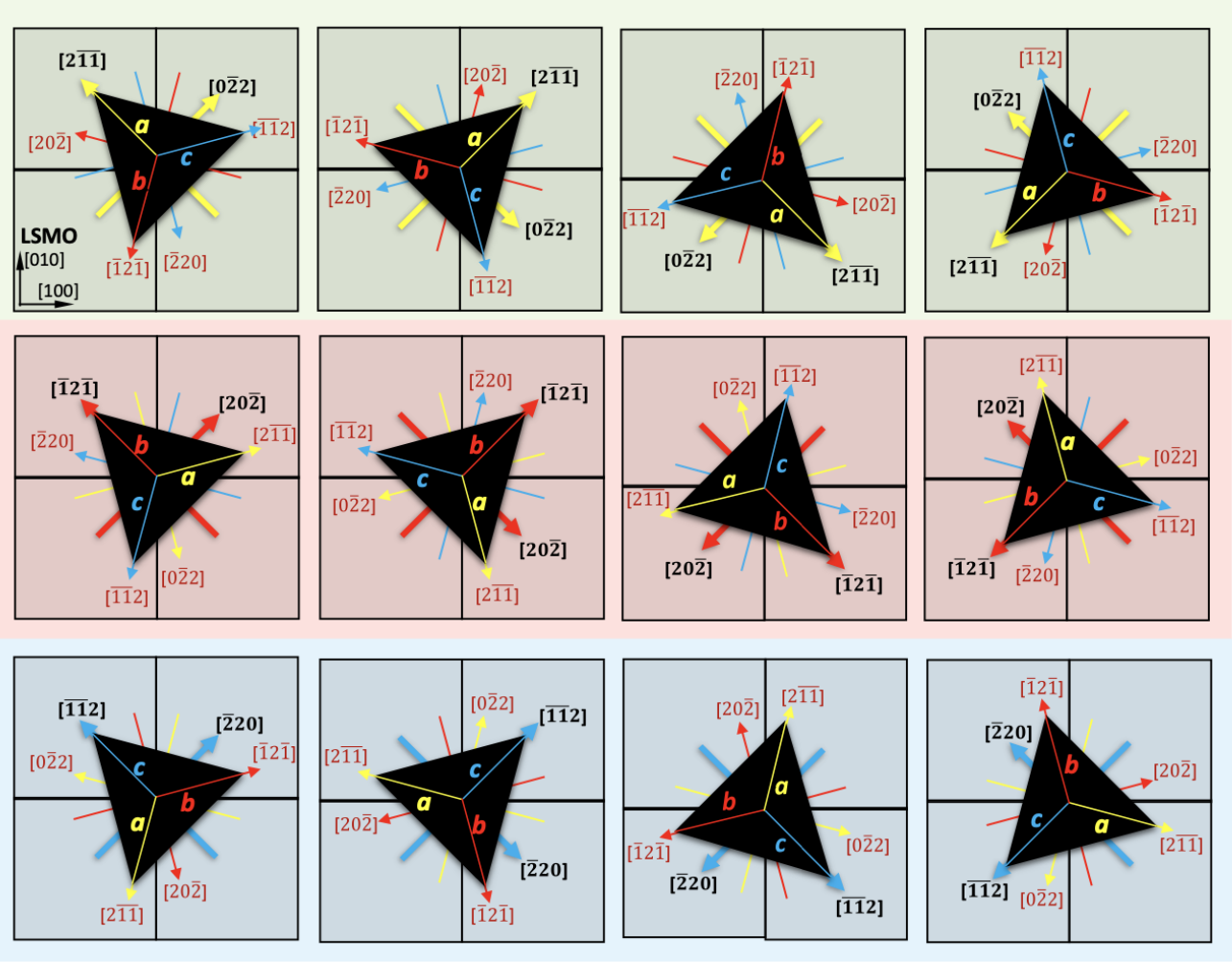
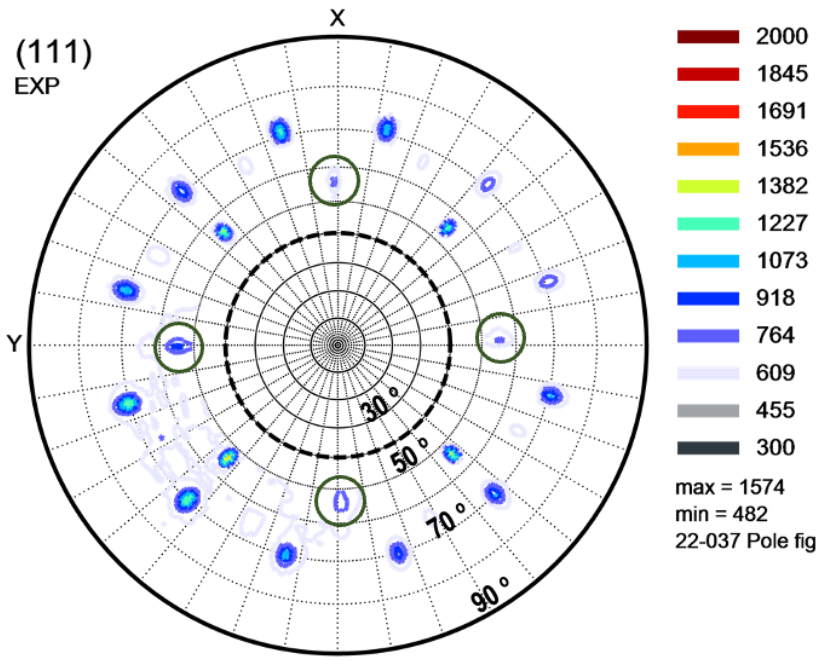


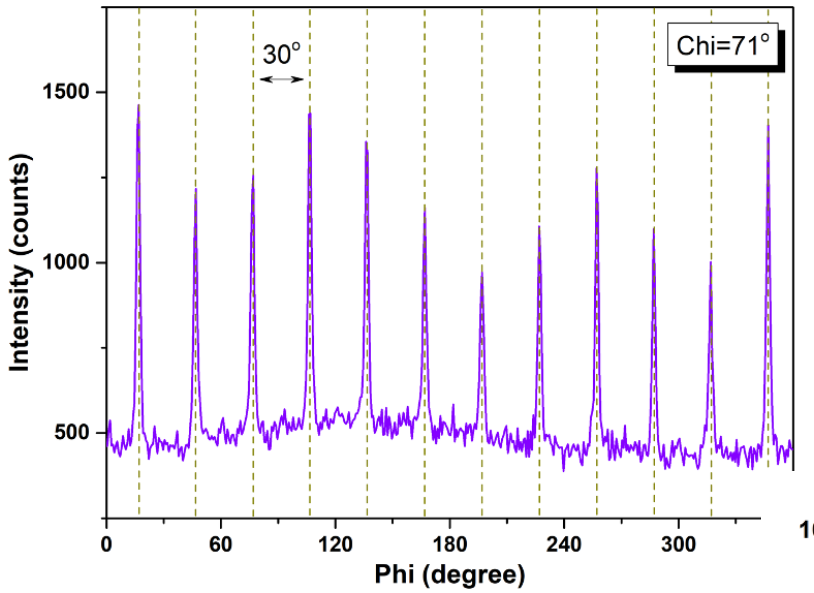
Figure S8. Sketch of the crystal variants present in epitaxial o-HZO(111) films on LSMO(001).

Let's assume that a, b, and c ([100], [010] and [001]) are inequivalent.

In the absence of a symmetry break from the substrate, you have not only the four domains shown in the left picture, but also, for each of them, the different permutations of the a, b and c axes.

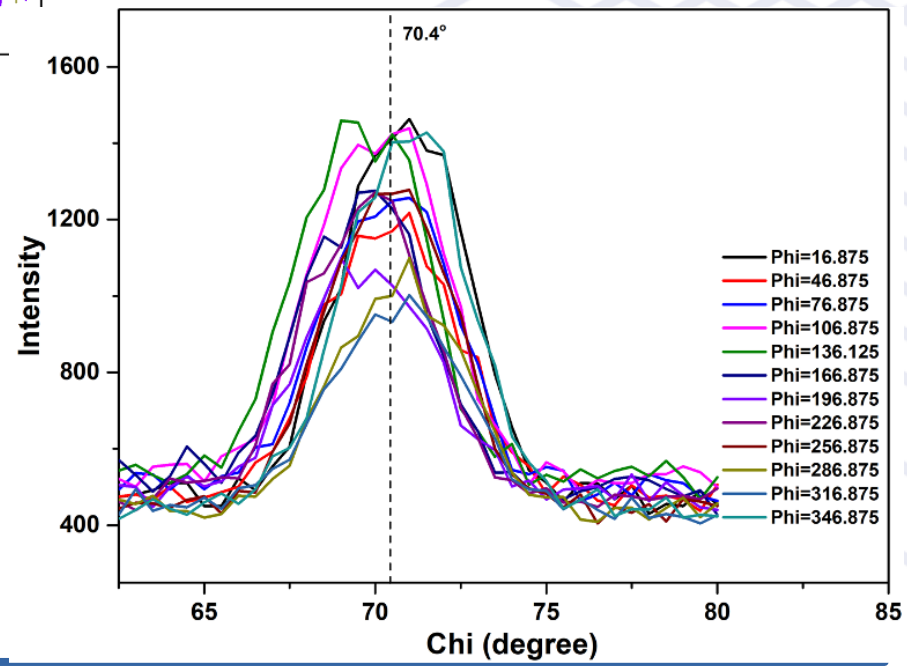
HZO on LSMO/STO 001 substrate





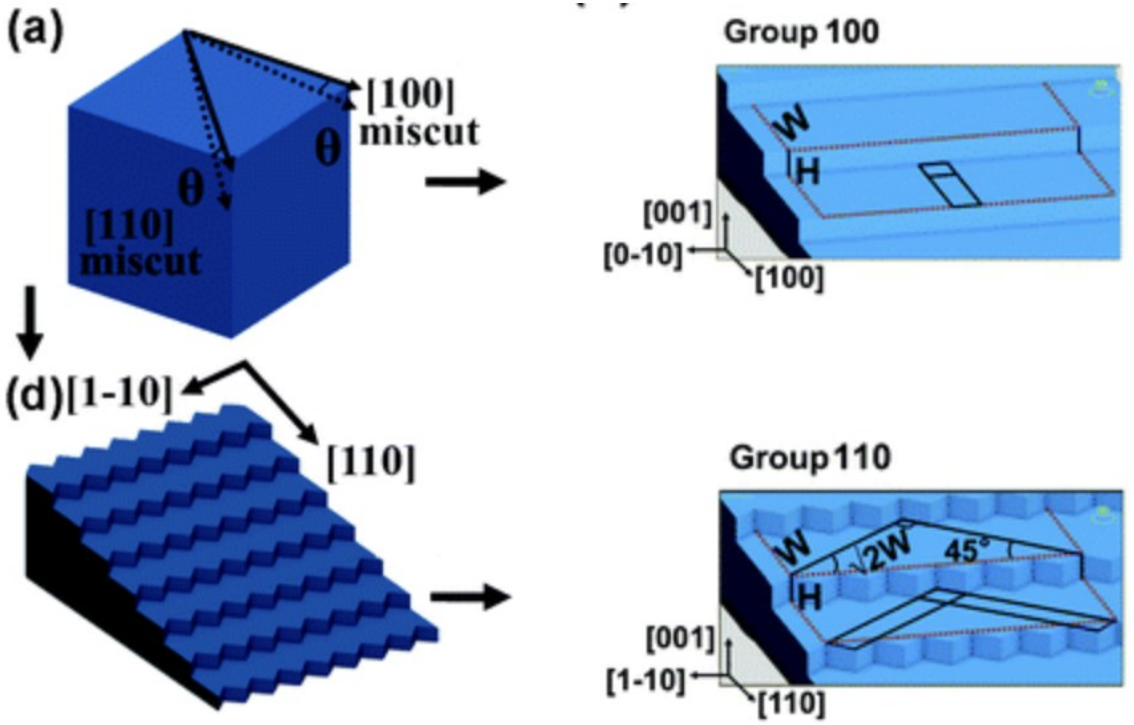
χ scan shows the expected 12 poles around 71°,
confirming the presence of 4 crystal domains in o-(111) HZO.
The 4 weak poles at 54 ° come from the {100} peaks.

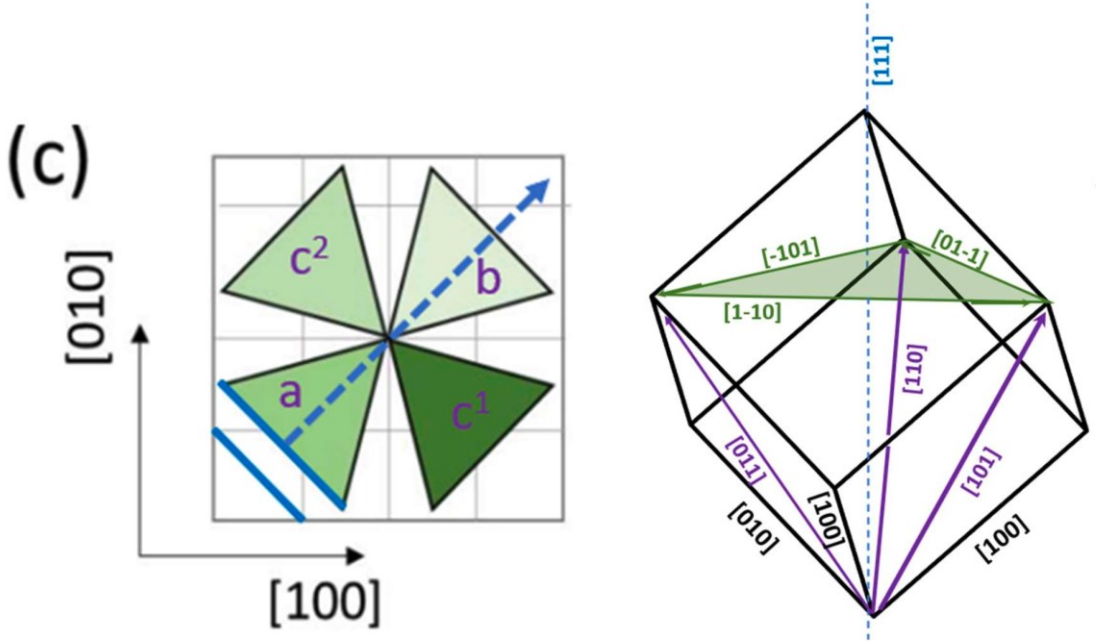
No symmetry broken is foreseen in χ scan.



HZO on vicinal substrates

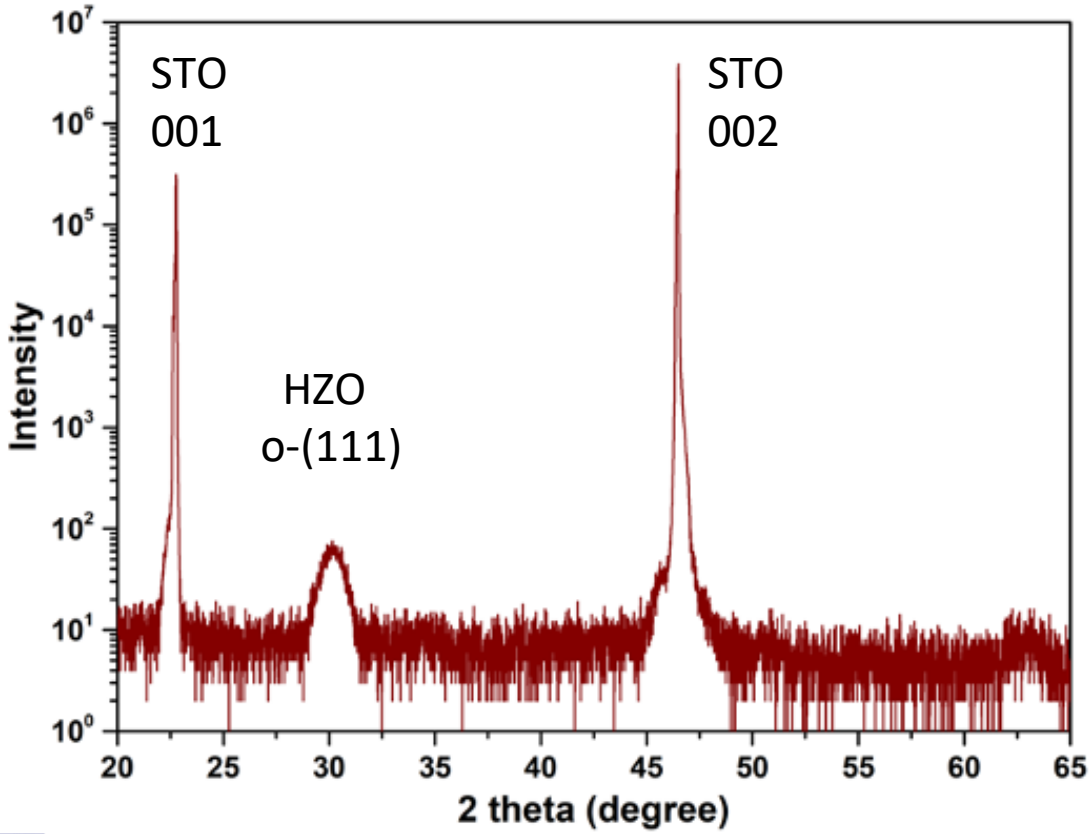
In the attempt of controlling the occurrence of the crystal domains, with a miscut along the 110 direction.



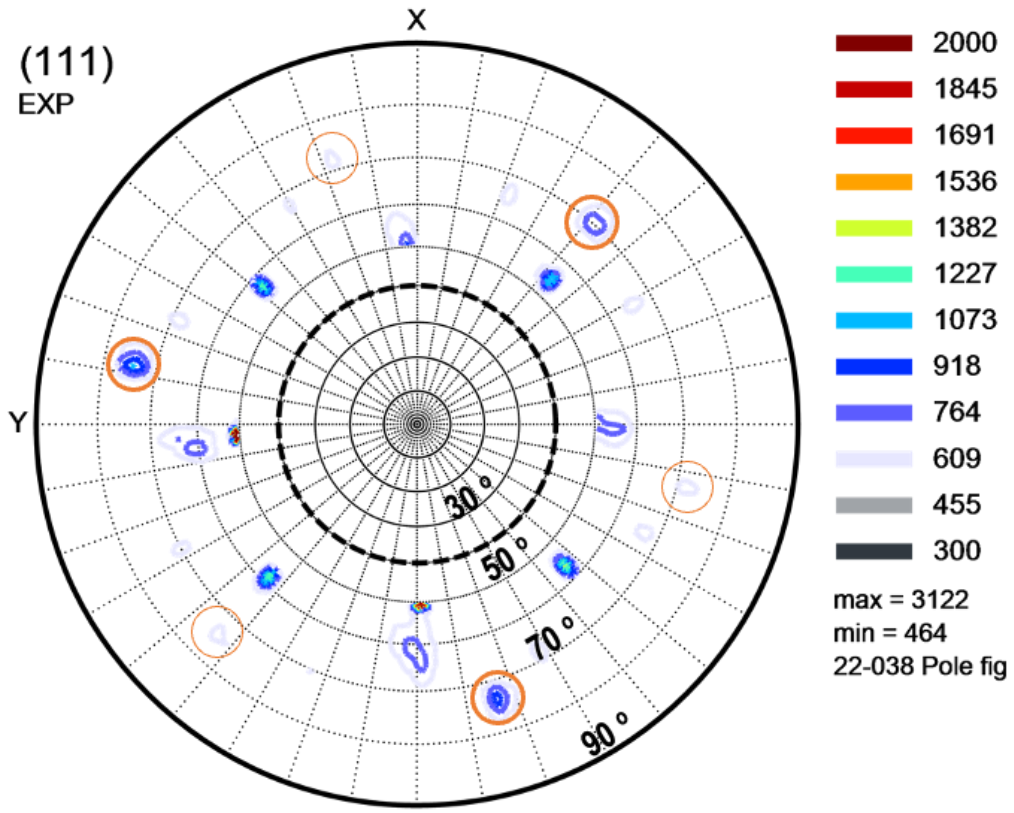


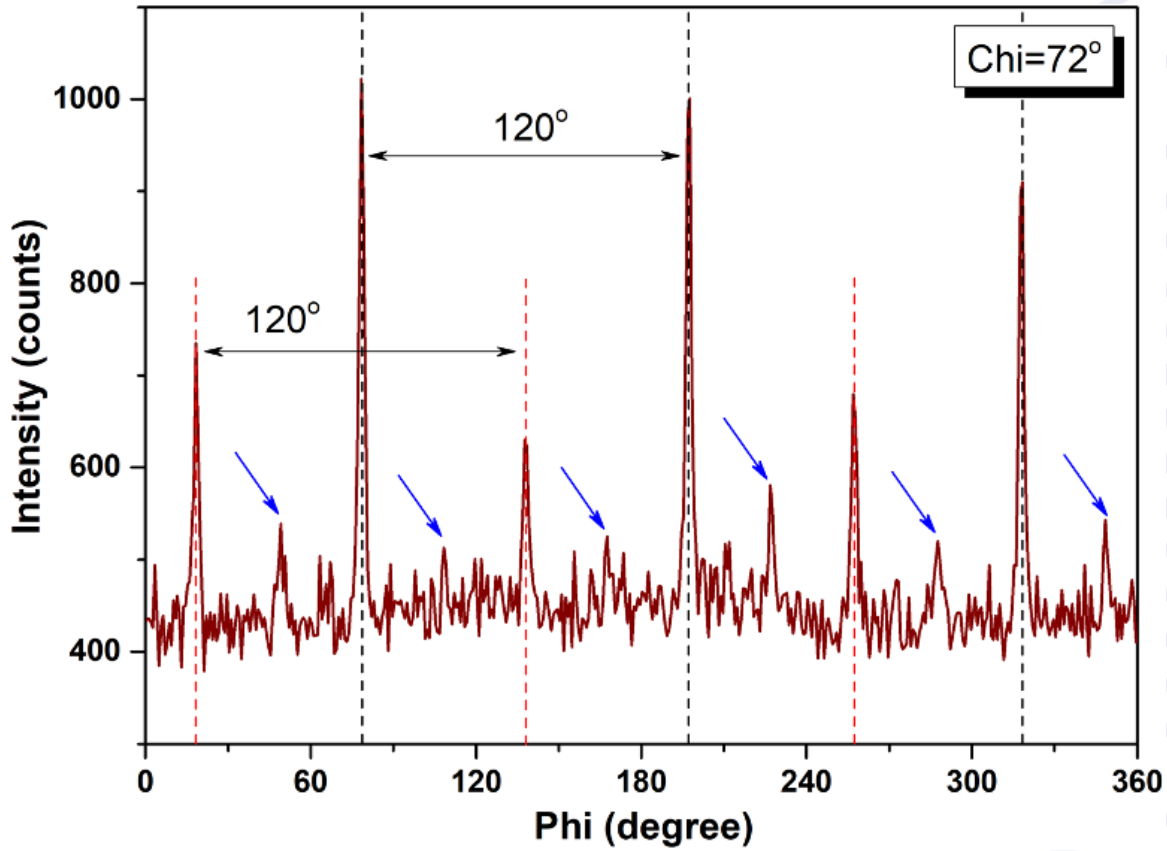
Vicinal substrate, miscut along (110), should enforce in-plane azimuth domains a and b to dominate, while suppressing domains c1 and c2.

HZO on STO 001 with 3°miscut along (110)



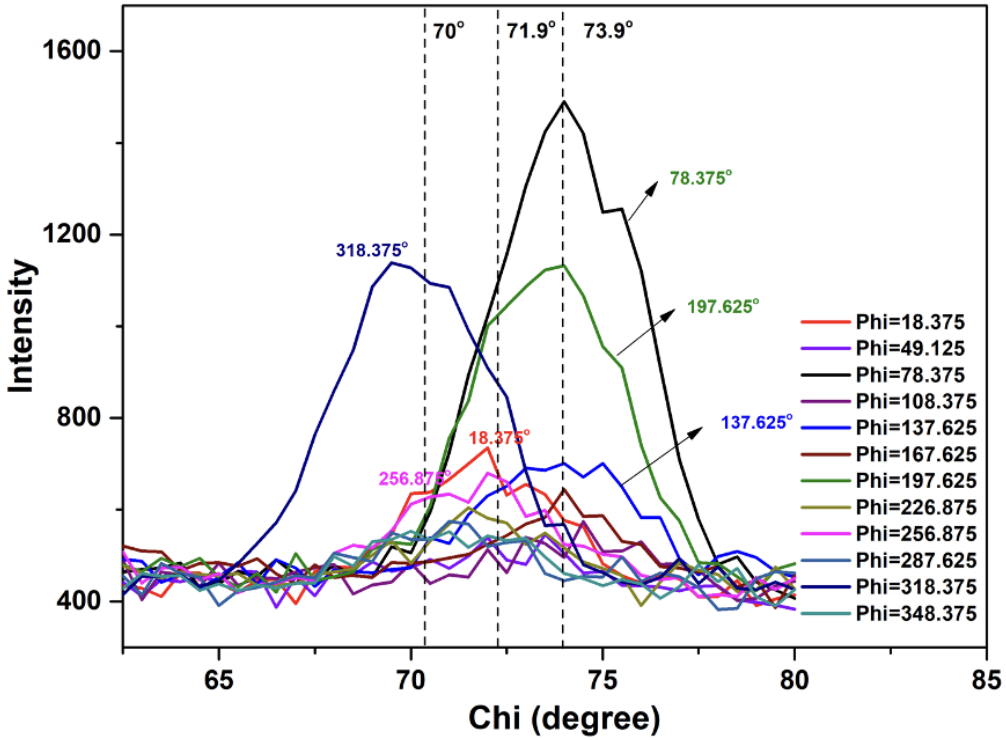
HZO on 3°miscut along (110)





At Chi= 72° , There are 3 rather strong poles and 3 weaker poles,
indicating one/two predominant domains with small fractions of other domains

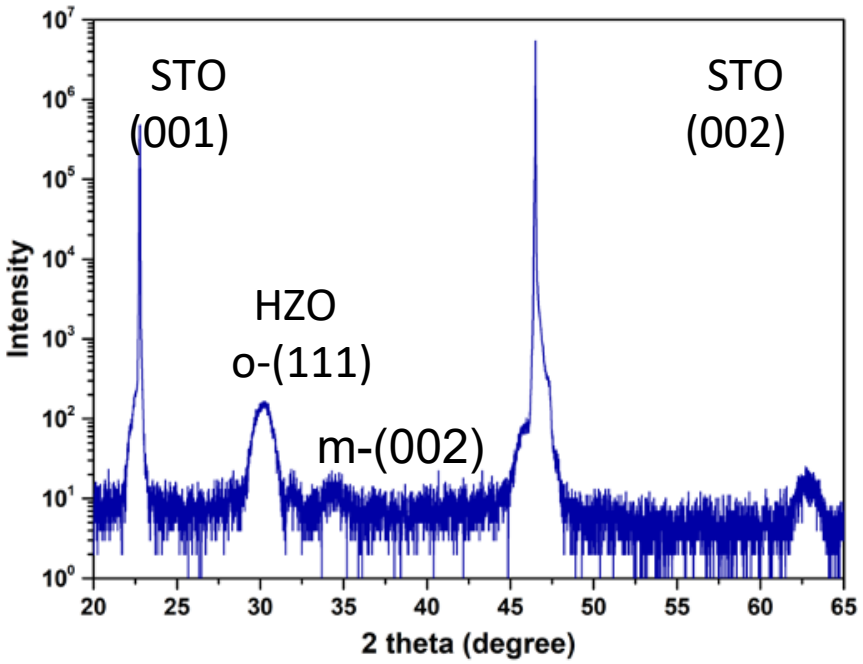
HZO on vicinal substrates

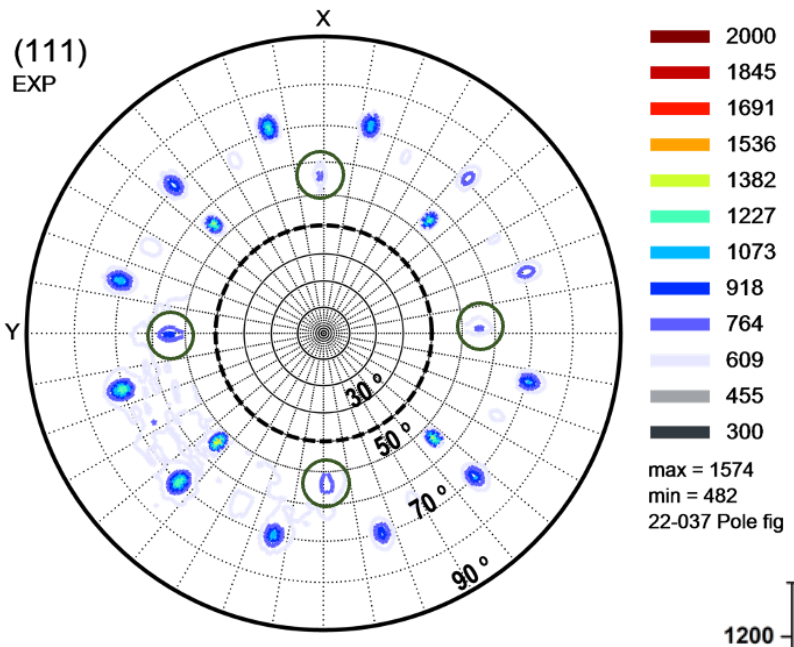


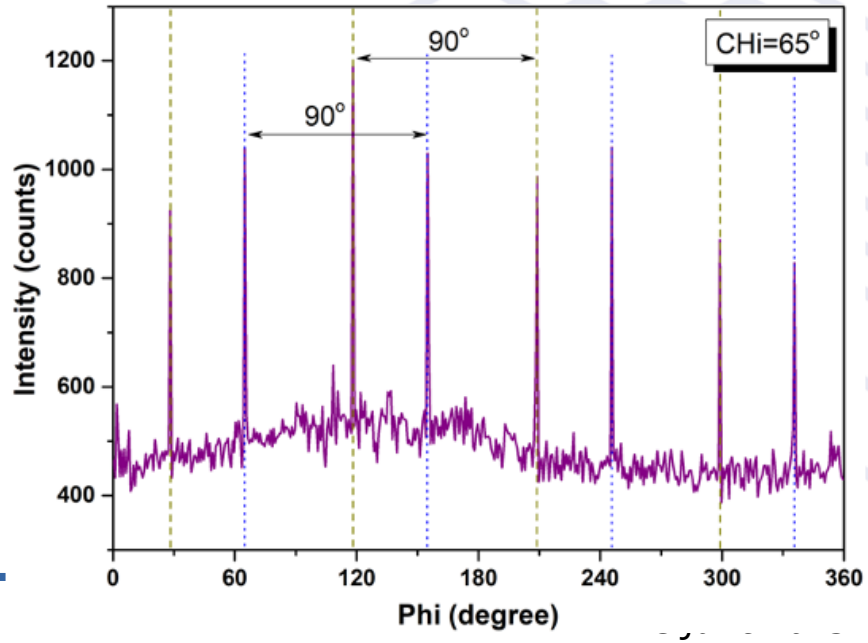
Assuming we had a purely orthorhombic structure with lattice parameters 5,040 ; 5,074 ; 5,269 A (values for non-epitaxial samples) we would have χ angles 68,32°, 71,34° and 72,00°. Therefore, the data on our samples are consistent with an orthorhombic cell with a strain-induced rhombohedral distortion that uniformly increases all χ angles by a couple of degrees.

The fact that we resolve different three χ angles, with χ values 120° apart, suggests that we also have, in our

HZO on STO 001 with 1°miscut along (11(







new set of peaks

Crystal variants and FE properties

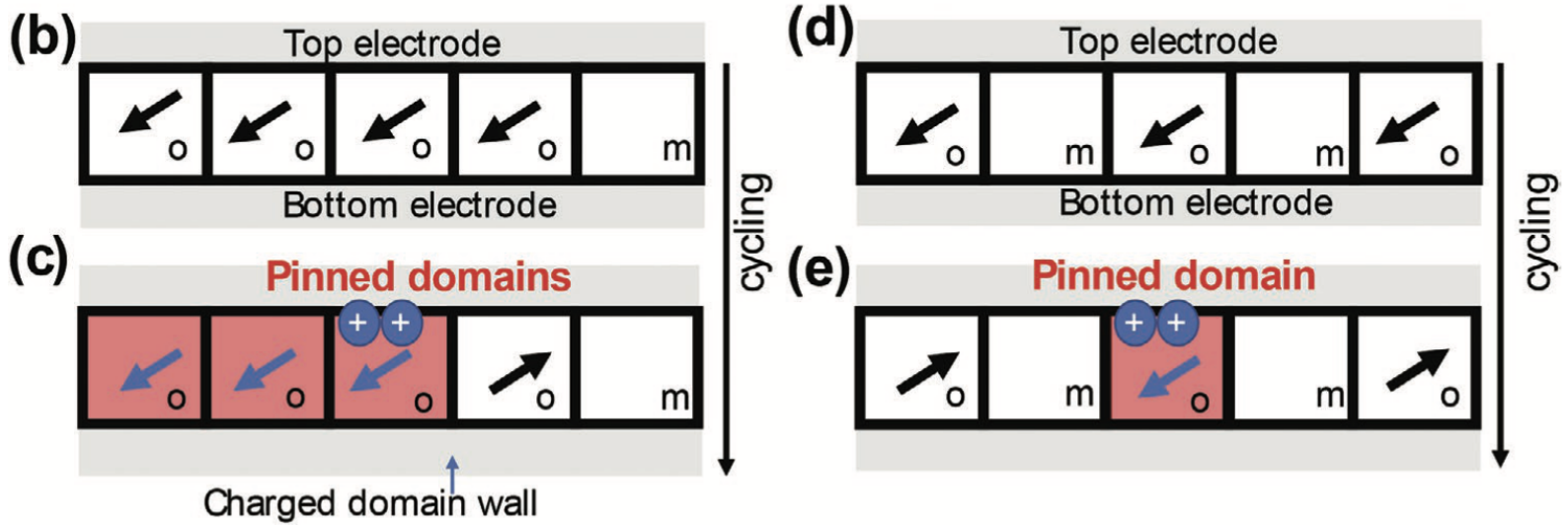


Figure 6. a) Cross-sectional STEM image of the HZO/LSMO/STO(001) sample, showing orthorhombic (o) and monoclinic (m) columnar grains. Grain boundaries are marked by yellow arrows. b–e) Sketch of the endurance degradation by fatigue in films with small b,c) and high d,e) amount of grains of paraelectric monoclinic phase. Oxygen vacancies are represented by blue circles. Blue and black arrows represent pinned and unpinned dipoles, respectively, oriented along [001] in the (111) oriented orthorhombic film.

As 12 crystal variants are present, the dipole vectors differ in the out- of-plane and the two in-plane components in contiguous crystal variant regions, with both Ex and Ey contributing to the electrostatic boundary conditions in the domain wall between two crystal variants.

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Conclusions

- Growth and characterization of HZO/LSMO film on STO (001) and GSO (001)

- Pr measured value of 8 uC/cm2 for HZO film of 6.5 nm

- Selection of the crystal variants through the employment of vicinal substrates:
  No significative results for 1° miscut along 110 direction
  One main domain selected for 3° miscut along 110 direction

Ongoing activities:
comparison of the FE properties between *standard multi-domains* and *single domain* HZO sample