

# Grain to grain heterogenities in PbZrTiO\_3 thin film as probed by in-situ biasing XRD

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### Abstract: Grain to grain heterogenities in PbZrTiO<sub>3</sub> thin film as probed by insitu biasing XRD

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Piezoelectric thin-films are those which generate mechanical strain in response to applied electric field and they are used for a wide range of technological applications. The case of polycrystalline thin films is particularly complex and delicate to model. A better understanding of the intergranular responses is necessary to evaluate the intergranular constraint and the anisotropic responses of individual grains [1]. However, this problem is sparsely experimentally documented due to the lack of adequate methods. Here, the behavior of a ten of single grains of Lead Zirconate Titanate (Pb(Zr<sub>x</sub>, Ti<sub>1-x</sub>)O<sub>3</sub>) has been evaluated thanks to the in-situ biasing Xray Diffraction (XRD) technique [2] using a synchrotron source and a sub-micronic X-ray beam. A small capacitor has been biased with DC voltage between zero and  $\pm 20V$  and at each step of bias a set of spotty Debye rings has been recorded. By selecting an appropriate region of interest, the evolution of a single grain peak can be extracted. The fine analysis of (200) pseudo-cubic peak allows to separate the evolution of different parameters of a/c tetragonal and rhombohedral domains during the electrical biasing. Finally, through the calculation of the center of gravity of the peaks, the effective piezoelectric coefficient ( $d_{33,eff}$ ) was deduced which shows a heterogeneity between different grains. This research contributes to a better understanding of the local behaviors in piezo/ferroelectric polycrystalline films and in the improvement of their performance for different applications.

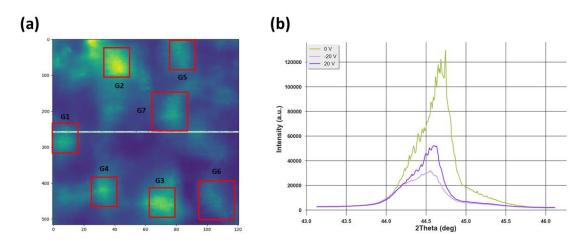


Figure 1: (a) High resolution pole figure where a tens a single grain are recorded (b) Example of the evolution of (200) peak at different bias values for grain 1

#### References

- [1] J. E. Daniels *et al.*, "Heterogeneous grain-scale response in ferroic polycrystals under electric field," *Sci Rep*, vol. 6, no. 1, p. 22820, Mar. 2016, doi: 10.1038/srep22820.
- [2] K. Nguyen, E. Bellec, E. Zatterin, G. Le Rhun, P. Gergaud, and N. Vaxelaire, "Structural Insights of Electrical Aging in PZT Thin Films as Revealed by In Situ Biasing X-ray Diffraction," *Materials*, vol. 14, no. 16, Art. no. 16, Jan. 2021, doi: 10.3390/ma14164500.

### **Presentation preferred**

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