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Multi-scale characterization of piezo/ferroelectric thin-films by in situ X-ray Diffraction during biasing

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Piezoelectric and ferroelectric thin films are ubiquitous in many applications such as sensors, actuators, pyroelectric devices or advanced memories. The case of polycrystalline thin films is particularly complex and delicate to model. Several effects (i.e. interface, substrate clamping, grain boundary, stress) affect the behavior of the domains at the local scale and by consequence impose the film macroscopic response.

It will be shown in this communication how in-situ X-ray diffraction during electrical biasing offers unique information to address these complex behaviors at different scales. The case of the prototypal Pb (Zr₄₈, Ti₅₂) O₃ or PZT films will be addressed as a general example. These films at the morphotropic phase boundary (MPB) are composed of two textured ferroelectric phases (one tetragonal and the other rhombohedral). First, it has been observed that interphase boundary motion is the predominant effect during the biasing. A grain to grain heterogeneity has also been observed and quantified [1]. Our results are based a combination of synchrotron beamtimes [2] as well as results from our in-situ lab source based setup [3]. Finally, methodologies and perspectives will be discussed.



Figure: (a) Schematic of in-situ biasing XRD setup. (b) High resolution pole figure where a tens a single grain are recorded (c) Example of the evolution of (200) peak at different bias for grain #3

References

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[2] K. Nguyen et al., "Structural Insights of Electrical Aging in PZT Thin Films as Revealed by In Situ Biasing Xray Diffraction", Material **14**, 4500 (2021); doi: 10.3390/ma14164500

[3] Allouche et al, Materials & Design 154, 340 (2018)





