Improvement of the X-ray characterisation of electroceramic thin films by the application of a novel combined analysis procedure

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The so-called combined approach, which is now proved to be a viable tool [1], is an alternative method of X-ray analysis that has not been applied to ceramic thin films until recently [2]. The advantage of this method, which consists in the combination of adequate refinement procedures, resides in the simultaneous and more accurate determination of the structure and texture of thin films, which allows to obtain important microstructural information not available by other means.

In this presentation we briefly explain the fundamentals of the combined approach, where quantitative texture analysis and Rietveld refinement are used in a cyclic process using the Materials Analysis Using Diffraction Package (MAUD) [3] developed by L. Lutterotti. Then we present the results of the application of this method to the study of several ferroelectric thin films. The development of preferential orientations or texture along the polar axis in these films, studied previously [4], determines the final properties of the material. However the application of more conventional analysis methods produces unsatisfactory results when separating the contributions of the different texture components, due precisely to a less precise determination of the structural parameters of the film. This problem is solved with the use of the combined approach, and the evolution of the contributions of the texture components along <001> (polar direction) and <100>, normally associated in the systems studied, is studied when the film is deposited on different substrates. The deduction of effective physical properties by an averaging process of the single crystal values, taken into account the calculated orientation distribution function, is also discussed.

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3. *http://www.ing.unitn.it/~luttero/maud/*4. J. Ricote, R. Poyato, M. Algueró, L. Pardo, M.L. Calzada and D. Chateigner. *J. Am. Ceram. Soc.* 86[9], 1571-1577 (2003).