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Advances in the microstructural and structural analysis by X-ray diffraction of ferroelectric thin films

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X-ray diffraction methods are widely used nowadays for the characterization of thin films with technological applications. Parameters that determine the physical behavior of films, like the crystalline structure of the present phases, the appearance of preferential orientations or residual stress, are available with this non-destructive microstructural characterization. The precise determination of these parameters by X-ray methods requires a previous knowledge of others, i.e., to determine the texture we need to know the crystalline structure, but to determine precisely the crystalline structure, we require a previous knowledge of the texture of the material. These problems lead most research laboratories to partially determine some of the parameters available by X-ray techniques. The use of the recently developed combined approach, which is able to determine all the parameters accessible by X-ray diffraction through the combination of adequate refinement procedures, allows the analysis of the complex layered structures of technological thin films. In this work we will show the results obtained on several polycrystalline ferroelectric thin films of Ca modified lead titanate with a new expert X-ray system, with both diffraction and reflectivity and that implements the methodology necessary for the combined analysis. The importance of this advance in the analysis of X-ray diffraction data is reflected in the solution of fundamental problems that could not be analyzed directly up to now. A good example is the reliable separation of the contributions of (001) and (100) reflections in modified lead titanate thin films. The overlap of these two reflections prevent the study of preferential orientations along the polar axis, <001>, and at the same time a precise structural determination. The use of the combined analysis allows us to study the influence of the stress produced by different substrates on the orientation, structure and residual stress of these ferroelectric thin films.