

X-RAY DIFFRACTION QUANTITATIVE ANALYSIS OF CA-MODIFIED LEAD TITANATE THIN FILMS COMBINING TEXTURE, STRUCTURE AND STRESS DETERMINATIONS

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The complete determination of the microstructure of a thin film includes analyses of the crystallographic preferred orientations and structures, internal stresses (residual and microstresses), particle sizes, ...

Most of the microstructural details can give specific contributions on the X-ray diffraction signals, but their combination in a single diagram, as in the case for most of the elaborated materials, makes their analyses particularly difficult. Unfortunately, one cannot avoid treating all of these contributions as a whole, since they are inter-dependant. For instance, refining the texture without knowing the exact structure can give rise to artefacts in the texture treatment, and inversely. The presence of residual stresses in a material can affect the results of structural determinations.

Only recently, a methodology has been developed which combines the principal aspects of the microstructural contributions to neutron diffraction data. When using X-rays, such an analysis is even more complex, mainly because of the high absorption coefficients of X-rays. Most of these problems are now resolved, and results of the so-called "combined" approach are presented here, on Ca-modified PbTiO₃ thin films.

