X-ray Combined QTA using a CPS applied to a ferroelectric ultrastructure

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The combined approach as implemented in MAUD is used in order to determine the microstructure, structure and texture of an ultrastructure, a complex stacking of several layers provoking strong peaks overlaps in the x-ray diagrams. We used a curved position sensitive detector to acquire all the necessary diagrams and a classical x-ray generator.

The sample studied is a Ca-modified PbTiO₃ ferroelectric layer (or PTC) deposited on a Pt/TiO₂/SiO₂/Si-(100) substrate elaborated by spin-coating. The PTC layer is a pseudo-cubic tetragonal perovskite, giving rise to problems in its texture analysis because of the strong intraphase overlaps. The Pt substrate moreover overlaps with some of the PTC peaks, all Pt peaks being covered partially by PTC, and few PTC's remaining for QTA. Cell-parameters are not finely controlable because of the non-stoichiometric structure, and the different layer thicknesses are only known from the deposition parameters. Different texture strength are present with different crystallite sizes and microstrains. This as a whole makes very difficult to obtain a reliable analysis of the ultrastructure. Using the combined approach, the refinement of the whole diagrams is achieved, including the determination of the texture (WIMV approach), the cell parameters, crystallite sizes and microstrain parameters, and layer thicknesses, for the two top layers.

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