Rietveld Texture and Stress Analysis of Thin Films by X-ray Diffraction

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Abstract

In many applications where thin films are involved, like in electronics or ferroelectricity, it is required quantitatively to characterize their texture and residual stresses. Moreover, commonly the films contain several layers and phases, and due to the severe overlapping of the reflection peaks and sharp texture, the analysis of both features is difficult or even not possible by the traditional pole figure- and $\sin\psi^2$ *-techniques. Rietveld texture and stress analysis is a viable methodology to overcome the overlapping problem and a dedicated system composed by a special diffractometer and software for the analysis has been developed to accomplish the task. The diffractometer is mainly composed by a goniometer with an open eulerian cradle coupled with a curved position sensitive detector covering 120° to collect a large part of the* 2θ *spectrum in a resonable time. The data are then processed by the program MAUD for Rietveld Texture and Stress Analysis to obtain the ODF, the macrostress tensor and all information about crystal structure and microstructure of the phases present in the layered film structure. The method take into account the thickness of the films and the sequence of the layers as well as the phase fraction of the phases inside each layer. For the texture analysis inside the Rietveld, different approaches are availables, from the simple March-Dollase formula to the conventional WIMV, up to a special version of WIMV for very sharp textures currently of interest in the electronic/ferroelectric field. This entire system has been tested and proved successfully for different cases and some analysis examples are presented to show the powerfull combination of all these methodologies with a dedicated instrument quantitatively to analyse films of interest for the industry of ferroelectric and electronic appliances.*