Combined texture-structure-microstructure-phase analysis of multi-phased bulks and thin films using x-ray and neutron diffraction: some case studies, Bi2223, $Ca_3Co_4O_9$, PCT and nano-Si.

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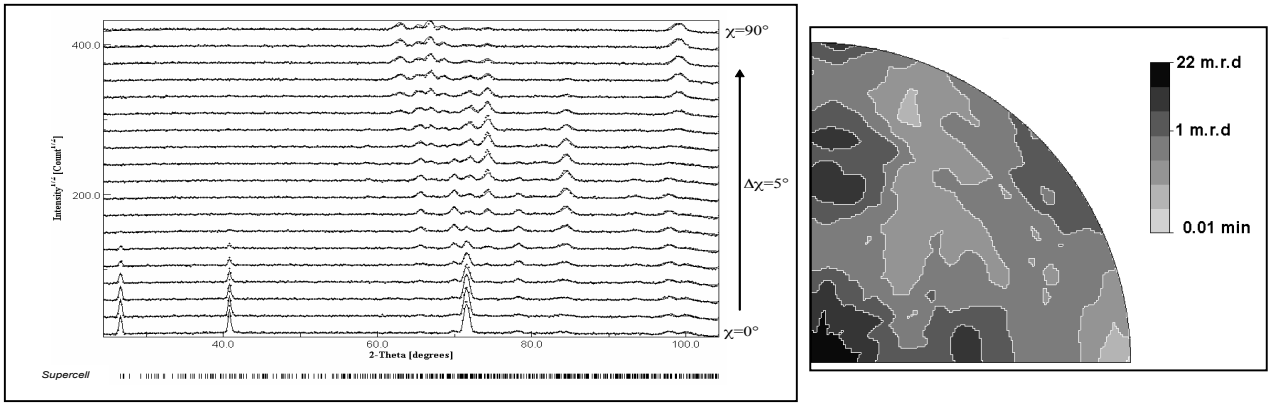
The controlled development of texture in polycrystalline materials appears to be more and more essential in ceramic and thin film processing, since potential applications require materials with macroscopic properties comparable to the intrinsic anisotropic tensors of the crystal structures. Texture analysis is consequently recognized as a really important tool in the characterisation of oriented samples. However, a quantitative texture analysis of these materials is usually not a simple task. In most cases, the diffraction spectra are very complex with many partially or fully overlapping diffraction peaks and with several crystallographic phases. The X-ray defocusing effect limits also the pole figure coverage and obstructs the analysis. To overcome this problem, the combination of Rietveld, WIMV and Popa approaches, for instance as implemented in the MAUD software (Materials Analysis Using Diffraction), permits a comprehensive new approach to crystal structure-texture-microstructure-phase-stress analysis. In this study, we report the application of this method to different ceramic materials with different textures, crystallographic structures, microstructures …. Orientation distributions (OD) were determined from neutron and X-ray diffraction using curved position-sensitive detectors (D1B (ILL) & INEL CPS 120). We demonstrate here the efficiency and reliability of iterative combination of algorithms for structure-phase determination (Rietveld), microstucture (Popa) and OD calculation (WIMV) in the case of oxide ceramic and thin film materials, and of silicon nanostructured films.



Example of combined analysis fit for the Co349 modulated structure of an oriented ceramic and corresponding inverse pole figure for the pressure direction