Comparison of different texture models in Rietveld analysis of diffraction data

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Abstract

The texture analysis by diffraction of X-rays or neutrons involves the measurement of either pole figures of some reflections or the collection of diffraction patterns at different sample orientations. The latter can be seen as a measurement of inverse pole figures and a suitable method to analyse this type of data is the Rietveld method. Its use increased in recent times due to the development of instrumentation based on line or large aerea detectors that most of the time don't produce regular complete or incomplete pole figures. Another reason is the presence of more phases and/or low symmetry compounds with high peaks overlapping in the diffraction pattern that make the pole figure measurement unsuitable.
The data coming from this kind of instruments is most of the time not uniform in term of texture space coverage and completeness. This lead to some problems when analysing the Orientation Distribution Function (ODF) and most of the time the proper method of inversion (from pole figure data to ODF) should be used. A certain number of inversion algorithms have been implemented in the Rietveld software package MAUD, from functional methods (spherical harmonics, standard functions, exponential harmonics) to discrete ones (WIMV, EWIMV). We have now added in MAUD the possibility to use also external packages and one of the first is MTEX that can also be used for the texture analysis inside the Rietveld refinement cycle.
We will present and analyse different examples to show what are the possibilities and limitations of the different texture inversion algorithms inside the Rietveld analysis. There is no one method that is better overall respect to the others. Different kind of data and problems may require the correct choice of algorithm in order to succeed and obtain a reliable and complete ODF.

Keywords: Texture analysis, diffraction, Rietveld method, MAUD, WIMV, spherical harmonics, MTEX

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