Geophysical Research Abstracts, Vol. 7, 08430, 2005
SRef-ID: 1607-7962/gra/EGU05-A-08430

Quantitative texture analysis of isostatically-pressed molybdite powders by means of neutron diffraction

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The modelling and/or correcting of preferred crystallographic orientation (PO), $i.e.$ texture in crystalline materials is of critical importance in powder diffraction analysis: for structure refinements and in the determination of bulk descriptors such as phase composition. The comparative evaluation of the March model and the generalized spherical harmonic (GSH) description for PO using Rietveld analyses of Debye-Scherrer neutron powder diffractometer (ND) data and BraggBrentano X-ray powder diffractometer (XRD) data have been recently conducted [1,2]. Extensive measurements were performed on suites of uniaxially pressed powders for both diluted (50% by weight silica gel) and undiluted (100%) molybdite (MoO_3) and calcite ($CaCO_3$) for which the compression was systematically varied. The results showed that the GSH description provides better crystallographic R_{WP}-factors and goodness-of-fit indeces for molybdite and calcite powders than the March model. Therefore, the GSH approach should be used for correction of the PO in XRD analysis, for both crystal structure refinement and phase composition analysis. Also, the ND-derived POs appear to describe the bulk material in uniaxially pressed material correctly, whereas the XRD Pos are heavily influenced by the pressing procedure.

The main problem of the GSH description for texture analysis arises from the fact that the harmonic expansion degree is limited by the finite number of measured points over the pole figure space and also by the presence of possible ghosts (artifacts in the ODF), particularly in cases of low crystal and sample symmetries and for sharp textures. To overcome this problem, the WIMV method was used to determine the best ODF reproducing the pole-figure texture values by assuming some properties of what is in essence the odd-order harmonic terms that cannot be determined from the diffraction experiment. Thus it is more efficient and reliable to determine the ODF using Rietveld refinement with the WIMV method than the GSH description [3]. We will describe the WIMV method on how to extract the ODF description directly from a simultaneous refinement with 1368 whole neutron powder diffraction patterns of isostatically pressed molybdite powders at 300, 350 and 400 Mpa held in a variety of orientations in the ILL D1B texture goniometer.

References

[1] Sitepu (2002). J. Appl. Cryst. 35, 274-277.
[2] Sitepu H, O'Connor, B.H. and Li, D.Y. (2005). J. Appl. Cryst. 38, 158-167.
[3] Sitepu, H., O'Connor, B.H., A. Benmarouane, Hansen, T. and Ritter, C. and Brockmeier, H.-G. (2004). Physica B. 350, e573-e576.