

**s10.m2.o1** Investigating Nanocrystalline Materials with Diffraction Line Profile Analysis. D. Louër, *Laboratoire de Chimie du Solide et Inorganique Moléculaire (UMR CNRS 6511), Université de Rennes I, 35042 Rennes cedex, France.*

Keywords: noncrystalline materials, line broadening analysis, profile fitting.

X-ray diffraction line broadening is traditionally used for the characterization of nanocrystalline materials. The analysis is based on the integral breadth of the diffraction lines or on the representation of line profiles by Fourier series. Improved algorithms and software for the decomposition of powder diffraction patterns into individual Bragg reflections and the availability of good quality diffraction data from high resolution instruments have resulted in a renewed interest in line broadening analysis<sup>1</sup>. The major benefit of profile fitting techniques is the extension of the analysis to a greater number of Bragg reflections, provided that the degree of line overlap is not too severe. Consequently, a more detailed description of the microstructural properties in terms of size and shape of coherently diffracting domains and structure imperfections can be expected from the analysis. Moreover, with the use of model-based methods a wealth of (3-dimensional) information has been reported in a few examples. The integral breadth procedure, considerably improved by the introduction of the Voigt function<sup>2</sup>, has the advantage of speed and convenience over the elaborate Fourier analysis, but only the last approach can give information on crystallite size distributions. The two approaches are nowadays integrated in profile fitting approaches<sup>3,4</sup>.

The use of these modern approaches will be illustrated by a number of recent applications to nanocrystalline materials, e.g. Ni(OH)<sub>2</sub>, AlN, CeO<sub>2</sub> and ZnO obtained from the thermal decomposition of various precursors<sup>5</sup>. The microstructural properties discussed for these examples include crystallite size and shape and structure mistakes. Examples of strain-free powders will be presented. In particular, the unique characterization of the size and shape of crystallites from X-ray diffraction line broadening will be emphasized through the study of the initial stage of crystallite growths. It will be shown that new concepts on the microstructural dependence of nanocrystalline oxides with the chemical nature of the precursor have been derived from thorough line broadening analyses.

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**s10.m2.o2** Investigation of mesoscale microstructures with diffraction techniques. P. Klimanek. *Freiberg University of Mining and Technology, Institute of Physical Metallurgy, 09 596 Freiberg/Sa., Germany*

Keywords: powder diffraction, microstructure analysis.

Processes of materials science and technology give frequently rise to the formation of complicated, locally inhomogeneous defect structures (e.g. dense dislocation clusters and walls, sub-boundaries, microtwins, deformation and/or shear bands etc.), whose experimental investigation and, in particular, quantitative characterisation is difficult. It requires the introduction of suitable microstructure models as well as the elaboration of a methodology of structure analysis which allows the detection of substructure evolution on different length scales and also the occurrence of scale transitions. In this connection two problems have to be solved:

- the identification and characterisation of individual lattice defects and/or special defect arrangements and
- the quantitative estimation of microstructure characteristics as, for instance, defect densities, lattice misorientations, dislocation-cell or subgrain sizes etc.

The lecture is concerned with the quantitative characterisation of mesoscale microstructures by means of diffraction techniques (i.e. analysis of X-ray or neutron diffraction – peak broadening, TEM, and application of EBSP for microtexture studies). In order to illustrate the potential of the diffraction analysis three problems are considered:

- (1) X - ray and TEM analysis of the dislocation content in plastically deformed metallic materials [1,2],
- (2) quantitative analysis of shear banding in cold-rolled  $\alpha$ -brass by means of X-ray and EBSP analysis [3,4], and
- (3) TEM identification of disclinations in cold – worked metals [5,6].

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