Whole Powder Pattern Fitting Methods focused on Nanocrystalline Materials

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The methods of diffraction data analysis from polycrystalline materials have reached maturity for samples at the micrometer size scale. Whole Powder Pattern Fitting (WPPF) techniques have become more and more efficient to meet the complex task of structural and microstructural sample characterization. However, when the particle size reduces to few nanometers, special size-related features occur and specifically tuned methods of analysis are needed to extract relevant information, like size, strain and structure concentrations, from powder diffraction patterns. The atoms on the surface may play the major role in very small nanoparticles (NPs), determining important strain contributions and size-related lattice parameters. In the most complex cases of some noble metal, non-crystallographic structures (icosahedron and decahedron) can occur.

WPPF methods will be presented to deal with powder diffraction data of randomly oriented nanocrystals.

Two different approaches will be described:

1) a dedicated approach dealing with noble metal fcc NPs, making use of the Debye function to calculate the diffracted intensity and based on a full-Newton least-squares techniques [1]; 2) a based-shaped convolution method dealing with spherical NPs with lognormal size distribution [2]. Applications will be shown in both cases.

[1] Cervellino A., Giannini C., Guagliardi A., *J. Appl. Cryst.*, 2003, **36**, 1148.
[2] Cervellino A, Giannini C., Guagliardi A., Ladisa M., *Phys. Rev B*, **2005**, *submitted*.

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