Deconvolution of X-ray Diffraction Profile by using the Regularization Technique

Vladyslav Piskarov, Joachim Wagner, Rolf Hempelmann, *Saarland University, Physical Chemistry, Germany.* E-mail: v.piskarov@mx.uni-saarland.de

The deconvolution of the instrumental function in X-Ray diffraction profile analysis is a basic step in order to obtain reliable results on the microstructure (crystallite size, lattice microstrain, *etc.*) and is a typical example of ill-posed inverse problems. The implementation of an eigen function method with different regularization techniques is investigated and a simple regularization algorithm is proposed.

A simulation of an instrumental-broadened profile superimposed with random noise and background signals is used to investigate the reliability and efficiency of the proposed technique. For the simulation an experimentally defined instrument function based on an accurate mathematical model for Cu emission profile, the geometry of the diffractometer and the physical properties of the specimen are used. The parameters for this instrumental function are obtained by least squares fitting of experimental data sets resulting from the reference materials LaB_6 and Al_2O_3.

Compared to established algorithms, the proposed route is faster and more reliable in terms of stability, especially in the case of large experimental noise. The evaluation of experimental diffraction data of nanocrystalline gold with respect to grain size and microstrain and the comparison with standard evaluation technique is done.

[1] Kurashov V.N., Kurashov A.V., Piskarev V.L., *Proc. SPIE*, 1997, **3317**, 36.
[2] Ida T., Toraya H., *J. Appl. Cryst.,* 2002, **35**, 58. [3] Sanchez-Bajo F., Cumbrera F.L., *J. Appl. Cryst.,* 2000, **33**, 259.
Keywords: powder diffraction, profile analysis, regularization