Anisotropic microstrain-like diffraction-line broadening due to composition variations and other origins, Andreas Leineweber* and Eric Jan Mittemeijer, *Max Planck Institute for Metals Research, Germany*. E-mail: a.leineweber@mf.mpg.de

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In the course of fitting procedures considering complete powder diffraction profiles (e.g. Rietveld refinement) often the problem arises to describe anisotropic diffraction-line broadening appropriately. Sometimes, purely empirical approaches are adopted, e.g. if the line-profile is not of interest itself. But more frequently 'size' and 'microstrain' broadening contributions and their anisotropies are dealt with separately. Often it is desired to extract the physical information supplied by the anisotropic line-broadening. For that purpose it is necessary to incorporate into the fit routines the anisotropies of 'size' and 'microstrain' broadening in a way compatible with their physical origins. In many cases of anisotropic microstrain broadening the width of a reflection on the 2θ scale varies for a certain direction of the diffraction vector with $\tan\theta_{hkl}$:

$$B_{hkl} = A(hkl) \times \tan\theta_{hkl} \tag{1}$$

where B_{hkl} quantifies the width of the reflection *hkl* (e.g. the full width at half maximum) and $A(hkl)$ is an anisotropy factor, which varies with the direction of the diffraction vector, but not with θ_{hkl}. Assuming no specific physical origin for the microstrains and their probability density function a phenomenological expression for the anisotropy factor was derived on the basis of statistical considerations [1,2]:

$$A(hkl) = d_{hkl}^2 \times \sqrt{\sum_{H+K+L=4} S_{HKL} h^H k^K l^L} \tag{2}$$

where d_{hkl} corresponds to the average *d*-spacing of the reflection *hkl*, and S_{HKL} are fit parameters with restrictions imposed due to crystal symmetry, and H,K,L are exponents for h,k,l. It can be shown that certain physical origins of microstrain which are caused by local variations of a single scalar variable ξ (e.g. composition, temperature ...) [3] lead to an anisotropy factor of

$$A(hkl) = d_{hkl}^2 \times \left| \sum_{H+K+L=2} D_{HKL} h^H k^K l^L \right| \tag{3}$$

with fitting parameters D_{HKL} which have again restrictions imposed due to crystal symmetry, and which are related to the width of the distribution of ξ and the derivatives of the components of the reciprocal metrical tensor with respect to ξ. Eq. (3) constitutes a special case of Eq. (2), and thus the physical origins of line broadening leading to Eq. (3) can also be fitted using Eq. (2), however with redundant fitting parameters. Practical examples for both symmetric and asymmetric anisotropic diffraction-line broadening according to Eq. (3) will be presented (in particular due to composition variations), as well as model cases for which specific physical origins of microstrain line-broadening lead to anisotropies compatible with Eq. (2) and/or (3). Furthermore, possible advantageous alternative formulations of Eqs. (2-3) will be discussed.

[1] Popa, N.C., *J. Appl. Crystallogr.* **31** (1998) 176.
[2] Stephens, P.W., *J. Appl. Crystallogr.* **32** (1999) 281.
[3] Leineweber, A. & Mittemeijer, E.J., *J. Appl. Crystallogr.* **37** (2004) 123.