Comments on "A Geometrical Correction for Precise Lattice Constant Determination" by Bradaczek, Leps, and Uebach

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The expression for diffracted X-ray intensity as a function of absorption and asymmetry derived by Bradaczek et al. [1] is already contained in the general integrated-intensity formula. It is interpreted incorrectly by these authors with regard to the correction of precision lattice constants.

In a recent paper Bradaczek, Leps, and Uebach [1] have derived the expression

$$E(\beta) \sim V(\beta)\,(1 + \tan\beta \cdot \cot\Theta)/2\,\mu$$

for the distribution of diffracted X-ray intensity E as a function of the angle position β of the crystal ($V(\beta)$ undistorted intensity distribution function, Θ diffraction angle, μ linear absorption coefficient). It is to be pointed out that this expression can be taken from the formula for the integrated intensity of a mosaic crystal in the Bragg case (cf. e.g. [2]) which is proportional to $[\mu\,(1 + |b|)]^{-1}$, where the asymmetry factor b is given by

$$b = \sin(\beta - \Theta)/\sin(\beta + \Theta)$$

and therefore

$$(1 + |b|)^{-1} = 1 + \tan\beta \cdot \cot\Theta\,,$$

β being the angle between crystal surface and reflecting planes (β positive if the reflected beam is broadened).

The "geometrical factor" $1 + \tan\beta \cdot \cot\Theta$ depends on two angle variables, β and Θ. Both dependences may lead to a distortion of the measured intensity distribution curve and hence to a peak displacement. The authors [1] have considered only the β dependence of the above relation and give the following expression for the peak displacement β'' of a curve $E(\beta)$ with half width w:

$$\beta'' = k\,w^2 \cot\Theta\,(1 + \tan^2\beta)\,(1 + \tan\beta \cdot \cot\Theta)^{-1}\,,$$

$$\beta'' = k\,w^2 \cot\Theta \quad \text{for} \quad \beta \ll \Theta$$

(with an obvious misprint, β'' instead of β, in their formula (9)). They conclude that the expression would hold for spectral and orientation distributions ("mosaicity"). It is valid however only for intensity distributions measured at constant angle Θ, i.e., for orientation distributions. To describe the corresponding peak displacement of a spectral distribution curve (Θ dependence) an analogous relation for the peak displacement Θ'' can be obtained:

$$\Theta'' = k\,w^2 \tan\beta\,(1 + \cot^2\Theta)\,(1 + \tan\beta \cdot \cot\Theta)^{-1}\,,$$

$$\Theta'' \to 0 \quad \text{for} \quad \beta \to 0\,.$$

The peak displacement of a measured intensity distribution curve (rocking curve) results from the convolution of both spectral and orientation distributions, each of them distorted by the corresponding angle depending factors.

The factor k in the above relations can not generally be assumed to equal unity as did the authors [1]. It has the value 0.125 for Cauchy and 0.180 for Gaussian response curves, respectively, i.e., the peak displacement by the geometrical factor is essentially smaller than claimed by these authors.

With the exception of paper [1] only the profile distortion by the Lorentz-polarisation factor has been considered in the lattice constant determination of single crystals up to now. The geometrical factor is another correction term to be applied. But following the interpretation by the authors [1], wrong values of it may be obtained. Thus the peak displacement equals zero for symmetrical reflections of perfect crystals. The factor is important essentially for strongly asymmetrical reflections (β being large). It must be pointed out, however, that still other angle dependent factors in the complete intensity formula may distort the intensity distribution curves. All the factors must be considered in order to describe the profile distortions exactly and to calculate the true peak displacements in high-

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precision measurements. Furthermore, for nearly perfect crystals the corresponding intensity formula as given by the dynamic diffraction theory [2] should be more relevant, which contains the angle dependent factors in different and more complicated form so that in general other values for the peak displacement result. The whole problem will be discussed elsewhere in more detail [3].

[1] H. Bradaczek, B. Leps, and W. Uebach, Z. Naturforsch. **37 a,** 448 (1982).
[2] P. B. Hirsch and G. N. Ramachandran, Acta Cryst. **3,** 187 (1950).
[3] H. Berger, to be published.