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# Comments on *Extinction-corrected mean thickness and integral width used in the program UMWEG98* by Rossmanith (2000)

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Comments are made on a paper by E. Rossmanith [*J. Appl. Cryst.* (2000), **33**, 330–333] concerning the use of asymptotic expressions for the extinction-corrected mean thickness.

In a recently published paper, Rossmanith (2000) accounts for expressions for the extinction-corrected mean thickness used in the program *UMWEG*98. A comparison with already existing models for the primary-extinction factor in perfect crystal spheres is also presented.

In particular, Rossmanith's kinematical formula for the extinction-corrected mean thickness as a function of the mean crystal thickness is compared with results based on asymptotic expressions for the primary-extinction factor, $y_p$, found by the present authors (Larsen & Thorkildsen, 1998) for the limiting cases $\theta_{oh} \to 0$ (pure Laue case) and $\theta_{oh} \to \pi/2$ (pure Bragg case). Here $\theta_{oh}$ denotes the Bragg angle. Rossmanith questions the result for the Laue case because it 'does not agree with the Al Haddad & Becker (1990) primary-extinction correction'. This is owing to a printing error in the expression for the asymptotic primary-extinction factor, equation (8), of Larsen & Thorkildsen (1998). The correct expression is

$$y_p(x, \theta_{oh} \to 0) \simeq (3/8x)\{1 + [\pi/(2\pi x)^{3/2}]\cos(4x - 5\pi/4) + 1/16x^2\}, \quad (1)$$

where $x = R/\Lambda_{oh}$, the ratio between the radius of the sphere and the extinction distance. The sign error in the oscillating term of the erroneous version of equation (1) is equivalent to a phase shift of $\pi$, as is evident from Fig. 1 of Rossmanith (2000). We acknowledge Rossmanith for drawing this to attention.

When it comes to the Bragg case, Rossmanith seems to question the result [equation (7) of Larsen & Thorkildsen (1998)] because it 'exceeds the kinematical upper limit'. This statement is somewhat confusing owing to the fact that our results are based on *dynamical theory* as formulated by Takagi (1962, 1969). The equivalence between the Takagi theory and the fundamental theory of dynamical diffraction has been established and demonstrated (Thorkildsen & Larsen, 1999). In the limits $\theta_{oh} \to \{0, \pi/2\}$, the diffraction geometry is quasi one-dimensional. For these two cases, the expression for the primary-extinction factor for a finite convex crystal of general shape, bathed in the incident beam, becomes

$$y_p^{(i)} = (1/V_{\rm cry}) \int_{A_\perp} {\rm d}u\,{\rm d}v\, t_{||}(u, v)\, y_p^{({\rm plate},i)}(x = t_{||}/\Lambda_{oh}) \quad (i = {\rm Laue,\ Bragg}) \quad (2)$$

where $A_\perp$ denotes the cross section of the crystal projected onto a plane $(u, v)$ normal to the direction of the incident/diffracted beam. The function $t_{||}(u, v)$ represents the crystal dimension along the incident beam. $V_{\rm cry}$ is the volume of the crystal. Applying equation (2) to a spherical crystal in the Bragg case gives equation (4) from (3) in the paper by Larsen & Thorkildsen (1998).

In our opinion, corrections for primary extinction, which is a dynamical feature, should be formally handled by a dynamical diffraction theory, rather than a kinematical approach.

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# Response to Larsen & Thorkildsen's comments on *Extinction-corrected mean thickness and integrated width used in the program UMWEG98*

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Some additional comments are made concerning the asymptotic expressions for the primary-extinction factor for a perfect spherical crystal.

In Fig. 1 of the paper by Rossmanith (2000), the ratio of the extinction-corrected mean thickness to the extinction length, $t_{\rm ext}/\Lambda$, of a perfect crystal sphere (solid lines therein) is compared with the results for the semi-infinite plane parallel plate (dotted lines). The asymptotic expressions given by Larsen & Thorkildsen (1998) for perfect crystal spheres, represented as dashed lines in Fig. 1 of Rossmanith (2000), were questioned by the author.

It is pointed out by Larsen & Thorkildsen (2000) that for the 'Laue case', the disagreement between their asymptotic expression and the Laue approximation solution is owing to a sign error in their original paper (Larsen & Thorkildsen, 1998). For large values of the ratio of mean thickness to extinction length, $\bar{t}/\Lambda$, the corrected expression given as equation (1) in the comments by Larsen & Thorkildsen (2000) now indeed agrees with the solid line 2 in Fig. 1 of Rossmanith (2000), which was derived using the Takagi theory.

For the 'Bragg case', on the other hand, the solid line 1 in Fig. 1 represents a kinematical upper limit for the $t_{\rm ext}/\Lambda$ ratio of a perfect crystal sphere totally bathed in the incident X-ray beam (the cross section of the incident beam is larger than the cross section of the sample for all sample diameters under consideration!), whereas the dotted curve 3 represents the dynamical solution for the symmetrical Bragg case of a semi-infinite plane parallel plate (the cross section of the incident beam is small compared to the infinite surface of the sample).

According Larsen & Thorkildsen (2000), equation (2) given in their comments can be used for the calculation of $y_p$ ($\theta \to \pi/2$) for a finite convex crystal of general shape bathed in the incident beam. It can easily be shown that by applying equation (2) to a needle-shaped crystal oriented parallel to the incident beam, the result

$$y_p^{\rm needle} = y_p^{\rm plate} \qquad (1)$$

is obtained, where $y_p^{\rm needle}$ is the extinction factor for the needle bathed in the incident beam and $y_p^{\rm plate}$ is the extinction factor for the semi-infinite plane parallel plate. Having in mind the definition of the extinction factor [Rossmanith, 2000, equation (12) therein], it follows that equation (1) and consequently equation (2) given in the comments of Larsen & Thorkildsen (2000) are correct only if identical intensity profiles are obtained during the $\omega$ scan for both the needle as well as the semi-infinite plane parallel plate. But, in view of the very different experimental conditions, it seems improbable that the profiles are identical, *whatever theory is used*, *i.e.* it should be expected that, because of the well known shape dependence of intensity profiles, they will differ outside the region of total reflection.

Similar arguments hold for all other convex-shaped crystals, which can be considered as made up of needles. As a consequence, neither equation (2) of Larsen & Thorkildsen (2000) nor the expressions given earlier by Larsen & Thorkildsen (1998) are exact (analytical) expressions for a perfect spherical crystal in the limit $\theta \to \pi/2$.

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