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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 ($\theta \rightarrow \pi/2$) 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 ω 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 $\theta \rightarrow \pi/2$.

References

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