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On the normalization of the resolution function for three-axis spectrometers.

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Abstract

It is demonstrated that a recent publication by Tindle [*Acta Cryst.* (1984), A**40**, 103–107] on the normalization of resolution functions for a three-axis spectrometer is in error. The complete normalization factor derived by this author is the same as that obtained in previous works. However, Tindle's interpretation of data for the peak reflectivity of mosaic crystals is incorrect. This error leads him to contradict erroneously previously published results.

The following considerations refer to the paper *A new instrumental factor in triple-axis spectrometry and Bragg reflectivity measurement* by Graham L. Tindle (1984). Tindle argues that the normalization given by Dorner (1972) is 'fallacious'. To clarify the situation, we concentrate on two points.

The first concerns the formula for the resolution (or transmission) of the monochromator for a three-axis spectrometer. In the present context it is not necessary to repeat the whole formula. We will consider only two relevant factors: the normalization P_{0M} and the peak reflectivity of the monochromator crystal $P_M(k_I)$. Here k_I is the most probable wavevector of the reflected neutrons, and the factors P_{0M} and $P_M(k_I)$ always appear as a product. In the notation of Dorner this product is given by

$$P_{0M}P_M(k_I) = \frac{\beta_0}{(4\eta_M'^2 \sin^2\theta_M + \beta_0^2)^{1/2}} \times \frac{F_f(k_I)}{F_i(k_I)}. \quad (1a)$$

In Tindle's paper the product is given by

$$P_{0M}^T P_M^T(k_I) = \frac{\beta_0}{(4\eta_M'^2 \sin^2\theta_M + \beta_0^2)^{1/2}} \times \frac{F_f(k_I)}{F_i(k_I)} \times \frac{1}{(2\pi)^{1/2}\eta_M}. \quad (1b)$$

Here, β_0 is the vertical divergence of the beam before the monochromator, θ_M the Bragg angle, η_M' and η_M the vertical and horizontal mosaic widths, F_f and F_i will be explained below.

The factor $[(2\pi)^{1/2}\eta_M]^{-1}$ in (1*b*) is erroneous, because the transmission function should not be normalized with respect to η_M. In fact the transmission depends on η_M: for η_M small compared to horizontal collimations, the transmitted flux increases linearly with η_M and for large η_M the transmission tends to an asymptotic value defined by the horizontal collimations.

Besides this error (Tindle does not explicitly mention this difference) *the formulae* (1*a*) *and* (1*b*) *are identical and thus yield the same resolution functions.*

The alleged difference between Tindle's result and that of Dorner concerns the definition of the peak reflectivity $P_M(k_I)$, point two of the present paper. The most commonly used notation reads

$$P_M(k_I) = \frac{F_f(k_I)}{F_i(k_I)}, \quad (2)$$

where $F_f(k_I)$ is the maximum flux reflected out of a well defined incoming beam with flux $F_i(k_I)$. Obviously, $P_M(k_I)$ can never become larger than one!

The definition of the peak reflectivity, which is a crystal property, and its experimental determination can be found in the literature (Dorner, 1971; Shapiro & Chesser, 1972; Boeuf, Gobert & Rustichelli, 1975; Freund, 1975; Freund & Forsyth, 1979; Freund, 1984). Here a well defined beam means that instrumental effects can be neglected with respect to the diffraction properties of the monochromator. This is equivalent to assuming a monochromatic and parallel incident neutron beam. On the other hand, the detector has to accept a large horizontal and vertical divergence. These definitions of $F_f(k_I)$ and $F_i(k_I)$ are the same as those given by Tindle.

Generally, $P_M(k_I)$ decreases with increasing k_I, which is due to both a decrease of the scattering power per unit length and an increase of the attenuation factor by inelastic scattering (Freund, 1983). A particular case in this context is pyrolytic graphite (PG). The reflectivity of PG has been investigated by Shapiro & Chesser (1972), Chesser & Axe (1973), Dorner & Kollmar (1974) and Freund (1984). The decrease of reflectivity is enhanced in PG by unavoidable and increasing parasitic Bragg scattering, which arises as k_I increases, and it depends on crystal quality, being more pronounced for large mosaic width. This behavior of PG is well understood by experienced neutron scatterers as an *intrinsic* feature of PG.

This is in complete disagreement with Tindle's suggestion 'that the variation should be regarded as a consequence of the process of measurement and not indicative of any intrinsic crystal property'. He defines the reflectivity P_M^T as

$$P_M^T(k_I) = \frac{1}{2\eta_M' \sin\theta_M} \times \frac{F_f(k_I)}{F_i(k_I)}, \quad (3)$$

a function which diverges for small Bragg angles. With this absurd definition he replots reflectivity data for PG by Chesser & Axe (1973) and obtains a k_I-independent P_M^T. This is certainly a fortuitous result for the particular specimen of PG.

In parallel with the new definition of P_M^T, Tindle endorses without criticism the normalization factor P_{0M}^T of Cooper & Nathans (1967),

$$P_{0M}^T = \left(\frac{1}{\beta_0^2} + \frac{1}{4\nu_M'^2 \sin^2\theta_M}\right)^{-1/2}, \quad (4)$$

which is missing the factor $(2\eta_M' \sin\theta_M)^{-1}$ as has been shown by Dorner (1972).

By transferring the factor $(2\eta_M' \sin\theta_M)$ from the normalization to the reflectivity, as Tindle does, *the overall resolution function remains unchanged.* But this

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manipulation leads him to incorrect arguments about the normalization of the instrumental resolution function.

In conclusion we contradict Tindle's statements about the normalization; it is clear that the formulation presented by Dorner (1972) is correct.

In formulating this short note I benefitted from profound discussions with my colleagues A. Freund and R. Pynn.

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Erratum

Acta Cryst. (1984). **A40**, 723

Graphic representation and nomenclature of the four-dimensional crystal classes. III. A notation for the crystal classes: erratum.

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Abstract

A printers error is corrected in Table 2 on page 407 of Whittaker [*Acta Cryst.* (1984), A**40**, 404–407]. The correct lines are

Family XVII

$wx/yzw[0111]^* w[0110]/z[0\bar{1}10]:wx[0110]$.

All information is given in the *Abstract*.

International Union of Crystallography

Acta Cryst. (1984). **A40**, 723–724

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