SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1983). A**39**, 818

Phase relationships in the chiral space groups $P4_1$ and $P4_3$. Correction of an error in *International Tables for X-ray Crystallography*, Vol. I.

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Abstract

Corrections are given to phase relationships for space groups $P4_1$ and $P4_3$ listed in *International Tables for X-ray Crystallography* [Vol. I. (1969). Birmingham: Kynoch Press].

The entries $l = 4n + 1$ and $l = 4n + 3$ to the phase relationships between $\alpha(\bar{h}kl)$ and $\alpha(khl)$ in space groups $P4_1$ and $P4_3$ listed in *International Tables for X-ray Crystallography* (1969) should be interchanged. This leads to the following phase relations:

$$\alpha(\bar{h}kl) = \pi + \alpha(h\bar{k}l) = \tfrac{1}{2}\pi + \alpha(khl) \quad [P4_1: l = 4n + 1; P4_3: l = 4n + 3]$$

$$\alpha(\bar{h}kl) = \pi + \alpha(h\bar{k}l) = \tfrac{3}{2}\pi + \alpha(khl) \quad [P4_1: l = 4n + 3; P4_3: l = 4n + 1].$$

The same corrections should be made in the paper on the discrimination between two enantiomorphously related space groups (Kroon, Pontenagel, Krabbendam & Peerdeman, 1982). They do not affect, however, the validity of the procedure suggested in that article.

References

International Tables for X-ray Crystallography (1969). Vol. I, 3rd ed., pp. 415–416, 417. Birmingham: Kynoch Press.

KROON, J., PONTENAGEL, W. M. G. F., KRABBENDAM, H. & PEERDEMAN, A. F. (1982). *Acta Cryst.* A**38**, 170.

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An alternative approach to the quantitative determination of grain-size distribution in X-ray diffraction? A comment.

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Abstract

The paper by Zhao, Lu & Lagally [*Acta Cryst.* (1982), A**38**, 800–802] is commented on and compared with a previous paper by Bertaut [*Acta Cryst.* (1950), **3**, 14–18].

In a recent publication with the title above, the authors (Zhao, Lu & Lagally 1982, abbreviated ZLL) quote my paper (in French, Bertaut, 1950) which relates the distribution of particle size m to the profile of Debye–Scherrer lines according to equation (22).

$$\frac{\partial^2 t(m)}{\partial m^2} = g(m). \qquad (22)$$

Here $g(m)$ is the distribution function of size m and $t(m)$ is the Fourier transform of the observed intensity profile $I(X)$. The paper also states (Bertaut, 1950) that the size distribution $g(m)$ can be obtained directly by Fourier transforming $X^2I(X)$, that is, the intensity multiplied by X^2.

ZLL rediscover this equivalence, after the lecture in Guinier's fine book (Guinier, 1963), call it an 'alternative approach' and obtain $g(m)$ in model calculations using Gaussian and Lorentzian functions $I(X)$.

Let us translate here the French text following (22) in view of another problem which in our mind is most important.

'One may ask the question if it is not possible to replace an always uncertain double differentiation in m space by a simpler operation in X space on $I(X)$, prior to its Fourier transformation.

Indeed the theory of Fourier integrals establishes the following correspondences

$$\begin{aligned} I(X) &\rightarrow t(m) \\ 2\pi i X I(X) &\rightarrow \frac{\partial t(m)}{\partial m} \\ -4\pi^2 X^2 I(X) &\rightarrow \frac{\partial^2 t(m)}{\partial m^2}. \end{aligned} \qquad (23)$$

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