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.


An erratum: Effective particle size as determined by the initial slope of the Fourier-coefficient-against-order curve for X-ray diffraction line profiles.

By G. B. MITRA and B. K. MATHUR, Department of Physics, Indian Institute of Technology, Kharagpur-721302, India

(Received 15 January 1976; accepted 8 March 1976)

Certain errors in a previous publication by the present authors [Mitra & Mathur (1975), J. Appl. Cryst. 8, 543-544] on the interpretation of the initial slope of the Fourier-coefficient-against-order curve for X-ray diffraction line profiles have been pointed out and corrected. The effect of Cauchy strain distribution on determination of particle size has also been investigated.

In a recent publication by the present authors [Mitra & Mathur (1975)] the problem of interpretation of the initial slope of the Fourier-coefficient-against-order curve for X-ray diffraction line profiles has been investigated. We have, however, detected some mistakes in the calculations which lead to considerable modification of the conclusions arrived at. By an unfortunate oversight, \( \frac{dA'(n)}{dn} \) has been equated to \( n\varphi^{n-1} \), while it should be \( \varphi^{n} \log \varphi, \) since \( A'(n) = \varphi^{n} \) according to equation (6) of Mitra & Mathur (1975). Hence equation (7) should be modified to:

\[
A'(n)\Big|_{n=0} = 1 \quad \text{and} \quad \frac{dA'(n)}{dn} \Big|_{n=0} = \log_{e} \varphi.
\]

This would lead to

\[
\frac{d}{dn} \left( \frac{A(n)}{A(0)} \right) \Big|_{n=0} = -\frac{1}{\langle N \rangle} + \log_{e} \varphi.
\]

If the strain profile is of Cauchy type,

\[
A'(n) = \exp \left( -\frac{\pi^2}{\sigma} \ln \langle S^2 \rangle \right) \quad \text{and} \quad \frac{dA'(n)}{dn} \Big|_{n=0} = -\frac{\pi^2}{\sigma} \langle S^2 \rangle,
\]

where \( l \) is the reflexion type, \( S \) is the r.m.s. strain and \( \sigma \) is the cut-off strain where Hooke's law becomes invalid. Thus for the case of the Cauchy profile for strain and in the presence of faultings,

\[
\frac{d}{dn} \left( \frac{A(n)}{A(0)} \right) \Big|_{n=0} = -\frac{1}{\langle N \rangle} - \frac{\pi^2}{\sigma} \langle S^2 \rangle + \log_{e} \varphi,
\]

while for the Gaussian profile,

\[
\frac{d}{dn} \left( \frac{A(n)}{A(0)} \right) \Big|_{n=0} = -\frac{1}{\langle N \rangle} + \log_{e} \varphi.
\]

For f.c.c. and b.c.c. systems \( \log_{e} \varphi \), according to Table 1 of Mitra & Mathur (1975), is given by (after necessary steps):

\[
\log_{e} \varphi = \frac{1}{2} \log_{e} (1 - 3\alpha - 2\beta),
\]

which, in the first approximation, after expanding for \( \log_{e} (1 - x) \) like terms, becomes

\[
\log_{e} \varphi = -\frac{1}{2} (3\alpha + 2\beta) = -(1.5\alpha + \beta),
\]

as derived by Warren (1959). Similar agreement with Warren's (1959) results is also obtained for h.c.p. systems if we write \( \varphi = -\beta/2 + q \) instead of \( (1 - \beta^2 + q^2)/4 \), which was wrongly introduced in Table 1 of Mitra & Mathur (1975) through oversight.

An interesting consequence of equations (1) and (2) is that they explain, at least to a considerable extent, the difference obtained in particle-size values calculated on the basis of Gaussian and Cauchy strain profiles, respectively. Combining equations (1) and (2), we find that,

\[
\left( \frac{1}{N_{\text{eff}}} \right)_{\text{Gaussian}} - \left( \frac{1}{N_{\text{eff}}} \right)_{\text{Cauchy}} = \frac{\pi^2}{\sigma} \langle S^2 \rangle.
\]

The right-hand side of equation (3) is of the order of \( 10^{-4} \) for \( \langle S^2 \rangle \approx 10^{-6} \), thus, \( (N_{\text{eff}})_{\text{Cauchy}} - (N_{\text{eff}})_{\text{Gaussian}} \approx 10^6 \times 10^{-4} = 10^2 \), taking both these quantities to be of the order of \( 10^3 \) a.u. This is corroborated by the findings of Michell & Haig (1957) and Michell & Lovegrove (1960).

References


