(*LPTa*)) has been calculated for several radiations (*LMPT*, Fig. 2) and is used as prescribed in these earlier papers.

The similarity between the angle factor previously derived for the integrated intensity formula in the classical case (*J* (2·31, 2·50)) (strictly monochromatic X-rays) and the angle factor for the case discussed here (where there is a spectral distribution in the incident beam) is manifest because the λ^3 factor appearing in the integrated intensity formula is offset by the absorption factor (*J* 2·50), which to the first order is proportional to λ^3. Thus the integrated intensity (*J* 2·50) is virtually independent of wavelength.

References

DARWIN, C. G. (1922). *Phil. Mag.* **43**, 800.

JAMES, R. W. (1950). *The Optical Principles of the Diffraction of X-rays*. London: Bell.

LADELL, J. & LOWITZSCH, K. (1960). *Acta Cryst.* **13**, 205.

LADELL, J., MACK, M., PARRISH, W. & TAYLOR, J. (1959). *Acta Cryst.* **12**, 567.

LADELL, J., PARRISH, W. & TAYLOR, J. (1959*a*). *Acta Cryst.* **12**, 253.

LADELL, J., PARRISH, W. & TAYLOR, J. (1959*b*). *Acta Cryst.* **12**, 561.

LANG, A. R. (1956). *J. Appl. Phys.* **27**, 485.

MILBERG, M. E. (1958). *J. Appl. Phys.* **29**, 216.

PARRISH, W. & WILSON, A. J. C. (1959). *International Tables for X-ray Crystallography*, Vol. II, Section 4.7.

PIKE, E. R. (1959). *Acta Cryst.* **12**, 87.

PIKE, E. R. & LADELL, J. (1961). *Acta Cryst.* **14**, 53.

PIKE, E. R. & WILSON, A. J. C. (1959). *Brit. J. Appl. Phys.* **10**, 57.

VICTOREEN, J. A. (1948). *J. Appl. Phys.* **19**, 855.

WILSON, A. J. C. (1950). *J. Sci. Instrum.* **27**, 321.

WILSON, A. J. C. (1958). *Proc. Phys. Soc.* **72**, 924.

ZACHARIASEN, W. H. (1945). *Theory of X-ray Diffraction in Crystals*. New York: Wiley.

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; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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The Lorentz factor in powder diffraction.*

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(*Received* 24 *March* 1960)

In a recent communication by Ladell, Parrish & Taylor (1959), a correction was suggested to be applied to the centroids of powder-diffraction lines for the purpose of counteracting the shift from true Bragg position caused by the effect of the Lorentz and polarization factors. More recently with M. Mack (Ladell, Mack, Parrish & Taylor, 1959) the same authors have published values of this correction calculated for various radiations. A similar correction was earlier reported by Pike (1959) in a theoretical study of the role of the Lorentz factor. There is a small discrepancy between the results of Pike and those suggested by Ladell *et al.*, and close inspection shows that the corrections are based upon different angular factors attributed to the Lorentz factor.

In restudying both papers to clarify the presumably divergent concepts of the Lorentz factor, an arithmetic error was discovered which has the effect of increasing the discrepancy. Although the discrepancy becomes smaller at higher angles, an apparent difference in lattice parameter of approximately one part in 10^5 is manifest if one of the corrections is preferred to the other.

In Pike (1959) the second-order terms in eq. (39) are in error by a factor of two; the correct expression should read

$$\psi - \psi_0 = -\frac{V}{\lambda^2}\tan^3\theta\left\{3 + 2\cot^2\theta - \frac{16\cos^2\theta\cos 2\theta}{1+\cos^2 2\theta}\right\}. \quad (1)$$

The asymptotic expressions quoted in the abstract are not affected by this error.

In Ladell, Parrish & Taylor (1959) and Ladell, Mack, Parrish & Taylor (1959) the suggested correction factor Δ_{LP} accounts not only for the Lorentz, polarization, and trigonometric factor associated with the powder method but also accounts for the effect of physical absorption, a wavelength-dependent factor (see Wilson, 1958). The theoretical basis for the suggested correction factor, Δ_{LP}, has been established in a later work (Ladell, 1961), but the role of absorption was not recognized in the earlier papers. To draw attention to this previously unrecognized property, the correction factor Δ_{LP} has been renamed Δ_{LPU} (Ladell, 1961).

In view of the foregoing it is now clear that the divergent angular factors previously reported take into account *different* effects. When the diffraction of powders is considered apart from absorption the angular factor is

$$B(2\theta) = \tan\theta(1+\cos^2 2\theta) \quad (2)$$

* This work was supported in part by the U.S. Army (Signal Corps), the Air Force through the Air Force Office of Scientific Research (ARDC), and the U.S. Navy (ONR).

as given by Pike (1959), eq. (16). If the absorption is included, the angular factor is given by

$$1/J(\theta) = (1+\cos^2 2\theta)/(\sin^2\theta\cos\theta) \qquad (3)$$

as in Ladell (1961), eq. (43), and Ladell, Parrish & Taylor (1957, 1959).

The methods of Pike (1959) can be easily extended to take into account the effect of absorption (in addition to the Lorentz, polarization and other factors) by substituting (3) for $B(2\theta)$ in his eq. (38). One obtains

$$(\psi-\psi_0)_U = -\frac{V}{\tilde{\lambda}^2}\tan^3\tilde{\theta}\left\{3-4\cot^2\tilde{\theta}-\frac{16\cos 2\tilde{\theta}\cos^2\tilde{\theta}}{1+\cos^2 2\tilde{\theta}}\right\}. \qquad (4)$$

(where the subscript 'U' has been used to indicate that the angular correction term now also accounts for absorption).

The correction term given by (4) can be compared with that reported by Ladell, Mack, Parrish & Taylor (1959) by calculating the spectral variance, $\tilde{V}$, and mean wavelength, $\tilde{\lambda}$, on their spectral model and substituting these quantities in (4).

Table 1. *Comparison of correction terms*

$\Delta_D+\Delta_{LPU}$ and $(\psi-\psi_0)_U$ for Cu $K\alpha$ radiation: $\tilde{\lambda}=1538{\cdot}745$ X.U., $\tilde{V}=3{\cdot}84957$

2θ	$(\psi-\psi_0)_U$	$(\Delta_D+\Delta_{LPU})$
120	−0·0016°	−0·0015°
130	−0·0032	−0·0033
140	−0·0065	−0·0066
150	−0·0157	−0·0164
155	−0·0272	−0·0279
160	−0·0530	−0·0554
162·5	−0·0789	−0·0821
165	−0·1252	−0·1336

Table 2. *Comparison of correction terms*

$\Delta_D+\Delta_{LPU}$ and $(\psi-\psi_0)_U$ for Cr $K\alpha$ radiation: $\tilde{\lambda}=2286{\cdot}450$ X.U., $\tilde{V}=4{\cdot}55732$

2θ	$(\psi-\psi_0)_U$	$(\Delta_D+\Delta_{LPU})$
120°	−0·0008°	−0·0008°
130	−0·0017	−0·0019
140	−0·0035	−0·0033
150	−0·0084	−0·0088
155	−0·0146	−0·0150
160	−0·0284	−0·0289
162·5	−0·0423	−0·0433
165	−0·0671	−0·0704

The correction term given by (4) was calculated for Cu and Cr $K\alpha$ radiation and is compared with the equivalent correction term $\Delta_D+\Delta_{LP}$ (Ladell, Mack, Parrish & Taylor, 1959, Figs. 1, 2). The results are given in Tables 1 and 2. These results indicate that the approximations which lead to the characterization of the correction in terms of the variance and mean wavelength are reasonable and that there is no significant difference between the numerical approach of Ladell, Mack, Parrish & Taylor (1959) and that of Pike.

References

Ladell, J., Parrish, W. & Taylor, J. (1957). Philips Laboratories Technical Report No. 122, privately communicated.

Ladell, J., Parrish, W. & Taylor, J. (1959). *Acta Cryst.* **12**, 253.

Ladell, J., Mack, M., Parrish, W. & Taylor, J. (1959). *Acta Cryst.* **12**, 567.

Ladell, J. (1961). *Acta Cryst.* **14**, 47.

Pike, E. R. (1959). *Acta Cryst.* **12**, 87.

Wilson, A. J. C. (1958). *Proc. Phys. Soc.* **72**, 924.

Acta Cryst. (1961). **14**, 54

The choice of axes in the amphiboles.

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(*Received* 2 *May* 1960)

One of us (Zussman, 1959) has previously pointed out some of the confusion which has arisen in the literature of the amphiboles as a result of the possibility of describing the Bravais lattice by two different cells which have closely similar axial parameters. As a result of this some earlier comparisons of the unit-cell parameters of different amphiboles are invalidated by the fact that the parameters in question refer to different unit cells. It has since come to our notice that there are other sources of confusion in the literature which are related to this matter, and it is the purpose of the present note to discuss these for the benefit of future work.

1. Space group

The two conventional choices of axes correspond to descriptions of the space group in the settings $C2/m$ and $I2/m$, and the most convenient way of specifying which choice of unit cell is being used on any occasion is to denote it as either the C-cell or the I-cell. Although $C2/m$ is the standard setting for this space group, most papers on amphibole structure have used the I-cell because it best illustrates the relationship to the pyroxene structure when the latter is referred (as it usually is) to a C-cell. The first published structure of an amphibole, that of tremolite (Warren, 1930), was referred to the I-cell, but was published before the introduction of the Hermann–Mauguin symbols, and the space group was therefore given in the Wyckoff notation 2Ci-3, and later commentators translated this into the standard form $C2/m$ without noticing that this would involve a change in the unit-cell parameters (e.g. Bragg, 1937). Thus the parameters of the I-cell have appeared in the literature in conjunction with a statement that the space group is $C2/m$.