Correction for the Satellite Group in the Variance Method of Profile Analysis

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Three methods are described of eliminating the influence of the satellite group in the variance method of X-ray line profile analysis. The first is to interpolate the line profile under the satellite group; however, the satellite group must be reasonably well distinguished from the \( \alpha_1 \) tail and from the background.

The second method is to correct the experimental variance-range curve by a graphical construction: this assumes that the satellite lines and the broadening function are Cauchy in form. The third method is to compute the necessary corrections to the slope and intercept of the linear variance-range function by using model spectral distributions with and without the satellite group. The first two methods are applied to profiles from powders of iron and iron alloys studied with iron radiation, the third method uses an analytical model of the spectral distribution of the iron \( K_\alpha \) multiplet. The corrections given by these methods to be made to the slope and the intercept of the variance-range function are nearly constant for all but the smallest amounts of particle-size broadening. It is also shown that particle sizes determined either from slope or intercept of the variance will be underestimated if correction is not made for the satellite group.

1. The interpolation method

The great extent to which the variance-range function is affected by the satellite group was first emphasized by Langford (1968) and again by Edwards & Toman (1969). In the latter paper it was shown that the elimination of the satellite group by interpolation is a viable way of dealing with this problem. As can be expected, this method is reliable only for measurements with low statistical fluctuation and high ratio of the intensity of the peak of the \( \alpha_1 \) line to that at the peak of the satellite group. This condition will be put in a more quantitative form later in this paper (§ 1) and it will be shown that the interpolation procedure is useful not only with single-crystal measurements but also in some cases with powder samples.

Furthermore a graphical method is described (§ 2) which is faster than the interpolation method (unless a computer is available) and applicable more often. Finally it is shown that a numerical computation (§ 3) using a model intensity distribution for the multiplet gives the required corrections to the intercept and slope of the linear variance-range function determined experimentally.

2. The graphical method

The measured intensity of the diffraction profile can be plotted either as a function of the diffraction angle...
2θ, or of the reciprocal coordinate ζ, or of the wavelength λ. Accordingly, the variance of the intensity distribution can be expressed in \( \Gamma'(2θ)^2 \) or in Å\(^{-2} \) or in Å\(^2 \), and we can transform the variance values in any one of these representations into those of another by multiplying them by the square of the appropriate derivative (if dispersion can be neglected). The correction for the influence of the satellite group can be best performed in the λ-representation because in this representation the intensity distributions for all reflections may be compared immediately as they differ only in the degree of broadening; the broadened profile can be represented by the convolution of the spectral distribution with the broadening function of the sample and with aberrations. If the variance is corrected for aberrations (Wilson, 1963) and if we assume a Cauchy form for the broadening function then all features of the resulting variance–range function, including the satellite correction, can be derived from the spectral distribution and from the width of the broadening function.

In Fig. 2 the diffraction pattern (i.e. the spectral distribution folded with the broadening function of the sample) of the Kα group is shown schematically. Let us assume for simplicity that \( P_{λ}(λ) \), the intensity distribution in the diffraction pattern of the \( α_{12} \) doublet, has definite zero and first moments and that \( P_{p}(λ) \), the intensity distribution in the diffraction pattern of the satellite group, is very narrow. is situated at distance λ\(_c\) from the common centroid and has definite zero, first and second moments. Further, let \( P_{d}(λ) + P_{s}(λ) \) be normalized to unity. (Note that \( P_{d}(λ) \) and \( P_{s}(λ) \) are not spectral distributions but the spectral distributions folded with a broadening function.)

If we express \( W'(σ) \), the variance of the whole Kα group, as a function of the truncation parameter σ, then

\[
W'(σ) = \int_{-σ}^{σ} \left[ P_{d}(λ) + P_{s}(λ) \right] 2^2 dλ, \tag{3}
\]

where \( W'(σ) \) is the variance as defined by Wilson (1965, equation 11). The contribution of the satellite group to \( W'(σ) \) is approximately \( \frac{1}{2} λ_c^2 A \) for \( σ = λ_c \) and \( λ_c^2 A \) for \( σ > λ_c \). Here, A is the fractional contribution of the satellite group to the integrated intensity of the whole Kα group. Because \( λ_c \) and A are spectral properties of the Kα group and do not depend on the sample (for an iron target \( A = 0.01 \) and \( λ_c = 10.0 \) mÅ), a simple and general graphical method for correction for the satellite group can be readily devised (Fig. 3). We subtract \( \frac{1}{2} λ_c^2 A \) from the uncorrected variance value at \( σ = λ_c \).

<table>
<thead>
<tr>
<th>Powder sample</th>
<th>hkl</th>
<th>µ/σ</th>
<th>Extent of removal</th>
<th>Uncorrected</th>
<th>Corrected</th>
<th>Correction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure iron</td>
<td>110</td>
<td>16</td>
<td>90%</td>
<td>-0.5</td>
<td>1.2</td>
<td>1.7</td>
</tr>
<tr>
<td>Pure iron</td>
<td>200</td>
<td>5</td>
<td>50</td>
<td>-0.8</td>
<td>0.3</td>
<td>1.1</td>
</tr>
<tr>
<td>Iron alloy (1)</td>
<td>110</td>
<td>13</td>
<td>70</td>
<td>1.3</td>
<td>2.4</td>
<td>1.1</td>
</tr>
</tbody>
</table>

Table 1. Interpolation method. The changes in intercept (Å\(^2 \) x 10\(^6\)) and slope (Å x 10\(^4\)) of the linear variance–range functions (iron radiation)

Fig. 1. Pure iron powder, 110 line. Ordinate scales are counts per 300 sec, with the satellite group on the enlarged (inner) scale. Dashed curve: result of interpolation under the satellite group.
(point \(A_0\)) and \(\lambda^2 A\) from the uncorrected variance value at \(\sigma > \lambda_c\) (point \(B_0\)). The straight line \(A_0B_0\) represents the corrected linear variance–range function, because the initial curvature of the corrected variance–range function is very small beyond \(\sigma > \lambda_c\) (about 10 mÅ for iron radiation) (Edwards & Toman, 1969).

This method is very simple, but in practice slight modification is necessary, because the satellite group is neither very narrow (its width in \(\lambda\)-representation is often considerably broadened by the broadening function of the sample) nor has it a definite second moment. But, as will be shown, the only change is to subtract \(\frac{1}{2} \lambda^2 A(1+\varepsilon)\) and \(\lambda^2 A(1+\delta)\) instead of \(\frac{1}{2} \lambda^2 A\) and \(\lambda^2 A\) when constructing points \(A_0\) and \(B_0\). Here \(\varepsilon\) and \(\delta\) are small numbers calculable from \(P_s(\lambda)\).

For the computation of \(\delta\) and \(\varepsilon\) we need to specify the analytical form of \(P_s(\lambda)\). As a reasonable model we shall take two normalized Cauchy functions of the same width \(2w_s\) centred at \(\lambda_c + \Delta\) and \(\lambda_c - \Delta\). The parameter \(w_s\) is given by

\[
w_s = w_t + w_b
\]

where \(2w_t\) is the spectral width of either component of the satellite group and \(2w_b\) is the width of the broadening function of the sample, if we assume that this function is Cauchy. \(P_s(\lambda)\) is thus

\[
P_s(\lambda) = \frac{A w_s}{2\pi} \left( \frac{1}{w_t^2 + (\lambda - \lambda_c - \Delta)^2} + \frac{1}{w_b^2 + (\lambda - \lambda_c + \Delta)^2} \right).
\]

From spectroscopic measurements, the values of \(w_t\) and \(\Delta\) can be derived (we found for iron that they are respectively \(0.6 \pm 0.1\) mÅ and \(0.80 \pm 0.07\) mÅ). The width \(2w_b\) is related to \(k\), the experimental slope of the variance–range function, by the relation \(k = 2/\pi(w_b + w_d)\), where \(2w_d\) is the mean value of the widths of the \(\alpha_1\) and \(\alpha_2\) lines (for iron about 0.9 mÅ). Noting the small difference between \(w_t\) and \(w_b\) and the fact that \(w_b\) in most cases where the satellite correction is important is several times larger than \(w_d\) and \(w_t\) and further that both \(\varepsilon\) and \(\delta\) depend only slightly on \(w_s\) (or \(k\)) (as will be evident later), one can accept \(w_s = \pi k/2\) as a fair approximation. Having fixed all constants in \(P_s(\lambda)\) we can proceed to the computation of \(\Delta W'_{s}(\sigma)\), the contribution of the satellite group to the variance. The result is

\[
\Delta W'_{s}(\sigma) = \frac{A}{2\pi} \left\{ 4\sigma w_s + [(\lambda_c + \Delta)^2 - w_s^2] \left[ \arctan \frac{(\sigma - \lambda_c - \Delta)/w_s + \arctan (\sigma - \lambda_c + \Delta)/w_s}{w_s^2 + (\sigma - \lambda_c + \Delta)^2} \right] 
+ [(\lambda_c - \Delta)^2 - w_s^2] \left[ \arctan (\sigma - \lambda_c + \Delta)/w_s 
+ \arctan (\sigma - \lambda_c - \Delta)/w_s \right] 
+ w_s \left[ (\lambda_c + \Delta) \arctan \frac{w_s^2 + (\sigma - \lambda_c - \Delta)^2}{w_s^2 + (\sigma - \lambda_c + \Delta)^2} 
+ (\lambda_c - \Delta) \arctan \frac{w_s^2 + (\sigma - \lambda_c + \Delta)^2}{w_s^2 + (\sigma - \lambda_c - \Delta)^2} \right] \right\}.
\]

Putting \(\sigma = \lambda_c a\) and taking into account the fact that \(\lambda_c \gg \Delta\) and \(\lambda_c \gg w_s\) we get for \(a > 1\):

\[
\Delta W'_{s}(a) = \lambda^2 A \left\{ \frac{\pi}{\arctan (a - 1)} \right\} \left\{ \frac{2\lambda_c}{\pi k} \right\} - \frac{k}{\lambda_c} \left( a - \ln \frac{a + 1}{a - 1} \right) \}.
\]

Fig.2. Schematic representation of the diffraction pattern of the whole Kα group (satellite group exaggerated). \(A\) is the centroid of the group.
Because in all practical applications \( k \) is many times smaller than \( \lambda_c \) the arctan terms are close to 1 and the second term is a small quantity. Therefore we can put \( AW'_{\delta}(a) = \lambda_c^2 A(1 + \delta) \). The values of \( \delta \) for iron radiation were computed for \( 5 \times 10^{-4} \text{ Å} \leq k \leq 20 \times 10^{-4} \text{ Å} \) and for \( 1.5 \leq \sigma \leq 2.5 \) and are shown in Fig. 4(a).

Similarly, for \( \sigma = \lambda_c \), we get from (6):

\[
AW'_{\delta}(\lambda_c) = A^2 \frac{2k}{k_c} \left(1 - \alpha \arctan \frac{4\lambda_c}{\pi k_1 + \alpha^2} \right) = \frac{1}{2} A\lambda_c^2 (1 + \varepsilon),
\]

where \( \varepsilon = \sigma / h_k \). Here again, \( \varepsilon \) is fairly small compared with 1; the numerical values for iron radiation are given in Fig. 4(b). This graphical method was applied to measurements on a series of iron samples (with Fe K\( \alpha \) radiation) and the resulting corrections are given in Table 2. In Fig. 5 the graphical method is applied to the variance–range function corresponding to the reflection 110 of pure iron (\( \mu g / \varphi = 16 \)).

### 3. Computation on model profiles

The satellite correction can be obtained by comparison of those variance–range functions computed numerically from suitable models of the intensity distribution with the satellite group, with those computed from model distributions without the group. In our computation, the model intensity distribution was the convolution of a model spectral distribution with an appropriate broadening function, which represented the influence of the sample.

The intensity distribution \( P_{\delta}(\lambda) \) representing the convolution of the spectral distribution in the doublet \( \alpha_1 \) with the Cauchy broadening functions, was constructed from two Cauchy functions, each characterized by its parameter \( w_i \) \((i = 1, 2)\) and its amplitude. The amplitudes were in the ratio 2:1 and the parameters \( w_i \) were of the form \( w_i = w_{s1} + w_{b1} \), where \( 2w_{s1} \) represents the spectral (unbroadened) width of the \( i \)th Cauchy function and \( 2w_{b1} \) represents the width of the broadening function. The \( w_{s1} \) were chosen to be 0.29 and 0.33 mA. These values give the same ratio of the widths of the \( \alpha_1 \) and \( \alpha_2 \) lines and the same slope of the variance–range function as that found experimentally for iron radiation (Edwards & Toman, 1969). The limited adequacy of this model is reflected by the fact that the half-widths of these model lines are substantially smaller than those observed (0.58 and 0.66 mA, compared with 0.86 and 0.99 mA). The separation of the peaks was taken as 3.96 mA, which corresponds to the experimental value.

### Table 2. Graphical method. The changes in intercept (Å\(^2\) \times 10\(^6\)) and slope (Å \times 10\(^4\)) of the linear variance–range functions (iron radiation)

<table>
<thead>
<tr>
<th>Powder sample</th>
<th>( hkl )</th>
<th>( \mu g / \varphi )</th>
<th>Uncorrected ( W'_0 )</th>
<th>( k )</th>
<th>Corrected ( W'_0 )</th>
<th>( k )</th>
<th>( \Delta W'_0 )</th>
<th>( \Delta k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure iron</td>
<td>110</td>
<td>16</td>
<td>-0.5</td>
<td>10.3</td>
<td>1.0</td>
<td>8.5</td>
<td>1.5</td>
<td>-1.8</td>
</tr>
<tr>
<td>Pure iron</td>
<td>211</td>
<td>7</td>
<td>0.1</td>
<td>8.8</td>
<td>1.2</td>
<td>7.5</td>
<td>1.1</td>
<td>-1.3</td>
</tr>
<tr>
<td>Iron alloy (1)</td>
<td>110</td>
<td>13</td>
<td>1.3</td>
<td>8.4</td>
<td>2.8</td>
<td>6.6</td>
<td>1.5</td>
<td>-1.8</td>
</tr>
<tr>
<td>Iron alloy (2)</td>
<td>110</td>
<td>8</td>
<td>-5.3</td>
<td>19.3</td>
<td>-4.4</td>
<td>17.7</td>
<td>0.9</td>
<td>-1.6</td>
</tr>
<tr>
<td>Iron alloy (1)</td>
<td>211</td>
<td>6</td>
<td>2.1</td>
<td>6.7</td>
<td>3.4</td>
<td>5.0</td>
<td>1.3</td>
<td>-1.7</td>
</tr>
<tr>
<td>Iron alloy (2)</td>
<td>211</td>
<td>4</td>
<td>-2.1</td>
<td>15.2</td>
<td>-0.8</td>
<td>13.5</td>
<td>1.3</td>
<td>-1.7</td>
</tr>
</tbody>
</table>

Fig. 3. Illustration of the graphical method of correcting for the satellite group.
Similarly, the intensity distribution $P_d(\lambda)$, representing the convolute of the spectral distribution in the satellite group with the Cauchy broadening function, was constructed from two Cauchy functions of the same amplitude and width. The parameter $w_b$ was given by $w_b = w_t + w_b$ where $w_b$ is the same parameter as used above in the distribution $P_d(\lambda)$ and $w_t$ was taken as 0.6 mA. The separation of the peaks in $P_d(\lambda)$ was 1.6 mA and their amplitude was adjusted to keep the integral of the $P_d(\lambda)$ distribution equal to 0.01 of the integral of the $P_d(\lambda)$ distribution. The distance apart of the centres of gravity of $P_d(\lambda)$ and $P_8(\lambda)$ was kept at 10.0 mA.

Fig. 6 shows the variance–range functions $W_{d+s}(a)$ based on the distribution $P_d(\lambda) + P_e(\lambda)$ and the variance–range functions $W_d(\sigma)$ based on $P_d(\lambda)$ only. Both sets were computed according to the first definition of the variance function (zero moment with infinite integration limits; see Wilson, 1965).

The next step was to approximate $W_{d+s}$ and $W_d$ by straight lines within the limits 7 mA ≤ $\sigma$ ≤ 10 mA. The difference of the slopes, $\Delta k = k_d - k_{d+s}$ is a measure of the effect of the satellite group and can be considered as a correction to be added to the measured slope of the variance function calculated when the satellite group is present (note: from this definition, $\Delta k$ is always negative). In a similar way $\Delta W_0 = W'_0 - W'_{d+s}$, the correction to the intercept, was obtained; $\Delta W_0$ should be added to the measured intercept. In Fig. 7 $\Delta k$ and $\Delta W_0$ are shown as functions of the width of the broadening function (full curves), which is here represented by the uncorrected value of the slope, $k_{d+s}$. Both $\Delta k$ and $\Delta W_0$ vary only slowly with the slope.

Conclusions

In this paper three different ways of correcting the satellite group are presented. The interpolation method has the obvious merit that it does not contain any assumption about the nature of the broadening function but it is useful only if the satellite group is reasonably well distinguished from the tail of the $z_1$ line and from the background, i.e. for the above cases, $\mu_0/\sigma > 10$.

The graphical method is quite simple in application, does not assume any particular form of the spectral distribution of the doublet, but does assume a Cauchy form for the satellite lines and for the broadening function. The greatest disadvantage of this method is its
use of the variance value at a rather high \( \sigma \), where the variance is very sensitive to the chosen value of the background level.

The method based on the model computations does not have this disadvantage, but all diffraction profiles are assumed to be Cauchy in form.

All three methods are compared in Fig. 7, where the corrections to intercept and slope obtained from the interpolation and graphical methods (as applied to various lines of five different iron powders) are compared with the corrections given by the model computation. It can be seen that the latter gives consistently smaller corrections, and this indicates, as mentioned above, the shortcomings of approximating all profiles – including the markedly asymmetric iron lines – as Cauchy in form. The other two methods are thus generally to be preferred in practice and so an attempt has been made in these two diagrams to draw curves (dashed) through the points derived from these methods, which curves may then be used to find directly the corrections necessary for any experimental variance–range curve. The average scatter of points about these ‘empirical correction curves’ is \( \pm 0.37 \) ordinate units in each case, which is quite large; again, this indicates (for the graphical method) the limitations of the approximations made, coupled with the unfortunate use of the variance value at a high \( \sigma \), where the variance is very sensitive to the choice of background level. Making these corrections will thus introduce unfortunately large relative errors into the corrected values of slope and intercept, but these two diagrams show that errors several times larger would be incurred by omitting the corrections altogether.

Finally it will be shown that correction for the satellite group is a necessary preliminary to determining particle sizes from the variance of powder profiles. In Fig. 6 let curve \( B \) represent the variance of some powder profile; also, curve \( A \) will represent the variance of the spectral distribution of the \( K\alpha \) doublet since the broadening is here zero. The correct procedure for deducing the particle size is to correct the variance \( B \) for the satellite group (by one of the above methods) to gain curve \( C \) and then to subtract the contribution of the spectral distribution of the doublet, represented by section \( KL \) of curve \( A \) (the true linear part). The correct particle size may then be determined from either the slope or the intercept of the remaining variance (assuming, as always, that the variance of instrumental aberrations has been allowed for).

If curve \( B \) is not corrected for the influence of the satellite group, the particle size determined as before is always underestimated; this was shown as follows. A variance–range function such as curve \( B \) was synthesized for a given particle size (200, 400, 600 or 800 Å) from the variance of the particle size broadening, the variance of the \( K\alpha \) doublet (as Edwards & Toman, 1969) and the variance of the satellite lines (approximated as Cauchy profiles). This was then analysed in two ways to re-extract the particle size – without making correction for the satellite group – by subtracting the contribution to slope and intercept of either section \( KL \) or section \( JK \) (the pseudolinear part) of curve \( A \). When the particle size is calculated from the resulting slope/intercept, the former method gives the amounts of underestimate shown in Table 3 whilst the latter method gives those shown in Table 4. This was done for four (correct) particle sizes for values of \( 2\theta \) corresponding to the first three lines of iron using iron radiation. The former method takes no account at all of the contribution of the satellite group: the

![Fig. 5. Pure iron powder, 110 line: the result of the graphical method. The corrected linear part \( A_0B_0 \) has intercept \( C \).](image-url)
latter method does take partial account of it, as shown by the smaller errors in Tables 4.

Table 3. Underestimates in particle size using the true linear part of the spectral distribution variance

(a) Particle size calculated from the variance slope (Å)

<table>
<thead>
<tr>
<th>Correct size</th>
<th>200</th>
<th>400</th>
<th>600</th>
<th>800</th>
</tr>
</thead>
<tbody>
<tr>
<td>2θ = 57° 5' (Fe(110) Kα)</td>
<td>11</td>
<td>49</td>
<td>115</td>
<td>206</td>
</tr>
<tr>
<td>2θ = 85 0 (Fe(200) Kα)</td>
<td>16</td>
<td>70</td>
<td>161</td>
<td>249</td>
</tr>
<tr>
<td>2θ = 111 52 (Fe(211) Kα)</td>
<td>21</td>
<td>87</td>
<td>183</td>
<td>290</td>
</tr>
</tbody>
</table>

(b) Particle size calculated from the variance intercept

<table>
<thead>
<tr>
<th>Correct size</th>
<th>200</th>
<th>400</th>
<th>600</th>
<th>800</th>
</tr>
</thead>
<tbody>
<tr>
<td>2θ = 57° 5'</td>
<td>10</td>
<td>68</td>
<td>195</td>
<td>353</td>
</tr>
<tr>
<td>2θ = 85 0</td>
<td>18</td>
<td>122</td>
<td>280</td>
<td>442</td>
</tr>
<tr>
<td>2θ = 111 52</td>
<td>27</td>
<td>158</td>
<td>329</td>
<td>515</td>
</tr>
</tbody>
</table>

Table 4. Underestimates in particle size using the pseudo-linear part of the spectral distribution variance

(a) Particle size calculated from the variance slope

<table>
<thead>
<tr>
<th>Correct size</th>
<th>200</th>
<th>400</th>
<th>600</th>
<th>800</th>
</tr>
</thead>
<tbody>
<tr>
<td>2θ = 57° 5'</td>
<td>3</td>
<td>19</td>
<td>56</td>
<td>114</td>
</tr>
<tr>
<td>2θ = 85 0</td>
<td>5</td>
<td>32</td>
<td>89</td>
<td>146</td>
</tr>
<tr>
<td>2θ = 111 52</td>
<td>7</td>
<td>43</td>
<td>101</td>
<td>162</td>
</tr>
</tbody>
</table>

(b) Particle size calculated from the variance intercept

<table>
<thead>
<tr>
<th>Correct size</th>
<th>200</th>
<th>400</th>
<th>600</th>
<th>800</th>
</tr>
</thead>
<tbody>
<tr>
<td>2θ = 57° 5'</td>
<td>3</td>
<td>31</td>
<td>120</td>
<td>248</td>
</tr>
<tr>
<td>2θ = 85 0</td>
<td>6</td>
<td>75</td>
<td>202</td>
<td>367</td>
</tr>
<tr>
<td>2θ = 111 52</td>
<td>9</td>
<td>89</td>
<td>255</td>
<td>427</td>
</tr>
</tbody>
</table>

The extreme underestimates for large particle size are unlikely to be perpetrated in practice: the variance-range functions would then look like curve D or curve E (Fig. 6) and the step due to the satellite group is quite evident. There would be a misrepresentation in approximating such a curve by a straight line (as we have done in computing the underestimate in particle size) which would not arise for a curve such as B: one would be very likely to make some correction (one of those described above) for the satellite group. Tables 3 and 4 do show, however, that the correction is still necessary in cases of appreciable particle-size broadening where the satellite-group step in the variance-range curve is not evident.

In summary, the following points concerning the practical application of the variance method may be

Fig. 6. Variance-range functions of model spectral distributions of iron (with and without the satellite group) folded with a broadening function of width 2w₀ (given in mA). Full curves: $W'_{d}(σ)$; dashed curves: $W'_{d}(σ)$. 
made:
(i) It has been found that for iron radiation the satellite group profoundly affects the form of the variance–range function of the spectral distribution (Edwards & Toman, 1969). In such a case, if no correction is made, only the slope of the variance curve beyond the satellite group can be used.

(ii) As indicated in this paper, some correction can be made for the satellite group; the slope and intercept of the corrected variance may then be used in the usual way.

(iii) However, there are difficulties in this procedure: the percentage correction is sometimes large (especially for intercepts, and if the crystallite size is large, see Tables 1 and 2), so it is frequently necessary to know the variance well beyond the satellite group (graphical method) and this is not always well defined, and the correction may not be known very precisely (see the scatter of points in Fig. 7). These three factors are thus a drawback to the usefulness of the variance method in such a case, especially in the use of the intercept.

(iv) We would emphasize that these conclusions apply for iron radiation only. Whether their validity can be extended to other radiations is at present not clear. The variance–range function for the Cu Kα multiplet, determined by Langford (1968), suggests that the satellite correction is less important for this radiation. His measurements, however, are of lower statistical significance than ours, and further spectroscopic work seems desirable before drawing any more general conclusions.

We are again indebted to Professor A. J. C. Wilson for his help in this work, and also to Dr J. I. Langford for much assistance by way of discussion. Our thanks are also due to the Science Research Council for a Senior Visiting Fellowship (K. T.) and a maintenance grant (H. J. E.).

References