Abstract
It is well known that the extraneous $K\alpha_2$ line complicates the interpretation of X-ray diffraction spectra. Experience has shown that the arms and weights calculated by Ladell’s method [Laddell, Parrish & Taylor (1959). Acta Cryst. 12, 561–567] have to be determined for each user’s X-ray diffractometer, rather than using the published coefficients, for an accurate $K\alpha_2$ elimination. When different materials are analyzed, the signal/noise ratio can be optimized by choosing a suitable target material. $K\alpha_2$ correction coefficients have been calculated for Cu, Co and Cr radiations using a fast Fourier calculation method.

1. Introduction
Ladell, Zagofsky & Pearlman (1975) reviewed the history of $K\alpha_2$ elimination techniques. They also showed that the $K\alpha_1$ profile is not exactly the same as the $K\alpha_2$ profile. Ladell, Parrish & Taylor (1959) gave an analytical representation of the $K\alpha_1$, $K\alpha_2$ doublet described by an asymmetrical function. More recently, Delhez & Mittemeijer (1975) showed the utility of an angle-dependent doublet separation within a given profile to perform the $K\alpha_2$ elimination. In this paper, some parts of the theory published by Ladell et al. (1959) have been followed but not the calculation procedure.

This paper should be considered more as an application of the Ladell et al. (1959) approach than as a new technique for the elimination of $K\alpha_2$ lines.

The two main contributions are:

straightforward application of a usual fast Fourier transform subroutine for $K\alpha_2$ elimination;

application of the Ladell et al. (1959) $K\alpha_2$ elimination in diffraction spectra for three radiations; Cu, Co and Cr.

2. Theory
The Ladell et al. (1959) analytical representation of the doublet spectral distribution can be briefly stated as follows. When the two peaks are shifted along an s scale so that the peak-top functions coincide and the intensity is adjusted to 1, the doublet can be described by the four relationships:

$$u_2(s) = \frac{1}{1 + c^2 s^2} \quad s < 0$$
$$u_2(s) = \frac{1}{1 + m^2 s^2} \quad s \geq 0$$
$$u_1(s - \delta) = \frac{1}{1 + a^2 s^2} \quad s < 0$$
$$u_1(s - \delta) = \frac{1}{1 + b^2 s^2} \quad s \geq 0$$

where $u_1$, $u_2$ are the $K\alpha_1$, $K\alpha_2$ shape functions, $s = \lambda/d$, $d =$ interplanar spacing, and $\delta = (\lambda \alpha_2 - \lambda \alpha_1)/d$. The peak top is positioned at the origin ($s = 0$). The parameters $a$, $b$, $c$, $m$ (full width at half maximum) have been calculated from a Cauchy-like function that fits each half peak of an observed resolved $K\alpha_1$, $K\alpha_2$ doublet.

Table 1 shows the peak parameters determined for the three radiations commonly used in LABORELEC [the inverses of $a$, $b$, $c$, and $m$ have been chosen in order to facilitate comparison with the data of Ladell et al. (1959)]. As the $K\alpha_1$ profile is observed during spectrum scanning, the algorithm will automatically eliminate the $K\alpha_2$ contribution to the $K\alpha_1$, $K\alpha_2$ doublet. The $K\alpha_2$ profile function must be determined from the $K\alpha_1$ profile function.

A convolution product defines the transformation $u_1(s) \rightarrow u_2(s)$:

$$u_2(s) = h(s) \ast u_1(s - \delta).$$

If $U(k)$ is the transform of $u(s)$, $H(k)$, the transform of $h(s)$, can be defined as

$$H(k) = U_2(k)/U_1(k).$$

The phase displacement concerning $\delta$ is not included in (3). A fast Fourier Transform subroutine has been applied to calculate $H(k)$.

The fast Fourier transform theory has been used to find the coefficients $U(k)$ calculated from a synthetic $K\alpha_1$, $K\alpha_2$ curve based on measured parameters so that signal fluctuations are diminished. 64 equally spaced points of the curve have been regularly chosen in order to perform the Fourier transform.

The first point is the intensity corresponding to an angular abscissa equal to five widths at half maximum.
The full period $R$ (ten widths at half maximum), divided in 63 steps, provides the 64 points for performing the calculation:

$$u_i(s) = \frac{1}{R} \sum_{k=0}^{k=63} U(k) \exp\left(\frac{-2\pi iks}{R}\right). \quad (4)$$

In practice, for the calculation conditions, the Fourier coefficients become very small after the first ten harmonics.

$$U_i(k) = \frac{1}{R} \sum_{s=-R/2}^{s=R/2} u_i(s) \exp\left(\frac{-2\pi iks}{R}\right) ds. \quad (5)$$

The $H(k)$ ($k$ chosen harmonics) can be easily calculated by dividing the $U_2(k)$ by the $U_1(k)$ coefficients.

A histogram of $h(s')$ (Fig. 1) can be plotted, where $s'=(\lambda_2-\lambda_1)/\lambda_1$ or, more exactly, in a discrete form $(\lambda_2-step \times n)/\lambda_1$ ($n$ is a positive or negative integer in the range $0 \rightarrow 63$). The histogram of $h(s')$ was normalized so that the sum of the ordinate was set equal to $\int h_2(s) ds/\int u_1(s-\delta) ds$.

In order to apply the convolution product, it is defined as a lever arm that represents the distance in $s'$ units from the origin where the corresponding weight factor $h(s')$ shall be applied. 64 pairs (arm/weight) have thus been calculated. The weights are principally concentrated around the origin $s_0$. Three, five or seven pairs are chosen near the origin and the sum of these pairs is again normalized in order to adjust the sum of the weights equal to the $K\alpha_2/K\alpha_1$ ratio (Table 2). The $K\alpha_2$ elimination algorithm can be applied following the relationship given by Ladell et al. (1959).

$$N(s) = \sum_{j=1}^{j=5} P(j)N[sA(j)],$$

$P(j)$ is the weight, $A(j)$ is the lever arm length, $s$ is the peak position, and $N(s)$ is the intensity reading at point $s$. The lever arm application $sA(j)$ will generate points which will be applied to regions (broken into $2\theta$ increments) where there are no data.

Mallory & Snyder (1978, 1979) have solved the mismatch of scales by applying a determined fraction of the calculated correction factor to the nearest-neighbour points of $sA(j)$. The nearest point to $sA(j)$ has the greatest part of the intensity $I(A)$ and the contribution of the intensity to the surrounding points is calculated by a linear interpolation based on the position of the point in $2\theta$. Figs. 2, 3 and 4 show the quality of the $K\alpha_2$ elimination performed by the program and applied for the three different radiations.

### 3. Programs

Two programs have been written to perform the calculation of the correction coefficients.

**SN.PARDI**

This program is written in Fortran IV. It determines the inverse of the half width at half height ($q$) of the Cauchy-like function $I(z) = 1/(1 + q^2 z^2)$ ($z = \lambda - \lambda_1$) for each peak.

A linear regression is carried out between $[1/(1/(z-1)]$ and $z^2$. The slightly smoothed intensities are introduced from the keyboard as well as the $d$ of the calibration crystal and the experimental peak maximum.

**SN.FOURI**

This program is written in Fortran IV. It calculates the weights and the arms for different radiations. The input data are: $1/a$, $1/b$, $1/c$, $1/m$, heights $K\alpha_1$, $K\alpha_2$, $d$ and the number of harmonics selected by the user.

The following information is found in the output:

- 64 Fourier coefficients expressed with their real and imaginary parts, the amplitude and the phase;
- the useful subroutine PLOTBAR allows one to visualize the amplitude of the Fourier coefficients for

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**Table 1. Experimental parameters of an α-quartz resolved doublet**

<table>
<thead>
<tr>
<th>Target</th>
<th>$1/a$</th>
<th>$1/b$</th>
<th>$1/c$</th>
<th>$1/m$</th>
<th>$I(K\alpha_2)/I(K\alpha_1)$</th>
<th>$d$ (Å)</th>
</tr>
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<tbody>
<tr>
<td>Cu</td>
<td>0.000577</td>
<td>0.000645</td>
<td>0.000658</td>
<td>0.000693</td>
<td>0.50</td>
<td>0.7913</td>
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<tr>
<td>Cu</td>
<td>0.0009358</td>
<td>0.0009277</td>
<td>0.001135</td>
<td>0.0009680</td>
<td>0.5152</td>
<td>0.9607</td>
</tr>
<tr>
<td>Cr</td>
<td>0.001250</td>
<td>0.001390</td>
<td>0.001680</td>
<td>0.001680</td>
<td>0.4854</td>
<td>1.2558</td>
</tr>
</tbody>
</table>

**Fig. 1. h(s') histogram. α-Quartz, d = 0.7913 Å, Cu radiation.**

Ordinate (weight): expressed in arbitrary units; abscissa (lever): $s' = (\lambda_2-step \times n)/\lambda_1$ ($n = 0 \rightarrow 63$).
Table 2. Calculated levers and weighting values for three radiations

<table>
<thead>
<tr>
<th></th>
<th>Cu</th>
<th>Co</th>
<th>Cr</th>
</tr>
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<tbody>
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<td>Three-bar histogram</td>
<td>Five-bar histogram</td>
<td>Seven-bar histogram</td>
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<tr>
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<td>- Weights</td>
<td>Arms</td>
<td>- Weights</td>
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</tr>
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<td>1.0025358</td>
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<td>1.0024862</td>
<td>0.17398778</td>
</tr>
<tr>
<td>1.0025854</td>
<td>0.095670579</td>
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<tr>
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the $K\alpha_1$ and $K\alpha_2$ lines and the $H(k)$ ratio as a function of the harmonic $0\rightarrow 63$. The histogram shown in Fig. 1 is also plotted as well as the $K\alpha_2$ profile calculated from the $K\alpha_1$ under a PLOTBAR pattern.

The Cu, Co and Cr arms and weights coefficients are used in the off-line program ADR2 (Mallory & Snyder, 1978) modified by Platbrood, Quitin & Barten (1981).

4. Equipment

A Siemens type $F$ powder diffractometer (Slo-syn stepping-motor goniometer equipped with filter) controlled by a Tektronix 4051 computer (32 kbytes) was used.

The computer was a Systems Engineering Laboratory SEL 32, 512 kbytes equipped with a Tektronix 4051 large display graphic terminal and a Calcomp pen plotter.

![Fig. 2. Graphic display of $\alpha$-quartz (Cu radiation) spectrum with and without $K\alpha_2$ elimination. Starred peaks $K\alpha_1$.](image)

![Fig. 3. Graphic display of $\alpha$-quartz (Co radiation). Spectrum with and without $K\alpha_2$ elimination ($d = 0.9607$ Å).](image)
5. Conclusion

The $Kz_2$ algorithm based on the computed arms and weights offers a number of advantages: short computation time for $Kz_2$ elimination, very small memory requirement in the main program and high-quality results.

The procedure described in this paper can also be applied to $Kz_2$ elimination where the $Kz$ profile is described by a more sophisticated expression [for instance a modified Lorentzian $I(z) = 1/(1 + az^2)$]. However, the results obtained with the Cauchy-like function show that a more sophisticated profile seems to be unnecessary.

The programs are available by writing to the authors.

The author is greatly indebted to H. Van de Velde and J. P. Bulens for discussions during the writing of the programs.

References