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Numerical evaluation of the double-reflection curve.*

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When the double-crystal diffractometer is operated in the parallel or $(n, -n)$ position with identical crystals at each axis, the double-reflection curve is given by

$$r_2(\beta) = \frac{\int_{-\infty}^{+\infty} [r_1^\sigma(\alpha).r_1^\sigma(\alpha-\beta)+r_1^\pi(\alpha).r_1^\pi(\alpha-\beta)]d\alpha}{\int_{-\infty}^{+\infty} [r_1^\sigma(\alpha)+r_1^\pi(\alpha)]d\alpha} . \quad (1)$$

In this expression, r_1 refers to single reflection, α and β are respectively the angular variables for single and double reflection, and superscripts σ and π refer to the perpendicular and parallel components of polarization (see, for example, James (1948)).

The single-reflection curve, $r_1(\alpha)$, frequently involves functions not amenable to simple algebraic manipulation. In this situation, the adoption of the elementary numerical method described in the following paragraphs should prove satisfactory.

The principal problem in the evaluation of (1) arises in the numerator since this integral must be established for each value of β that is of interest. Ordinarily, the σ and π components must be treated separately in such an evaluation. However, the mathematical forms are comparable in both cases and it will suffice in the following to treat the general integral

$$\int_{-\infty}^{+\infty} r_1(\alpha).r_1(\alpha-\beta)d\alpha . \quad (2)$$

Let the functions $r_1(\alpha)$ and $r_1(\alpha-\beta)$ be defined for values of the variables according to

$$\alpha = n_\alpha.\delta\alpha \quad \text{and} \quad \beta = n_\beta.\delta\alpha ,$$

where $\delta\alpha$ is an angular increment appropriately chosen to define all appreciable values of $r_1(\alpha)$ in the range

$$-n_\alpha^*.\delta\alpha \le \alpha \le n_\alpha^*.\delta\alpha .$$

The value of (2) when n_β is an odd integer is approximately given by

$$\delta\alpha.\sum_{m=-n_\alpha^*+(|n_\beta|-1)/2}^{m=n_\alpha^*-(|n_\beta|+1)/2} [r_1(m-(|n_\beta|-1)/2.r_1(m+(|n_\beta|+1)/2)] . \quad (3)$$

If n_β is an even integer, (2) is approximately equal to

$$\delta\alpha.\sum_{m=-n_\alpha^*+|n_\beta|/2}^{m=n_\alpha^*-|n_\beta|/2} [r_1(m-|n_\beta|/2).r_1(m+|n_\beta|/2)] . \quad (4)$$

When $r_1(\alpha)$ is an even function, i.e., when $r_1(\alpha) = r_1(-\alpha)$, the iteration for all the sums given by (3) can be conveniently expressed in the form of a triangular matrix. As a particularly simple example, let the function $r_1(\alpha)$ be defined at eleven equally spaced points along α such that $n_\alpha^* = 5$. Values of $r_1(\alpha)$ for $n_\alpha > 5$ are negligible. The matrix then has the form

$$\begin{array}{c||lll}
n_\beta & & & \\
1 & r(0).r(1) & & \\
3 & r(1).r(2) & r(0).r(3) & \\
5 & r(2).r(3) & r(1).r(4) & r(0).r(5) \\
7 & r(3).r(4) & r(2).r(5) & \\
9 & r(4).r(5) & &
\end{array}$$

One-half the sum in (3) for a given value of n_β is obtained by adding all the small products in the given n_β row from left to right as far as the row extends and then downward as far as the last column extends. Thus, the values of the integral in (2) become:

$$\int (n_\beta = 1) = 2.\delta\alpha[r(0).r(1)+r(1).r(2)+r(2).r(3) +r(3).r(4)+r(4).r(5)] ,$$

$$\int (n_\beta = 3) = 2.\delta\alpha[r(1).r(2)+r(0).r(3)+r(1).r(4) +r(2).r(5)] ,$$

$$\int (n_\beta = 7) = 2.\delta\alpha[r(3).r(4)+r(2).r(5)] ,$$

etc.

A similar matrix can also be developed for the situations in which n_β is an even integer. The rules for summation need only be modified in this case to the extent that one-half the weight is assessed the first (central) small product.

An evaluation of a large number of double-reflection curves has been completed with the technique described. The single-reflection curves in these computations covered a broad range of shapes between that of a step function and an error function. Although the single-reflection curve was defined by only $n_\alpha^* = 29$ points, it was found that the integrated double reflection, as established by the even integers for n_β, checked the corresponding quantity established by both the odd and even integers to within better than six significant figures in all cases. In turn, these values for the integrated double reflection agreed with the quantity

$$\int r_2(\beta)d\beta = \frac{\left\{\int r_1^\sigma(\alpha)d\alpha\right\}^2 + \left\{\int r_1^\pi(\alpha)d\alpha\right\}^2}{\int r_1^\sigma(\alpha)d\alpha + \int r_1^\pi(\alpha)d\alpha}$$

to within 0·2%.

The numerical evaluation of the double-reflection curve has been demonstrated to be practical with either hand or automatic digital techniques.

* This technique was treated in a dissertation by the author entitled *Diffraction of X-rays by Non-ideal Mosaic Crystals and the Structure of Plastically Deformed and Annealed Crystals of Zinc* submitted to the University of California, Berkeley, California, 1 September 1956.

Reference

James, R. W. (1948). *The Optical Principles of the Diffraction of X-rays*. London: Bell.