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Generalization of the Classical 'Parallel' Condition: Zero-Wavelength-Dispersion 'Counter' Profile Measurement

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Abstract

In the classical two-crystal system with monochromator (M) and specimen (c) crystal axes parallel, measurement with zero-wavelength dispersion (ZWD) is possible at only one value of scattering angle, $\theta_c = \theta_M$, the so-called 'parallel' condition. The procedure is highly selective and therefore of limited applicability. If one examines the situation where the ω rotation axis of c is rotatable (Φ) about the monochromator beam incident on c, the condition can be generalized so that appropriate choice of Φ will allow ZWD measurement anywhere in the range $0 \leq \theta_c \leq \theta_M$, thus releasing this valuable procedure from its earlier severe constraints. The setting condition for Φ is $\cos \Phi = -(\tan \theta_c)/(\tan \theta_M)$.

Introduction

Recently, we have shown how measurements of 'film' profiles,

$$I(\Delta 2\theta) = \int_{\Delta\omega_1}^{\Delta\omega_2} I(\Delta\omega, \Delta 2\theta^{(0)}) \mathrm{d}(\Delta\omega),$$

can be carried out so that they do not involve wavelength dispersion (Mathieson & Stevenson, 1986*b* - hereafter MS86*b*). With this procedure, Bragg reflections from a small single crystal, c, are intercomparable irrespective of the scattering angle, θ_c. As a result, variation of the reflectivity curve [=mosaic spread distribution for imperfect crystals; see Mathieson (1984)] from reflection to reflection can be identified and a more direct estimation of the reflectivity curve for individual reflections in a given orientation is feasible (see Mathieson & Stevenson, 1986*a*). The procedure proposed in MS86*b* for 'film' profiles is applicable also where a monochromator is involved.

'Counter' profiles – examination from the $\Delta\omega$, $\Delta 2\theta$ viewpoint

The question arises as to whether a similar type of capability is feasible for the measurement of 'counter' profiles,

$$I(\Delta\omega) = \int_{\Delta 2\theta_1}^{\Delta 2\theta_2} I(\Delta\omega, \Delta 2\theta^{(0)}) \mathrm{d}(\Delta 2\theta).$$

The analysis in MS86*b* shows that, for the non-monochromator case, the wavelength dispersion component makes a contribution at all θ_c (except $\theta_c = 0°$) and so, apart from that trivial case, the zero-wavelength-dispersion (ZWD) condition is not attainable.

When a monochromator crystal is introduced between the source and the specimen single crystal, interaction of the dispersion of the two crystals offers the potential to overcome that limitation. In the classical treatment of the two-crystal spectrometer (diffractometer) (Compton & Allison, 1935) which deals with extended-face crystals and the configuration where the two crystal axes are parallel, it was shown that the ZWD condition does exist but that it is highly selective, occurring only at the so-called 'parallel' condition where $\theta_c = \theta_M$. At any other value of θ_c, the wavelength dispersion makes a systematic contribution to the 'counter' profile.

Consider (Fig. 1) the more general situation where the ω rotation axis of the small specimen single crystal, c, and hence the associated zero-layer diffraction

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plane, can be rotated about the beam from the monochromator crystal to an angle Φ (Mathieson, 1968, 1985). In the present treatment, crystals M and c are considered as having zero mosaic spread. In Fig. 2(a) the locus of the wavelength dispersion band, $\Delta\lambda = \lambda_+ - \lambda_-$, is depicted in $\Delta\omega, \Delta 2\theta^{(0)}$ space [for terminology see Mathieson (1983)] for the case where $\Phi = 0°$ and the dispersion of c interacts with that of M in the same diffraction plane. Here, the locus of λ has its origin, λ_-, at O while the other extremity, λ_+, lies on the line $O'Z'_-$ at a point which is determined by the value of $t = (\tan\theta_c)/(\tan\theta_M)$. The line $O'Z'_-$ is linearly subdivided in terms of t. $t=0$ at O' where $\theta_c = 0°$. As θ_c increases, the λ_+ extremity is displaced along $O'Z'_-$ to (say) L'_-, the locus of λ then being OL'_-. When $t = -0{\cdot}50$, the λ locus is OA'; when $t = -1{\cdot}0$, it is OB'. In the latter case, it is evident from Fig. 2(a) that the whole of the $\Delta\lambda$ band interacts simultaneously and so that λ component makes a zero contribution to the 'counter' profile. This condition corresponds to the classical 'parallel' case. Away from this special condition, *e.g.* at OL'_-, the λ component straddles a range of $\Delta\omega$ settings, does not interact simultaneously and hence contributes to the size of the 'counter' profile.

When $\Phi = 90°$, the relationship of the disposition of M and c is different. Fig. 2(b) depicts the situation in relation to $\Delta\omega, \Delta 2\theta^{(0)}$ space. The λ_+ extremity of the λ dispersion of M now lies in a plane below and parallel to the (λ_-) diffraction plane of c. For $\theta_c = 0°$, the λ_+ extremity is at O'', below O and perpendicular to the $\Delta\omega, \Delta 2\theta^{(0)}$ plane. The locus of λ_+ is $O''Z''_-$ which is parallel to $O'Z'_-$. So the λ locus corresponds to (say) OL''_-. In this configuration, there is only one location where the $\Delta\lambda$ band interacts simultaneously, namely at $\theta_c = 0°$. At that setting, the receiving aperture in front of the detector must have sufficient height to accept the $\Delta\lambda$ band. Hence, in generalizing the situation, the condition to which we must look is not that the λ locus lie parallel to the $\Delta 2\theta$ axis but that it lie in a plane which passes through the $\Delta 2\theta$ axis and is perpendicular to the $\Delta\omega, \Delta 2\theta$ plane. This corresponds to the projection of the λ locus on the $\Delta 2\theta$ axis.

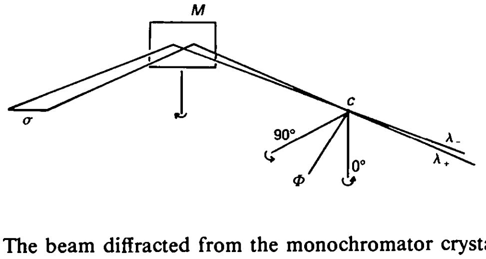
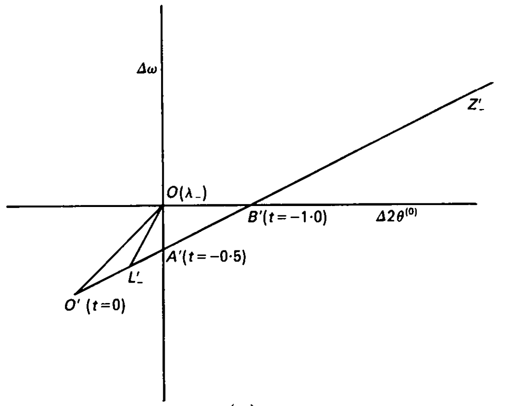
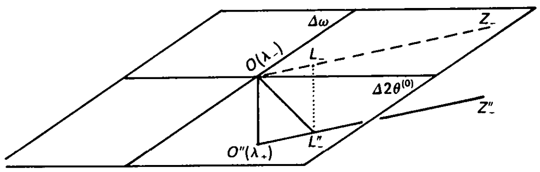


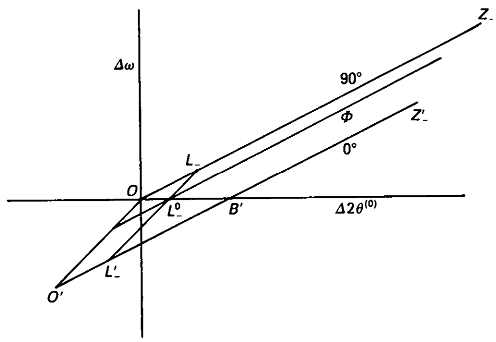
Fig. 1. The beam diffracted from the monochromator crystal, M, is incident on the specimen single crystal, c, at right angles to its rotation axis. The ω rotation axis of c is capable of being tilted around the beam at any orientation angle, Φ, at least between 0 and 90°. $\Phi = 0°$ corresponds to the rotation axis of c being parallel to that of M.



(a)



(b)



(c)

Fig. 2. (a) For the case $\Phi = 0°$, the variation in wavelength dispersion, $\Delta\lambda = \lambda_+ - \lambda_-$, with change in θ_c is demonstrated diagrammatically in $\Delta\omega, \Delta 2\theta^{(0)}$ space. The origin O corresponds to the lower extremity, λ_-, while the other extremity, λ_+, has as its locus the line $O'Z'_-$. The line $O'Z'_-$ lies at a slope of 1 in 2 to the $\Delta 2\theta^{(0)}$ axis and is subdivided linearly in terms of $t = (\tan\theta_c)/(\tan\theta_M)$. O' corresponds to $t = 0$, *i.e.* $\theta_c = 0°$. A' corresponds to $t = -0{\cdot}50$ while B' corresponds to $t = -1{\cdot}0$, the classical 'parallel' condition. The wavelength dispersion for any given value of t corresponds to the line joining O to the appropriate point on $O'Z'_-$ with that value of t, *e.g.* OL'_-. (b) For the case $\Phi = 90°$, the extremity, λ_+, lies in a plane parallel to the $\Delta\omega, \Delta 2\theta^{(0)}$ plane through $O(\lambda_-)$. The locus of λ_+ is $O''_-Z''_-$, O'' corresponding to $\theta_c = 0°$. The line OZ_- is in the $\Delta\omega, \Delta 2\theta^{(0)}$ plane and parallel to $O''Z''_-$. So the λ component corresponds to (say) OL''_- and OL_- is its projection onto the $\Delta\omega, \Delta 2\theta^{(0)}$ plane. (c) This illustrates how the extremity, λ_+, of the λ component, projected on the $\Delta\omega, \Delta 2\theta^{(0)}$ plane, moves in $\Delta\omega, \Delta 2\theta$ space as Φ changes from $\Phi = 0$ to 90°. At some appropriate value of Φ, the locus of L intersects the *plane* through the $\Delta 2\theta^{(0)}$ axis and normal to the $\Delta\omega, \Delta 2\theta^{(0)}$ plane. At this value, the λ locus OL^0_- lies in the vertical plane and therefore the $\Delta\lambda$ band interacts simultaneously. Its contribution to wavelength dispersion is therefore zero.

On this basis, as Φ is varied from 0 to 90°, the general point L'_- traces out the line L'_-L_- in Fig. 2(c). At some value of Φ, this line will cross the plane through the $\Delta 2\theta$ axis. The λ locus is then OL''^0_-, in projection OL^0_-. The whole of the $\Delta\lambda$ band interacts simultaneously and so the λ component makes a zero contribution to the 'counter' profile for this setting of Φ. The setting condition for Φ is that $\cos \Phi = -t$; see equation (4) in Mathieson (1985).

Hence, by the appropriate choice of Φ, one can bring any reflection with scattering angle θ_c to the ZWD condition. The only limitation is that $\theta_c \leq \theta_M$.

Discussion

While the classical 'parallel' condition has valuable properties for the measurement of reflectivity curves and for the establishment of accurate structure-factor values, there are restrictions in its use. Normally, one wishes to measure for a specimen crystal a number of different Bragg reflections which span a range of θ_c. If only one monochromator crystal is available, then measurement in the ZWD condition cannot be attempted. The alternative is to obtain a number of monochromator crystals with Bragg angles exactly matched to those of the specimen crystal - a task difficult in practice. The scheme outlined here would provide suitable flexibility to extend the capability of zero-wavelength-dispersion measurement.

Fig. 2, especially Fig. 2(c), shows that the range of application of the procedure lies within the region $0 \leq \theta_c \leq \theta_M$. Hence the larger θ_M is, the wider is its range of application and the greater its usefulness. The advantage of high θ_M for matters of resolution has been advocated on many occasions - the present proposal would appear to provide further reason for the use of high-θ_M monochromator crystals.

To effect this type of measurement requires that the four-circle diffractometer necessary to orient the specimen crystal (and detector) be itself mounted in a cradle which is capable of rotation about the beam for the monochromator crystal at least over the range $\Phi = 0$ to 90°. Thus, the basic requirement is a five-circle device.

The procedure suggested here would appear to be of interest to some users of synchrotrons where ZWD operations could be of value to explore variability in reflectivity curves and hence extinction conditions; see Fig. 4 in Höche, Schulz, Weber, Belzner, Wolf & Wulf (1986).

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Functional Form of Some Ideal Hypersymmetric Distributions of Structure Factors

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Abstract

The hypercentric or hyperparallel distribution of structure factors of order n [Rogers & Wilson (1953). *Acta Cryst.* **6**, 439-449] can be expressed in terms of Meijer's G functions [Erdélyi (1953). (Editor.) *Higher Transcendental Functions*, Vol. I, Ch. V. New York: McGraw-Hill]:

$$P_n(F) = (2^{n-2}\pi^n\Sigma)^{-1/2} \times G^{n,0}_{n-1,n}(F^2/2^n\Sigma\,|\,\tfrac{1}{2},\dots,\tfrac{1}{2};0,0,\dots,0),$$

where F is the modulus of the structure factor. This reduces to the known centric and bicentric distributions for $n = 1, 2$.

Introduction

The simplest hypersymmetric distribution, the bicentric, was introduced by Lipson & Woolfson (1952). They expressed it as an integral and evaluated it numerically. Their work was extended to higher hypersymmetries (hypercentric and hyperparallel) by Rogers & Wilson (Wilson, 1952; Rogers & Wilson, 1953), who showed that the bicentric distribution could be expressed in terms of the known Bessel function K_0. For the higher members of the series Rogers & Wilson gave integral representations, moments and Gram-Charlier expansions. The purpose of this note is to express the higher members in terms of the known but not very familiar G functions

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