C.M. BRAKMAN

ON THE INTERPRETATION
OF DIFFRACTION
LINE-SHIFT MEASUREMENTS
ON RED CUBIC MATERIALS
8. Het verdient aanbeveling de mogelijkheid te scheppen om hoogleraren na hun 60e levensjaar te ontheffen van het actief groepsleiderschap. Zij dienen vervolgens in staat te worden gesteld om hun intellectuele levenswerk samen te vatten in één of meerdere boeken van blijvende, wetenschappelijke waarde.

9. Indien men de universiteit aanduidt met 'Kerk van de Rede' rijst de vraag of de minister van onderwijs als paus of als inquisiteur gezien moet worden.


10. Respect voor eigendommen van andere (rechts)personen is geen aangeboren instinct. Het aanleren ervan zou een wezenlijk element moeten zijn van iedere opvoeding. De maatschappelijke kosten van vandalisme en aanverwant gedrag zijn hoog. Het verdient aanbeveling om te trachten via het basisonderwijs een verandering ten goede te bewerkstelligen.

C.M. Brakman


Stellingen

behorende bij het proefschrift

'On the Interpretation of Diffraction Line-Shift Measurements on Textured Cubic Materials'

1. Gediffraateerde intensiteit hangt alleen af van de waarde van de orientatie distributie functie (odf) gemiddeld over de rotatiehoek om de verstrooiingsvector. Diffractie hangt ook nog af van de eerste en tweede orde variatie van de odf met betrekking tot deze rotatiehoek. Hierdoor kan het voorkomen dat de hkl intensiteits-poolligur textuurvrij is terwijl de hkl diffractiek-poolfigur getextureerd gedrag vertoont. Het is echter niet aannemelijk dat in dat geval kristallografische textuur en elastische anisotropie een verklaring vormen voor de zogenaamde 'psi-splitting'.

2. Bij preparaten bestaande uit kristallen die behoren tot een puntgroep met alleen rotationele symmetrie-elementen, kan men de gemeten intensiteits-poolfiguur opgebouwd denken uit die van de links- en rechtshandige kristallen. De verhouding tussen de fracties links- en rechtshandige kristallen is dan een functie van de stand van de verstrooiingsvector. De impliciete veronderstelling van Bunge dat deze verhouding constant zou zijn, moet niet aannemelijk worden geacht.


3. Bij de plastische vervorming van metalen ontwikkelen de kristallografische textuur en de inwendige spanningen zich gelijktijdig en vermoedelijk gecorreleerd. Over de samenhang is weinig bekend. Voor de opheldering hiervan is een plasticiteitsmodel nodig dat rekening houdt met de wederzijdse beinvloeding van textuurontwikkeling en opbouw van de inwendige spanningen.
4. Met behulp van MoKα straling en de \{651 + 732\} dubbelreflectie vinden Hauk en Vaessen de spanningen: σ₁ = -104 MPa en σ₂ = -138 MPa in koud-gewalst laag-koolstofstaal. Zij stellen terecht dat de niet-lineariteiten in de diffractierek als functie van sin² ψ gemeten met de \{211\} reflectie en CrKα aan hetzelfde staal, nooit met deze spanningstoestand in combinatie met elastische anisotropie verklaard kunnen worden. Op grond hiervan wordt aangenomen dat plastic anisotropie de oorzaak is van niet-lineaire diffractierek versus sin 2 ψ.


5. In tegenstelling tot de opvattingen van vele auteurs in het vakgebied van de inwendige spanningsbepaling, is het gebruik van de macroscopische elastische constanten ν en E, al dan niet voorzien van een index hkl, in uitdrukkingen voor diffractierek (d.w.z. een microscopische grootheid) af te raden.


6. In de techniek worden oppervlakkelagen op metalen voorwerpen aangebracht om afhankelijk van de toepassing, weerstand tegen slijtage, corrosie en/of vermoeie te verkrijgen. Zulke lagen worden vaak gemaakt door inbrengen door diffusie van een chemisch element bij verhoogde temperatuur. In tegenstelling tot de procedure volgens Plüntitz et. al. moet, voor processen waar de laag uit meer dan één fase bestaat, de bepaling van de kinetische parameters voor diffusie in één van de fasen, geschieden met een model dat de koppeling van de kinetische parameters van alle fasen in rekening brengt.


7. Het is experimenteel bewezen dat de ductilititeit van (o.a. staal-) plaatmateriaal voldoende is voor dieptrekken in één trek met zeer grote dieptrekverhouding. Zelfs aan lage-kwaliteit plaatmateriaal zijn trekverhoudingen van 6 en 8 bereikt. Bij deze laboratoriumexperimenten werden laagsmeltende metalen gebruikt als medium om wrijvingskrachten en druk op het plaatmateriaal over te brengen. De industrie heeft behoefte aan dieptrekken in één trek, economisch en reproduceerbaar, tot verhoudingen van 3~4, zonder de noodzaak van verwijdering van het medium na afloop van het proces. Een oplossing dient te worden gezocht in het gebruik van die vloeistoffen als medium die zich bij hoge proces-snelheden gedragen als vaste stoffen.

ON THE INTERPRETATION OF DIFFRACTION LINE-SHIFT MEASUREMENTS ON TEXTURED CUBIC MATERIALS

APPLICATION OF THE ORIENTATION DISTRIBUTION FUNCTION AND IMPLICATIONS FOR RESIDUAL STRESS DETERMINATION

\[ \text{Formula} \]

\[ \text{Equation} \]
ON THE INTERPRETATION OF DIFFRACTION LINE-SHIFT MEASUREMENTS ON TEXTURED CUBIC MATERIALS

APPLICATION OF THE ORIENTATION DISTRIBUTION FUNCTION AND IMPLICATIONS FOR RESIDUAL STRESS DETERMINATION

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Delft, op gezag van de Rector Magnificus, Prof. drs. P.A. Schenck in het openbaar te verdedigen ten overstaan van een commissie door het College van Dekanen daartoe aangewezen, op maandag 26 september 1986, te 14.00 uur

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Erratum

P. 1, line 23: add after 'crystallites': and the occurrence of preferred orientation of the crystallites.
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Summary.  

Samenvatting.
1. INTRODUCTION.

This thesis deals with:

(i) explanation of diffraction strain phenomena obtained on poly-crystalline materials exhibiting preferred orientation of the crystallites.
(ii) determination of residual stresses from such diffraction strain data.

Residual stresses arise in a wide variety of materials. They often develop as a consequence of inhomogeneous plastic deformation occurring during processing. Inhomogeneous distribution of temperature during cooling after thermal treatment leads to similar effects. Other causes occur as well in practice.

These internal stresses can strongly influence service-life. The case of residual stresses in components subject to cyclic loading is well-known, for instance. Therefore, non-destructive determination of such stresses is of great importance. It can lead to enhanced service-life and better use of materials.

For non-destructive stress determination mainly diffraction methods are used. One can only measure lattice-spacings, from which strains are easily obtained; stresses can be determined only indirectly using diffraction techniques. The so-called diffraction strains can be calculated using lattice-spacing data of the unstrained material. The shift of the diffraction line profile is a direct measure for the strain. Stresses are determined from the diffraction strains using the appropriate (i.e. elastic) stress-strain relationship. The diffraction method most commonly used is the so-called sin^2Ψ method which has been developed in the 1930's in Germany by (among others) Glocke [1], Möller & Martin [2] and Schiebold [3].

For polycrystalline materials two causes of anisotropy have to be distinguished: the elastic anisotropy of the individual crystallites. The latter phenomenon is usually indicated by 'crystallographic texture' or 'texture' for short. If however, such a textured specimen consists of elastically isotropic crystallites the macroscopic strain of the specimen in a given direction and the strain of individual crystallites in this direction will be identical.

A texture-free specimen consisting of elastically anisotropic crystallites is macroscopically isotropic. In the following section we will consider the latter type of specimen.
1.1 The $\sin^2\psi$ method.

For the *macroscopic* normal-strain component in the $\psi,\phi$ direction (Fig. 1) of a biaxially stressed specimen it can be written:

$$
\varepsilon_{\psi,\phi} = -(\nu / E) (\sigma_1 + \sigma_2) + \{(1+\nu) / E\} \sigma_\phi \sin^2\psi
$$

(1)

where $\sigma_1$ and $\sigma_2$ are principal stresses and $E$ and $\nu$ stand for the macroscopic elastic constants and:

$$
\sigma_\phi = \sigma_1 \cos^2\phi + \sigma_2 \sin^2\phi
$$

The strain thus depends linearly on $\sin^2\psi$. From a plot of the strain vs. $\sin^2\psi$ the stresses can be determined. The case of a triaxial stress-state is not essentially different. Eq.(1) is independent of any assumptions about elasticity models. It is just Hooke's law written for the strain in the general $\psi,\phi$ direction caused by a biaxial stress.

In the case of *diffraction* methods employed the direction $\psi,\phi$ is parallel to [hkl] in the diffracting crystal. Eq. (1) reads:

$$
\varepsilon_{\psi,\phi} = (d_{\psi,\phi} - d_0)/d_0 = s_1(hkl)(\sigma_1 + \sigma_2) + 1/2 s_2(hkl)\sigma_\phi \sin^2\psi
$$

(2)

where $d_{\psi,\phi}$ and $d_0$ stand for the hkl-interplanar lattice spacings of the material in the loaded and unloaded conditions, respectively. The symbols $s_1(hkl)$ and $1/2 s_2(hkl)$ denote the so-called diffraction elastic constants. They depend on hkl. They can be calculated on the basis of an elasticity model and the single crystal elastic constants. The stresses can be determined from the diffraction strain provided the $\psi$- and $\phi$- dependency is correct. In some cases [6,7] the $s_1$ and $1/2 s_2$ obtained using known stresses are not identical to those calculated. The symbol on the left-hand side of eq.(2) stands for the *diffraction* strain.
Fig. 1. Definition of angles $\psi$ and $\phi$ with respect to the principal axes of the (macro) stress tensor. In most cases the principal axes of the stress tensor are taken to be coincident with the specimen's axes of symmetry. The angles determine the orientation of the scattering vector with respect to this reference system.

In the diffraction experiment, only a fraction of the crystallites contribute to the diffracted intensity. The experiment automatically selects only those crystallites with an hkl reciprocal lattice vector parallel to the scattering vector. As a consequence the experiment only 'sees' the strains of these grains and therefore, eqs. (1) and (2) may yield quite different results for the stresses even in materials without preferred orientation of the crystallites. The diffraction elastic constants $s_1$ and $1/2 s_2$ equal their macroscopic counterparts of eq.(1) only in special cases.
Eq. (2) predicts linear behaviour of the diffraction strain vs. \( \sin^2 \psi \). This equation has been used for non-destructive stress analysis for a long time [4,5]. The case of the full stress tensor has also been treated in the literature [6]; this case is omitted here. In a lot of practical examples eq. (2) is obeyed. However, an increasing amount of literature data of the past 15 years displays non-linear diffraction strain behaviour vs. \( \sin^2 \psi \) [7,8].

1.2 Problems in applying the linear \( \sin^2 \psi \) method.

Fig. 2. Non-linear lattice strain distributions vs. \( \sin^2 \psi \): (a) after cold-rolling (b) after tangent deformation. After Dölle [6].

(i) **Non-linearity** impedes straightforward calculation of the stresses by means of eq.(2). Non-linearity has been reported [6,9] for many materials exhibiting preferred orientation of the crystallites. The corresponding type of non-linearity is referred to as 'oscillatory' behaviour and also 'Schlangenkurve' (Fig. 2a).
The so-called 'ψ-splitting': different diffraction strain values observed for equal but opposite values of ψ. In Fig. 1 this amounts to different diffraction strain values observed in the directions ψ,ϕ and ψ, ϕ+π. It often arises after shearing-type deformations like grinding and wear. Non-linearity can occur simultaneously. Crystallographic texture is not a prerequisite for this phenomenon [6,7]. (Fig. 2b).

1.3 Causes of non-linearity and ψ-splitting.

(i) Crystallographic texture. Its consequences constitute the main theme of this thesis.

(ii) Shear stresses. If eq. (2) is written for the full stress tensor it follows that shear stresses operating in planes perpendicular to the specimen's surface normal introduce a term linear in sin 2ψ. This explains the ψ-splitting [7,10] if the existence of such stresses is accepted. It has been pointed out [11] that this is physically impossible in the case of single-phase materials because the conditions of mechanical equilibrium would be violated.

(iii) Plastic anisotropy. This may arise simultaneously with crystallographic texture in the plastic deformation history of the specimen. On processing, adjacent grains with different crystallite orientations undergo different deformations. After the processing, stresses develop in order to retain intergranular coherence. The corresponding residual stresses of this type are referred to by 'Spannungen 2. Or Art' (stresses of the second kind) or 'pseudomacro-stresses'.[12,13,14]

1.4 Scope of this thesis.

The present treatment deals with the explanation of non-linearity of measured diffraction strains vs. sin²ψ in terms of crystallographic texture in conjunction with the elastic anisotropy of the crystallites. Diffraction strain is an average of the single crystallite strains of those grains contributing to the diffraction. For these crystallites the hkl-direction is parallel to the scattering vector (i.e. the ψ,ϕ direction). Different crystallite orientations (different rotation angles about hkl) exhibit different strains in a homogeneous stress field due to single crystal elastic anisotropy.
For texture-free specimens the averages of the contributing crystallite strains can be shown to be on a straight line vs. $\sin^2\psi$. In the case of specimens exhibiting crystallographic texture the mean value depends on the crystallite orientations' frequency of occurrence. This frequency is a description of the texture of the specimen. It operates as a weight function with respect to the single crystallite strains.

It is the purpose of this thesis to quantitatively take into account crystallographic texture using the crystallites' orientation distribution function (odf) as a weight function. It represents an improvement of the so-called 'ideal orientations' method which is not adequate for most practical materials. The so-called series-expansion method [15] of the odf is used for practical calculations.

It will be shown that introduction of the odf in general leads to non-linear diffraction strain behaviour vs. $\sin^2\psi$.

The odf is also treated as a 5-term Fourier-series with respect to the rotation angle about the scattering vector. This allows a clear treatment of the problem in terms of simple physical concepts.

The analysis is applied to single-phase cubic materials. An assumption has been made concerning the stress-state of the material and the elasticity model relating stresses to strains. Macro-stresses (residual or applied) are taken as the cause of the strains observed. Macro-stresses are assumed to be constant over distances large compared to the grain size. The Kröner model of elastic polycrystal coupling [16] cannot be applied in analytical form to the case of textured materials. Instead, the Reuss [17] and Voigt [18] elasticity models have been used.

The Voigt model assumes constant strain throughout the specimen, the Reuss model assumes constant stress. In the Voigt model case the diffraction strain is asserted to be equal to the macroscopic strain. Eq. (2) is equivalent to eq. (1) then.

Both models have been adapted and applied to the textured materials case. Even then the Voigt model diffraction strain expression is linear with respect to $\sin^2\psi$. This is expected since Hooke's law written for an anisotropic specimen still yields linear behaviour of macroscopic strain with respect to $\sin^2\psi$. In the Reuss model equations non-linearity enters through the odf. Generally, non-linearity is predicted correctly. The amplitudes are too large, however.
The Voigt model diffraction strain expressions only exhibit the fourth-order series-expansion coefficients of the odf. In the Reuss model case the series-expansion has to be truncated as a consequence of the limited accuracy of the odf. In the Reuss model diffraction strain expressions a new type of surface spherical harmonic arises.

The Reuss model has been applied to the case of multiple coinciding reflections claimed [7,13] to yield linear behaviour vs. $\sin^2\psi$ even in the presence of texture. Results obtained indicate that linearity depends on the type of the texture: general behaviour in this sense cannot be expected.

The so-called Hill [19] average of the Reuss and Voigt model predictions is applied in the experimental analysis of a textured steel sheet specimen loaded in a tensile test device on an X-ray diffractometer.

It is concluded that the elastic anisotropy in conjunction with crystallographic texture can explain non-linear diffraction strain behaviour observed on textured materials. A good approximation to experimental data is observed. For residual stress determination the Hill approximation can be used.

However, the so-called plastic anisotropy as a cause for non-linearity vs. $\sin^2\psi$ in textured cold-rolled steels cannot be neglected [13, 20]. Generally, both elastic and plastic anisotropy may simultaneously be the cause of non-linearity vs. $\sin^2\psi$ in these materials. Construction of a model allowing systematic separation of both elastic and plastic anisotropy seems profitable. The elastic anisotropy treatment given here can provide the basis for such a model.
REFERENCES.

2. RESIDUAL STRESSES IN CUBIC MATERIALS WITH ORTHORHOMBIC OR MONOCLINIC SPECIMEN SYMMETRY: INFLUENCE OF TEXTURE ON Ψ SPLITTING AND NON-LINEAR BEHAVIOUR.
Residual Stresses in Cubic Materials with Orthorhombic or Monoclinic Specimen Symmetry: Influence of Texture on $\psi$ Splitting and Non-linear Behaviour

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Abstract

A quantitative formulation is given of the X-ray diffraction determination of (elastic) lattice deformation in a direction determined by two angles $\psi$ and $\varphi$ with respect to the specimen frame: the so-called $\sin^2\psi$ method giving full credit now to crystallographic texture. In most cases of practical X-ray stress analysis, (residual) stresses are evaluated by the traditional $\sin^2\psi$ method using quasi-isotropic X-ray elastic constants depending on the lattice plane $\{hkl\}$ chosen for the measurement but not on the directions $\varphi$ and $\psi$. For the case of a textured specimen, however, the single-crystal elastic bitensor components should be coupled to the orientation distribution function (o.d.f). At variance with most papers published on this subject, which describe the texture using ideal texture components, a general method is developed making full use of relevant o.d.f. theory. It is demonstrated that for orthorhombic specimen symmetry no $\psi$ splitting occurs in contrast with the case of monoclinic specimen symmetry. The theory developed is used to explain some experimental results published previously. All calculations use Reuss's theory of elasticity which neglects the mutual coupling of the crystallites.

The following equation has found widespread use:

$$
\langle \varepsilon_{zz} \rangle = \frac{d_{\varphi\varphi} - d_0}{d_0} = \frac{1}{2} S_2(hkl) \sigma_0 \sin^2\psi + S_1(hkl)[\sigma_{11} + \sigma_{22}]
$$

(1)

for the case that only $\sigma_{11}$ and $\sigma_{22} \neq 0$. Here

$$
\sigma_0 = \sigma_{11} \cos^2\varphi + \sigma_{22} \sin^2\varphi
$$

(1a)

d$_{\varphi\varphi}$ = measured lattice parameter in direction $\varphi$, $\psi$

d$_0$ = measured lattice parameter in a stress-free specimen of the same material.

The definitions of the X-ray elastic constants $S_1(hkl)$ and $S_2(hkl)$ read:

$$
S_1(hkl) = S_{1122} + S_0 \Gamma(hkl)
$$

(4)

$$
\frac{1}{2} S_2(hkl) = S_{1111} - S_{1122} - 3S_0 \Gamma(hkl)
$$

(5)

$$
\Gamma(hkl) = \frac{h^2k^2 + h^2l^2 + k^2l^2}{(h^2 + k^2 + l^2)^2}
$$

(6)

$$
S_0 = S_{1111} - S_{1122} - 2S_{1212}.
$$

(7)

Note that, generally speaking, the X-ray elastic constants are the coefficients that should be multiplied by all relevant stress-tensor components in order to find the total elastic strain in the measuring direction $\psi$, $\varphi$. $S_{1111}$, $S_{1122}$ and $S_{1212}$ are the well-known elements of the compliance tensor with respect to cubic crystal axes. Note that (4) and (5) represent X-ray elastic constants in the Reuss approximation.

The mean lattice strain $\langle \varepsilon_{zz} \rangle$ is measured in the $Z$ direction of the measurement ($L$) frame (Fig. 2). This axis is determined by the angles $\psi$ and $\varphi$ with respect to the specimen frame. Equation (1) predicts that a plot of $d_{\varphi\varphi}$ vs $\sin^2\psi$ should be a straight line. In practice, however, deviations from linearity are often observed: (i) non-linear behaviour of $\langle \varepsilon_{zz} \rangle$ vs $\sin^2\psi$; (ii) $\psi$ splitting: different values of $\langle \varepsilon_{zz} \rangle$ for $-\psi$ and $+\psi$ (Fig. 1).

In the literature attempts have been made to explain $\psi$ splitting assuming stress gradients (more specifically...
\( \sigma_{13} \) and \( \sigma_{23} \) in the surface layers of the specimen (Dölle, Hauk & Neubauer, 1978; Cohen, Dölle & James, 1979; Dölle & Hauk, 1979). However, the equations of mechanical equilibrium require that at the surface of the specimen the following condition should hold: \( \sigma_{13}(z) = \sigma_{23}(z) = \sigma_{33}(z) = 0 \) for \( z = 0 \). Furthermore, if it is assumed that the stress-tensor components and the strain-tensor components only depend on \( z \) the following conditions should hold as well (Timoshenko & Goodier, 1970):

\[
\frac{\partial \sigma_{13}(z)}{\partial z} = \frac{\partial \sigma_{23}(z)}{\partial z} = 0.
\]

Even if there were any body forces present in the \( Z \) direction, this would only lead to a gradient in \( \sigma_{33} \). Hence, from a theoretical point of view it would be interesting to look for an explanation of the experimental data not taking into account gradients in the stress-tensor components \( \sigma_{13} \) and \( \sigma_{23} \). Now it can be argued that under these assumptions in the case of orthorhombic specimen symmetry no \( \psi \) splitting can occur whereas any 'lower' specimen symmetry introduces the possibility of \( \psi \) splitting. This line of thought was implicitly proposed by Dölle & Hauk (1978, p. 415) and more explicitly by van Baal (1982). With reference to the symmetry of the problem it may be argued that \( \sigma_{12} = 0 \) even in the layers below the surface. In that case (\( \sigma_{13} \) and \( \sigma_{23} \) taken \( \equiv 0 \) as well) the reference frame of the principal stresses will always be coincident with the specimen symmetry axes. If the elastic bitensors for orthorhombic and monoclinic specimen symmetry (Nye, 1972) are taken into account, it is easily seen that in the orthorhombic case the reference frame of principal strains is coincident with the specimen symmetry axes in contrast with the monoclinic case (Penning, 1981). Thus, in the latter case macroscopic shear strains \( \varepsilon_{13} \) occur. The fact that \( \varepsilon_{13} \neq 0 \) now gives rise to \( \psi \) splitting (van Baal, 1983). Furthermore, the explanation for the \( \psi \) splitting given in the literature (Dölle & Hauk, 1978; Dölle & Cohen, 1980a; Peiter, 1976) that the reference frame of the principal stresses is tilted away from the specimen symmetry axes leads to the assumption of stress gradients as well because in that case \( \sigma_{13} \) and \( \sigma_{23} \) should be \( \neq 0 \) on the specimen reference frame. Still, at the surface \( \sigma_{13} \), \( \sigma_{23} \) as well as \( \sigma_{33} \) should be equal to zero. Therefore, this line of thought will not be followed here.

It is the purpose of this paper to present a full quantitative treatment of the phenomena mentioned above for the cases of orthorhombic and monoclinic specimen symmetries giving full credit to crystallographic texture. The resulting expressions will be applied to explain some experimental data published previously (Hauk, Krug & Vaessen, 1981; Dölle & Cohen, 1980a, b).

In the treatment the following assumptions are made:

1. The X-ray radiation used does not penetrate beyond the depth of the deformed surface layer.
2. The texture is homogeneous over the penetration depth of the X-rays.
3. The specimen principal directions (symmetry axes) are the principal directions of the residual stress tensor as well. After rolling these are RD, TD and ND, after grinding, milling, etc. one has SD, TD and ND (Fig. 2).
4. Only \( \sigma_{11} \) and \( \sigma_{22} \) are taken to be \( \neq 0 \). This assumption leaves the existence of gradients in \( \sigma_{11} \) and \( \sigma_{22} \) possible. In that case one measures a mean value of these stresses integrated over subsequent layers below the surface (Dölle & Hauk, 1979). Gradients in the stresses \( \sigma_{13} \) and \( \sigma_{23} \) are taken \( \equiv 0 \). The influence of a non-zero \( \sigma_{33} \) in the layers below the surface will briefly be considered. It will be demonstrated here that available experimental evidence can be explained qualitatively without taking into account any shear stresses or \( \sigma_{33} \).
5. The model of elasticity formulated by Reuss (1929) is thought to be valid, i.e. stress continuity across the grain boundaries is assumed and (implicitly) there is no elastic coupling between the crystallites. It will be argued, however, that the analysis given can be easily extended to the Voigt (1928) or Kröner (1958, 1967) models.

Although the treatment given is applied in particular to b.c.c. crystals the analysis may be easily extended to f.c.c. crystals as well. The model of texture representation formulated by Bunge (1969, pp. 20–90) is used.

2. Definition of angles, reference frames and transformation matrices

Throughout this paper, as far as possible, the same notation will be used as was given in the paper by Dölle & Hauk (1978). In the specimen (\( P \)) frame the \( L_1 \) direction is determined by the angles \( \psi \) and \( \varphi \) (Fig. 2). The rotation about the \( L_1 \) axis of the measurement (\( L \)) frame is given by the angle \( \varphi_2 \). The system of

Fig. 1. Non-linear lattice strain distributions as \( \sin^2 \psi \): (a) after cold-rolling; (b) after tangent deformation. After Dölle (1979).
Euler angles is defined in accordance with Gelfand, Minlos & Shapiro (1963, p. 5) and Bunge (1969, pp. 20–90). For the rotation \( g_1 \), which transforms the specimen (P) frame into the measurement (L) frame, \( g_1 = (\varphi + \pi/2, \psi, \varphi_2) \), where \( \varphi_2 \) can be chosen freely. The associated transformation matrix now reads:

\[
\begin{pmatrix}
\sin \varphi \cos \varphi_2 & \cos \varphi \cos \varphi_2 & \sin \psi \sin \varphi \\
-\cos \varphi \cos \psi \sin \varphi_2 & -\sin \varphi \cos \psi \sin \varphi_2 & \sin \varphi \cos \psi \\
-\sin \varphi \sin \psi \cos \varphi_2 & -\cos \varphi \sin \psi \cos \varphi_2 & \cos \psi \sin \varphi
\end{pmatrix}
\]

(8)

This matrix is found if one multiplies the transformation matrices of the subsequent rotations \( \{\varphi + \pi/2, 0, 0\} \), \( \{0, \psi, 0\} \) and \( \{0, 0, \varphi_2\} \) in the following order:

\[
g_1 = g_{\varphi_2} \times g_\psi \times g_{\varphi + \pi/2}.
\]

(9)

The orientation of the crystal corresponding to diffracted intensity in the direction of \( L_3 \) for the \( hkl \) reflection is generated from the measurement (L) frame by means of rotation \( g_2 \). If one defines the \([hkl] \) direction in the crystal by means of the angles \( \varphi_\beta \) and \( \beta_\beta \) (Fig. 2) the rotation \( g_2 \) can be put equal to

\[
g_2 \rightarrow \{\varphi_2, \varphi_\beta, \pi/2 - \beta_\beta\}.
\]

(10)

Just as \( \varphi_2, \varphi_\beta \) can be chosen freely, this can be easily understood if one realizes that the definition of a direction leaves one parameter free as far as the orientation of a reference frame is concerned. Note that the angles \( \varphi + \pi/2 \) and \( \pi/2 - \beta_\beta \) in the Euler rotation operators \( g_1 \) and \( g_2 \) are needed to ensure that \( L_3 \) and \([hkl]\) have the correct orientations \( \psi, \varphi \) and \( \varphi_\beta, \beta_\beta \) with respect to the specimen frame and the crystal reference axes. Both \( \varphi_2 \) and \( \varphi_\beta \) are rotations about \( L_3 \). We now obtain:

\[
g_2 =
\begin{pmatrix}
\cos \varphi_\beta \sin \beta_\beta & \sin \varphi_\beta \sin \beta_\beta & \sin \psi \cos \varphi_\beta \\
-\sin \varphi_\beta \cos \varphi_\beta \cos \beta_\beta & -\cos \varphi_\beta \cos \varphi_\beta \cos \beta_\beta & \cos \psi \cos \varphi_\beta \\
-\sin \varphi_\beta \cos \varphi_\beta \sin \beta_\beta & -\cos \varphi_\beta \cos \varphi_\beta \sin \beta_\beta & \sin \psi \sin \varphi_\beta
\end{pmatrix}
\]

(11)

For completeness it is emphasized that the row vectors in (8) and (11) are the basis vectors of the new reference frame in terms of the old one. For the strain in a single crystal in the \( L_3 \) direction we now write

\[
e_{zz} = S_{zzij} \sigma_{ij},
\]

(12)

where \( S_{nnij} \) is the compliance tensor in terms of the measurement (L) frame and \( \sigma_{ij} \) is the stress tensor in terms of the measurement (L) frame. The \( S_{zzij} \) may be computed from the single-crystal compliances using

\[
S_{zzij} = C_{km} C_{kn} C_{ij} S_{mnop} \quad \text{(where } S_{zzij} = S_{zzij})
\]

\[
= S_{1122} \delta_{ij} + 2 S_{1212} \delta_{3i} \delta_{3j} + S_{0} C_{ik} C_{ik} C_{jk}.
\]

(13)

Here the \( S_{mnop} \) are the single-crystal compliances with respect to the crystal axes and the \( C_{ij} \) are the elements of the inverted matrix \( g_2 \). Because the determinant of these rotation matrices is always equal to +1 the inverse of \( g_2 \) is found by simply transposing. Finally, one obtains

\[
e_{zz} = (S_{1122} + S_{0} C_{ik} C_{ik} \sigma_{ik}) \delta_{xx} + (S_{1122} + S_{0} C_{ik} C_{ik} \sigma_{yy})
\]

\[
+ (S_{1212} + 2 S_{1212} + S_{0} C_{ik} C_{ik} \sigma_{yz})
\]

\[
+ 2 S_{0} C_{ik} C_{ik} \sigma_{xy} + 2 S_{0} C_{ik} C_{ik} \sigma_{xy}
\]

(14)

\[
= S_{1122} \delta_{ij} + 2 S_{1212} \delta_{3i} \delta_{3j} + S_{0} C_{ik} C_{ik} C_{jk}.
\]

(13)

The magnitude of the stresses \( \sigma_{ij} \) in terms of the stresses on the specimen (P) frame are given in Appendix I.

3. Texture representation using Bunge's method

For this section the reader is referred to Bunge (1969, p. 215). Here the following items will be used:

\[
f(g) = \sum_{l, m, \nu} C^*_l \tilde{T}^*_ \nu(g)
\]

(15)

\[
\tilde{T}^*_ \nu(g) = \sum_{m, n} \tilde{A}^*_m \tilde{A}^*_n \tilde{T}^*_ \nu g(m, n)
\]

(16)

for the case of orthorhombic specimen symmetry and

\[
f(g) = \sum_{l, m, \nu} C^*_l \tilde{T} \nu(g)
\]

(17)

\[
\tilde{T} \nu(g) = \sum_{m, n} \tilde{A}^*_m \tilde{A}^*_n \tilde{T} \nu g(m, n)
\]

(18)

for monoclinic specimen symmetry. Here \( f(g) \) is the value of the orientation distribution function (o.d.f.) in a specific orientation \( g \) normalized as \( \int f(g) \, dg = 1 \); \( C^*_l, C^*_m \) are, from pole-figure measurements, determined expansion coefficients of \( f(g) \); \( \tilde{T}^*_ \nu \), \( \tilde{T} \nu \) are generalized symmetrical spherical harmonics. These are invariant with respect to crystal and specimen symmetry operations; \( \tilde{A}^*_m \) are cubic symmetry coefficients given, for instance, by Bunge & Ehler (1966); \( \tilde{A}^*_l, \tilde{A}^*_n \) are orthorhombic and monoclinic specimen symmetry coefficients. These can be derived from...
Table 1. Orthorhombic specimen symmetry coefficients $\tilde{A}_i^σ$

<table>
<thead>
<tr>
<th>$n$</th>
<th>0, ±2, ±4, ±6,...</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v$</td>
<td>1, 2, 3, 4,...</td>
</tr>
<tr>
<td>$\tilde{A}_i^σ$</td>
<td>$1, \sqrt{2}, \sqrt{2}, \sqrt{2}$</td>
</tr>
</tbody>
</table>

Table 2. Monoclinic specimen symmetry coefficients $\tilde{A}_i^σ$

<table>
<thead>
<tr>
<th>$s$</th>
<th>0, ±1, ±2, ±3,...</th>
</tr>
</thead>
<tbody>
<tr>
<td>$σ$</td>
<td>1, 2, 3, 4,...</td>
</tr>
<tr>
<td>$\tilde{A}_i^σ$</td>
<td>$1, \sqrt{2}, 1, 1$</td>
</tr>
</tbody>
</table>

Bunge (1969, p. 244), $T_{ijkl}^m(g_2)$ is a matrix element of the irreducible representation of weight $l$ of the rotation group in $R_3$. See Gelfand et al. (1963, p. 82). The coefficients $\tilde{A}_i^σ$ and $\tilde{A}_i^σ$ are given in Tables 1 and 2.

4. Derivation of $S_{\epsilon ij}$ with respect to the measurement ($L_1$ frame) (in the Reuss approximation)

For the mean strain obtained from all crystallites giving diffraacted intensity in the $\psi_{1}$ direction and having an $\langle hkl \rangle$ direction parallel to $L_2$, from (12),

$$\langle \epsilon_{xy} \rangle = S_{\epsilon xx} \sigma_{xx} + S_{\epsilon xy} \sigma_{xy} + 2S_{\epsilon xz} \sigma_{xz} + 2S_{\epsilon yy} \sigma_{yy}$$

Now it is defined that

$$S_{\epsilon ij} = \frac{\sum_{\psi} \int S_{\epsilon ij}(\phi_2, \psi, \beta_2) f(g_2 g_1) d\phi_2}{\int f(g_2 g_1) d\phi_2}$$

The integration in (20) has to be carried out only for all those orientations having an $\langle hkl \rangle$ direction parallel to $L_2$. Applying an analogous reasoning as was given by Bunge (1969, p. 236) the integral in the denominator is found to be equal to $2π P_{hh}(\psi, \phi)$, where $P_{hh}(\psi, \phi)$ is the normalized (in terms of 'times random') X-ray diffraction intensity of the $\langle hkl \rangle$ pole figure measured in a direction determined by $\psi$ and $\phi$.

For a further evaluation of the dependence of $S_{\epsilon ij}$ on $\phi_2, \psi_2$ and $\beta_2$ should be known. The necessary $S_{\epsilon ij}$ are given in (13). The needed $C_{hh}^2$ etc. are obtained from the inversion of matrix $g_2$ [[11]]. Note that the matrix elements $C_{hh}$ of the inverted matrix $g_2$ in (11) do not depend on the angle of integration. They are a function of $\psi_2$ and $\beta_2$ only. Hence they can be expressed by Miller indices $hkl$. See Dölle (1979, p. 496). From this it follows that the $S_{\epsilon ij}$ and consequently the X-ray elastic constants explicitly depend on $hkl$.

Also the following is needed:

$$f(g_2 g_1) = \sum_{l,m} C_l^{m+1} T_l^m(g_2 g_1)$$

$$= \sum_{l,m} C_l^{m+1} \sum_{n=-l}^{l} \tilde{A}_m^l \tilde{A}_n^l$$

$$\times \sum_{i=-l}^{l} T_{ijkl}^m(g_2) T_{ijkl}(g_1).$$

Here the well-known addition theorem has been used. See, for instance, Gelfand et al. (1963, p. 89). Further, it is mentioned that

$$T_{ijkl}^m(g_2) = \exp i(\ell \phi_2) P_{ijkl}^m(\cos \psi_2) \exp i[m(\pi/2 - \beta_2)]$$

$$T_{ijkl}^m(g_1) = \exp i[n(\phi + \pi/2)] P_{ijkl}^m(\cos \psi_1) \exp i(\ell \phi_1).$$

$$P_{ijkl}^m(\ell \phi) = \text{Jacobi polynomial as defined by Gelfand et al. (1963, p. 88).}$$

Equation (21) has been written in accordance with orthorhombic specimen symmetry. In the case of monoclinic specimen symmetry one has to use, of course, its monoclinic equivalent. For the orthorhombic case, (20) using (21)–(23) transforms into

$$S_{\epsilon ij} = \sum_{l,m} C_l^{m+1} \tilde{A}_m^l \tilde{A}_n^l \exp i[m(\pi/2 - \beta_2)]$$

$$\times \exp i[n(\phi + \pi/2)]$$

$$= \sum_{l,m} \frac{\sum_{i=-l}^{l} \exp i(\ell \phi_2) P_{ijkl}^m(\cos \psi_2) P_{ijkl}^m(\cos \psi_1)}{2\pi P_{hh}(\psi, \phi)}$$

$$\times \frac{\sum_{i=-l}^{l} \exp i(\ell \phi_2) S_{\epsilon ij} d\phi_2}{2\pi P_{hh}(\psi, \phi)}.$$

Note that both $S_{\epsilon ij}$ and $\sigma_{ij}$ depend on $\phi_2$ but $\langle \epsilon_{xy} \rangle$ does not in (19). Again, the integration is to be carried out with respect to $\phi_2$ only regarding those crystals having an $\langle hkl \rangle$ direction parallel to $L_2$. The summation over $l$ is truncated in most cases at $l_{max} = 22$.

4.1. Check for the case of a random specimen

In the analysis given the case of a random specimen should be contained as a special case. In (20) the integrals over the o.d.f. vanish because $f(g) = 1$ now. Hence, one finds immediately

$$S_{\epsilon ij} = \frac{1}{2\pi} \int \frac{2\pi}{0} S_{\epsilon ij}(\phi_2, \psi, \beta_2) d\phi_2.$$

In this case (19) should give the same result as (1). The angle $\phi_2$ can be kept fixed while carrying out the integration with respect to $\phi_2$. In this case

$$\langle \epsilon_{xy} \rangle = \frac{1}{2\pi} \int \frac{2\pi}{0} S_{\epsilon ij} d\phi_2,$$

$$\langle \epsilon_{xy} \rangle = \frac{1}{2\pi} \int \frac{2\pi}{0} S_{\epsilon ij} d\phi_2.$$
It can be proven that (25) and (26) yield the same result. Using (13) and Appendix II it may be found for (19):

$$\langle \epsilon'_{zz} \rangle = (\sigma'_{xx} + \sigma'_{yy})S_{zzzz} + \sigma'_{zz}S_{zizz}.$$  \hspace{1cm} (27)

Assuming only $\sigma_{11}$ and $\sigma_{22}$ $\neq 0$ and using (25) and Appendix I it is found, after elaboration,

$$\langle \epsilon'_{zz} \rangle = [S_{1122} + \frac{1}{2}S_0(1 - C_{4}^z)](\sigma_{11} + \sigma_{22}) + [S_{1111} - S_{1122} - (3/2)S_0(1 - C_{4}^z)]\sigma_0\sin^2\psi,$$  \hspace{1cm} (28)

where $C_{4}^z = C_{4}^2C_{4}^z$ (summation over repeated $k$) is invariant with respect to the permutation of $hkl$ since

$$C_{4}^z = \frac{h^4 + k^4 + l^4}{(h^2 + k^2 + l^2)}.$$  \hspace{1cm} (29)

The $C_{4}^z$'s are just the elements of the third row of the inverted form of matrix $g_z$ [[11]]. In other words, the $C_{4}^z$'s are the coordinates of the $L_3$ direction in terms of the crystal reference axes.

With $\Gamma(hkl) = \frac{1}{2}(1 - C_{4}^z)$ (28) reads

$$\langle \epsilon'_{zz} \rangle = [S_{1122} + S_0\Gamma(hkl)](\sigma_{11} + \sigma_{22}) + [S_{1111} - S_{1122} - 3S_0\Gamma(hkl)]\sigma_0\sin^2\psi = (\sigma_{11} + \sigma_{22})S_4(hkl) + \frac{1}{2}\sigma_0\sin^2\psi S_2(hkl).$$  \hspace{1cm} (30)

It is immediately seen that (30) is identical to (1).

4.2. Cubic invariance

The direction of the $hkl$ vector is determined by the angles $\phi_2$ and $\beta_2$ with respect to the cubic axes (Fig. 2). It can be argued that choosing another permutation of $hkl$ is the equivalent of fixing different 'labels' to the cubic axes while the 'physical' orientation of the crystal remains the same. Hence, choosing a different permutation of $hkl$ as a vector parallel to $L_3$ is the same as imposing a cubic symmetry operation upon an existing crystal reference frame. This is possible because the angles $\phi_2$ remains free. If a cubic symmetry operation is carried out after the rotations $g_1$ and $g_2$ in (21) the value of $f(g)$ does not change. In a similar way it can be argued that the compliances $S_{zzij}$ (being physical quantities) do not change after such a cubic symmetry operation. Hence, it follows that even for the most general case of 48 equivalent $[hkl]$ directions it is sufficient to treat only one specific $[hkl]$ direction (the most convenient one) as a vector parallel to $L_3$.

For instance, it is found that in the case of the $hkk$ reflection it is very advantageous to choose the $[hkk]$ direction as a vector parallel to $L_3$. In that case $\beta_2 = \pi/4$ and since $m$ is a multiple of 4 it is found now that in (24) only expressions like

$$\sum_{m=-1}^{1} A_{m}^{nn}(\gamma - 1)^{m/4} P_{m}^{n-1}(\cos \phi_2)$$  \hspace{1cm} (31)

occur. It can be shown that (24) is subject to cubic invariance as well. Thus, for the 211 reflection the $[112]$ direction will be used and for the 310 reflection the most convenient choice is [031] or [013].

4.3. $S_{zzij}$ for $l = 0$

It can be shown, using the inverse of matrix $g_z$ in (11), that generally speaking the $S_{zzij}$ only depend on $\sin \phi_2$, $\cos \phi_2$, $\sin 2\phi_2$ and $\cos 2\phi_2$ as far as $\phi_2$ is concerned. As a result, in the integral in (24) factors like $\delta_{l-1}$, $\delta_{l+1}$ occur ($\delta_{l,l}$ stands for the Kronecker delta). These factors lead to Jacobi polynomials like \(P_n^{m-1}(\cos \phi_2)\) but $P_{m-1}^{n-1}(\cos \phi_2)$. However, these are not defined for $l = 0$. Hence, in the sequel dealing with (24) in two cases the term with $l = 0$ will be separated. This looks like an 'isotropic part'. We have here $C_{0,0} = A_{0,0} = A_{0,0} = A_{0,0} = 1$.

For $S_{zzxx}\sigma_{xx} + S_{zzzy}\sigma_{yy}$, the term with $l = 0$ equals

$$[S_{1122} + S_0\Gamma(hkl)]((\sigma_{11} + \sigma_{22}) - \sigma_0\sin^2\psi)/P_{m\phi}(\psi, \phi).$$  \hspace{1cm} (32)

For $S_{zzzz}$ (being independent of $\phi_2$) the series development is superfluous. It follows from (20) that $S_{zzzz} = S_{zzzz}$. Hence the contribution $S_{zzzz}\sigma_{zz}$ to (19) can be obtained directly.

For $S_{zzxx}, S_{zzyy}$ and $S_{zzzz}$, it is seen from (II-4)--(II-6) that no $\phi_2$-independent part occurs. Hence, in (24) the contribution for $l = 0$ is always equal to zero as far as these compliances are concerned.

In (24) all series evaluations can start with the lower bound $l = 4$ because $C_{4}^z = 0$ and (32) has to be incorporated in the final result for (19).

5. ($hkl$) dependency of $\psi$ splitting and non-linearity

Texture dependency is determined by whether $S_{zzij}$ [[13], (14) and (20)] depends on $\phi_2$ or not. If the $S_{zzij}$ were independent of $\phi_2$, the integrals on the o.d.f. cancel in (20). Hence, in that case $S_{zzij} = S_{zzij}$. It will be demonstrated that both non-linearity and $\psi$ splitting can be explained by texture phenomena.

As far as $\psi$ splitting is concerned one has to realize that if a negative $\psi$ is operated on the diffractometer this cannot be accounted for in a straightforward manner in the present analysis. In this treatment the angle $\psi$ is taken as an Euler angle [cf. (8) and (9)] and thus the angle $\psi$ is only defined on the interval $[0, \pi]$. Hence, a negative value of $\psi$ could (mathematically speaking) not occur. However, it can be shown now that a negative $\psi$ on the diffractometer can be accounted for by taking the rotation $g_2$ equal to $\{\phi + 3\pi/2, \psi, \phi_2\}$ in (8) and (9). This generates exactly the

*The 321 b.c.c. reflection is not used very often as a measuring reflection and has therefore been neglected here.
same orientation now $\psi$ is taken positive and so is $\sin \psi$. Hence, the angle $\phi$ should only be substituted by $\phi + \pi$ in the resulting equations for examination of the consequences of negative $\psi$.

5.1. The 200 and 222 reflections

These reflections may be used for the general case of the 2h00 and 2h2h2h reflections.

5.1.1. The 200 reflection. For this case, $\beta = k\pi/2$; $\varphi = k\pi/2$; $k = 0(1)3$ (for definition of angles see Fig. 2).

It immediately follows from Appendix II that $C_{2h}C_{2h} = C_{2h}C_{2h} = C_{2h}C_{2h} = C_{2h}C_{2h} = 0$ and $C_{2h}C_{2h} = 1$ for all permutations of 200. Hence, it is found that the 200 reflection is not affected by any texture influence at all because from (14) it follows that $S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = 0$. From (19),

$$\langle \sigma_{zzz} \rangle = (\sigma_{zzz} + \sigma_{zzz})S_{1zzz} + S_{zzz}(S_{1zzz} + 2S_{1zzz} + S_{zzz}).$$

(33)

If only $\sigma_{11}$ and $\sigma_{22}$ are taken $\neq 0$ this transforms (Appendix I) into

$$\langle \sigma_{zzz} \rangle = (\sigma_{11} + \sigma_{22})S_{1222} + \frac{1}{4}\sigma_{11}\sin^2 \psi S_{2222}.$$

(34)

Hence, only isotropic X-ray elastic constants occur for the 200 reflection.

It is seen (by substituting $\phi + \pi$ for $\phi$) that no $\psi$ splitting can occur and the behaviour of $\langle \sigma_{zz} \rangle$ vs $\sin^2 \psi$ will be linear. Note, however, that if $\sigma_{11}$ and $\sigma_{22}$ were taken as non-zero it follows using Appendix I that both $\psi$ splitting and non-linearity would still occur.

5.1.2. The 222 reflection. For this case it is found that $\beta = k\pi/4$; $k = 1(2)7$ and $\varphi = k\pi/4$ or $\pi/2$ and $\alpha = 3^{-1/2}$ or $\pi/2$ and $\alpha = 3^{-1/2}$. For all crystallographic permutations of 222 one finds: $C_{2h}C_{2h} = C_{2h}C_{2h} = C_{2h}C_{2h} = C_{2h}C_{2h} = 1/3$ and $C_{2h}C_{2h}C_{2h} = C_{2h}C_{2h}C_{2h} = C_{2h}C_{2h}C_{2h} = 0$. There is no $\psi_2$ dependency so $\langle \sigma_{zzz} \rangle$ will not depend on texture and again $S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = S_{zzz} = 0$. From (14) it follows (Appendix I) that

$$\langle \sigma_{zzz} \rangle = (\sigma_{11} + \sigma_{22})S_{1222} + \frac{1}{4}\sigma_{11}\sin^2 \psi S_{2222}.$$

(35)

Only isotropic X-ray elastic constants occur for the 222 reflection. Again, it may be concluded that neither $\psi$ splitting nor non-linear behaviour occurs if only $\sigma_{11}$ and $\sigma_{22}$ are taken $\neq 0$. Note that if $\sigma_{11}$ and $\sigma_{22}$ were taken as non-zero it follows from Appendix I that $\psi$ splitting and non-linear behaviour would still occur.

5.2. The 110 reflection

This reflection is used for the general case of the $hh0$ reflection. For this case it is found that

$$\begin{align*}
110 & \beta = k\pi/4 \quad k = 1, 3, 5, 7 \quad \text{and} \quad \varphi_0 = \pi/2 \\
011 & \beta = \pi/2 \text{ or } 3\pi/2 \quad \text{and} \quad \varphi_0 = \pi/4 \text{ or } 3\pi/4 \\
101 & \beta = 0 \text{ or } \pi \quad \text{and} \quad \varphi_0 = \pi/4 \text{ or } 3\pi/4.
\end{align*}$$

Now,

$$C_{2h}C_{2h} = C_{2h}C_{2h} = 0 \quad \text{and} \quad C_{2h}C_{2h} = \frac{1}{2}$$

for all permutations.

$$C_{2h}C_{2h}C_{2h} = \pm \frac{1}{2} \sin 2\varphi_2;$$

$$C_{2h}C_{2h} = \frac{1}{2} \sin^2 \varphi_2 \text{ or } \frac{1}{2} \cos^2 \varphi_2;$$

$$C_{2h}C_{2h} = \frac{1}{2} \cos^2 \varphi_2 \text{ or } \frac{1}{2} \sin^2 \varphi_2.$$
Here \( N(l) = (l + 2)/2 \) and \( M(l) \) has been given by Bunge (1969, p. 33). Both coefficients \( C^\text{Mo}_l \) and \( S^\text{Mo}_l \) are valid for orthorhombic specimen symmetry only. They depend on the texture (the coefficients \( C^\varphi_l \)), the \( hkl \) reflection (\( \varphi_B \) and \( \beta_B \)) and \( j \). For \( (S^\text{Mo}_l \sigma_{xx} + S^\text{Mo}_l \sigma_{yy} + S^\text{Mo}_l \sigma_{xy}) \), \( j \) is equal to 2, whereas for \( (S^\text{Mo}_l \sigma_{xx} + S^\text{Mo}_l \sigma_{xy}) \), \( j \) is always equal to 1. The sums \( S(l, \mu, j, \varphi_B, \beta_B) \) depend on the \( hkl \) reflection but also on the crystallographic permutation of \( hkl \). [However, the treatment of \( j \) for one permutation is sufficient (§ 4.2).] Now,

\[
\langle \varepsilon_{zz} \rangle = (\sigma_{11} + \sigma_{22})S_{1}(110) + \frac{1}{2} \sigma_\varphi \sin^2 \psi S_{2}(110) \\
+ S_0(\sigma_{11} - \sigma_{22}) \sin 2\psi \cos \psi \\
\times S^\text{Mo}_1(\psi, \varphi, 2)/[8P_{110}(\psi, \varphi)] \\
+ S_0[(\sigma_{11} - \sigma_{22}) \cos 2\psi - \sigma_\varphi \sin^2 \psi] \\
\times C^\text{Mo}_1(\psi, \varphi, 2)/[8P_{110}(\psi, \varphi)].
\]

(39)

Note that in this equation the isotropic terms [analogous to (1)] are written first and the texture-dependent terms (where expressions \( C^\text{Mo}_l \) and \( S^\text{Mo}_l \) occur) are written at the end. This will be done systematically in all relevant cases.

Substitution of \( \varphi + \pi \) for \( \varphi \) in (37)–(39) shows immediately that no \( \psi \) splitting occurs in this case. Clearly, it follows from the last two terms of (39) that generally speaking non-polar behaviour of \( \langle \varepsilon_{zz} \rangle \) vs \( \sin^2 \psi \) occurs owing to the factors \( P_l^1 j, 2^{\varphi - 1}(\cos \psi) \) \( \pm P_l^2 j, 2^{\varphi + 1}(\cos \psi) \). These are nth-degree polynomials in \( \cos \psi \). Hence it depends on the magnitude of the o.d.f. expansion coefficients \( C^\varphi_l \) whether the Jacobi polynomials add 'higher-order' oscillations to the graph of \( \langle \varepsilon_{zz} \rangle \) vs \( \sin^2 \psi \) or not. It can be shown that choosing a different permutation of \( hkl \) does not change (39) although it does change the sums \( S(l, \mu, j, \varphi_B, \beta_B) \), the Jacobi polynomials \( P^M_l \) (cos \( \varphi_B \)) and the expressions for the \( S^\text{Mo}_l \). Note that using the expressions for \( \sigma_{xx}, \sigma_{yy} \), and \( \sigma_{xy} \) from Appendix 1 it follows that if \( \sigma_{13} \) and \( \sigma_{23} \) are non-zero, there is still a possibility of \( \psi \) splitting in the orthorhombic case.

5.2.2. Monoclinic specimen symmetry. Now Table 2 is used and, instead of \( n \) and \( v \), \( s \) and \( \sigma \) are used. Because monoclinic specimen symmetry is 'lower' than orthorhombic symmetry one has more o.d.f. expansion coefficients here. For instance, for \( l = 4 \) there are three coefficients \( C^\psi_l \) and five coefficients \( C^\varphi_l \). It should be understood that the \( C^\psi_l \) differ from the \( C^\varphi_l \). The first are obtained from a cubic–monoclinic o.d.f., whereas the latter are obtained from a cubic–orthorhombic o.d.f. Still, the \( C^\psi_l \) are real quantities. This follows from the fact that the \( C^\psi_l(\pi) \) may be chosen real and the fact that the o.d.f. itself has to be real as well. Although there are a lot of papers in the literature on the subject of cubic–orthorhombic o.d.f.'s (Bunge, 1969, pp. 111–127; Tobisch \& Mücklich, 1974; Masson, Parinière, Penelle \& Pernot, 1973; Ruer \& Baro, 1979; Roe, 1965) very little can be found on the subject of cubic–monoclinic o.d.f.'s. A treatment of some monoclinic pole figures is given by Williams (1962), Zaalberg, Dautzenberg \& Klostermann (1978), Krause \& Demirci (1978a) and Bunge (1971).

In close analogy with (37) and (38),

\[
C^\text{Mo}(\psi, \varphi, j) = \sum_{l = 4}^{M(l)} \sum_{\mu = 1}^{M(l)} S(l, \mu, j, \varphi_B, \beta_B) \\
\times \sum_{\varphi = 1}^{l + 1} C_l^\varphi(2 - \delta_{x,1})^{1/2}(-1)^{\sigma - 1} \\
\times [P_l^1 j, \sigma - 1(\cos \psi)] \\
+ P_l^2 j, \sigma - 1(\cos \psi)] \sin(\sigma - 1) \varphi.
\]

and

\[
S^\text{Mo}(\psi, \varphi, j) = 2^{1/2} \sum_{l = 4}^{M(l)} \sum_{\mu = 1}^{M(l)} S(l, \mu, j, \varphi_B, \beta_B) \\
\times \sum_{\varphi = 1}^{l + 1} C_l^\varphi(-1)^{\sigma - 1} \\
\times [P_l^1 j, \sigma - 1(\cos \psi)] \\
- P_l^2 j, \sigma - 1(\cos \psi)] \sin(\sigma - 1) \varphi.
\]

(41)

It is mentioned that for both orthorhombic and monoclinic symmetry the expressions for \( C^\text{Mo}_l, S^\text{Mo}_l, \text{etc.} \) become even more complex if one cannot choose the angle \( \beta_B \) equal to \( \pi/4, \pi/2 \) or \( \pi \). For the 110 reflection this is always possible, as was mentioned at the beginning of 5.2. In this case where \( (011) \) has been chosen \( \beta_B \) is equal to \( \pi/2 \) so for (36) it is found that

\[
S(l, \mu, 2, \pi/4, \pi/2) = \sum_{m = 1}^{l + 1} \hat{A}_m^\mu P_m^l(2 - 1/2).
\]

(42)

Note that \( S^\text{Mo}_l, C^\text{Mo}_l, \text{etc.} \) are always real.

Instead of (39), one finds now

\[
\langle \varepsilon_{zz} \rangle = (\sigma_{11} + \sigma_{22})S_{1}(110) + \frac{1}{2} \sigma_\varphi \sin^2 \psi S_{2}(110) \\
+ S_0(\sigma_{11} - \sigma_{22}) \cos 2\psi \sin \psi \\
\times S^\text{Mo}_1(\psi, \varphi, 2)/[8P_{110}(\psi, \varphi)] \\
+ S_0[(\sigma_{11} - \sigma_{22}) \cos 2\psi - \sigma_\varphi \sin^2 \psi] \\
\times C^\text{Mo}_1(\psi, \varphi, 2)/[8P_{110}(\psi, \varphi)].
\]

(43)

Substituting \( \varphi + \pi \) for \( \varphi \) in (40), (41) and (43) shows that for even \( \sigma \) the sign is reversed in the last two terms of (43). Clearly, this leads to \( \psi \) splitting being predicted in the monoclinic-specimen-symmetry case. Obviously, for odd \( \sigma \) the 'normal' orthorhombic behaviour, i.e. no \( \psi \) splitting, is predicted. As a general result it is concluded that \( \psi \) splitting occurs in the monoclinic case, whereas non-linear behaviour can be expected as well for the same reasons as mentioned in § 5.2.1.

Note that the 110 reflection is a 'hybrid' case
because the compliances $S'_{zzzz}$ and $S_{zzzz}$ behave like those for the 200 and 222 reflections, where both linear behaviour and no $\psi$ splitting were predicted. Note that a $\psi$ splitting could still be due to non-zero $\sigma_3$ and/or $\sigma_{23}$.

5.3. The 211 reflection

This reflection is used for the general case of the $hkk$ reflection.

The most convenient choice for the vector parallel to $L_3$ is $[112]$. Hence, $\varphi = \arccos(2/3)^{1/2}$ and $\beta = \pi/4$. Now it is found for (36)

$$S(l, \mu, j, \arccos(2/3)^{1/2}, \pi/4) = \sum_{m=-t}^{t} \Delta^m \mu^{r/m} (1)^m = (2/3)^{1/2}.$$ (44)

In this case all $S'_{zzij}$ except $S'_{zzzz}$ depend on $\varphi'$. 

5.3.1. Orthorhombic specimen symmetry.

$$S'_{zzzz} = S_{zzzz} + S_{zzzyy} + 2S_{zzxy} \sigma'_{xy}$$

$$= S_l[(\sigma_{11} - \sigma_{22}) \cos 2\varphi - \sigma_{66} \sin^2 \psi]$$

$$+ C_{\text{GR}}^{21}(\psi, \varphi, 2)/[24P_{211}(\psi, \varphi)]$$

$$+ S_0(\sigma_{11} - \sigma_{22}) \sin 2\varphi \cos \psi$$

$$+ S_{11}^{21}(\psi, \varphi, 2)/[24P_{211}(\psi, \varphi)].$$ (45)

Now the quantity $2S'_{zzxx} \sigma'_{xx} + 2S'_{zzxy} \sigma'_{xy}$ has to be evaluated as well. After rearranging,

$$2S'_{zzxx} \sigma'_{xx} + 2S'_{zzxy} \sigma'_{xy}$$

$$= S_0^{21}(\sigma_{11} - \sigma_{22}) \sin 2\varphi \sin \psi$$

$$+ C_{\text{GR}}^{11}(\psi, \varphi, 1)/[12P_{211}(\psi, \varphi)]$$

$$+ S_0^{21}(\psi, \varphi, 2)/[12P_{211}(\psi, \varphi)].$$ (46)

where $S_0^{21}$ and $C_{\text{GR}}^{21}$ should be used in the sense of (37) and (38) and where $j$ is equal to 1. Just like (39), (46) is independent of $\varphi_2$ as required. For the total result for the 211 reflection one should add the first two terms of (39) to (45) and (46). This yields [using $\Gamma(211) = \Gamma(110) = 1/4$]

$$\langle \epsilon_{zz} \rangle = (\sigma_{11} + \sigma_{22}) S_l(211) + \frac{1}{2} \sigma_{66} \sin^2 \psi S_2(211)$$

$$+ S_0[(\sigma_{11} - \sigma_{22}) \cos 2\varphi - \sigma_{66} \sin^2 \psi]$$

$$+ C_{\text{GR}}^{21}(\psi, \varphi, 2)/[24P_{211}(\psi, \varphi)]$$

$$+ S_0(\sigma_{11} - \sigma_{22}) \sin 2\varphi \cos \psi$$

$$+ S_{11}^{21}(\psi, \varphi, 2)/[24P_{211}(\psi, \varphi)]$$

$$+ S_0^{21}(\psi, \varphi, 2)/[12P_{211}(\psi, \varphi)].$$ (47)

Just as for the 110 reflection it is concluded from (47) that for the orthorhombic case no $\psi$ splitting is predicted. Note that for the 211 reflection the coefficients $S_{0211}(\psi, \varphi, j)$ and $C_{\text{GR}}^{21}(\psi, \varphi, j)$ are always real as required. Note that non-zero $\sigma_3$ and/or $\sigma_{23}$ could still give rise to $\psi$ splitting.

5.3.2. Monoclinic specimen symmetry. Instead of (47),

$$\langle \epsilon_{zz} \rangle = (\sigma_{11} + \sigma_{22}) S_l(211) + \frac{1}{2} \sigma_{66} \sin^2 \psi S_2(211)$$

$$+ S_0[(\sigma_{11} - \sigma_{22}) \cos 2\varphi - \sigma_{66} \sin^2 \psi]$$

$$\times C_{\text{MO}}^{11}(\psi, \varphi, 2)/[24P_{211}(\psi, \varphi)]$$

$$+ S_0^{21/2}(\sigma_{11} - \sigma_{22}) \sin 2\varphi \cos \psi$$

$$\times C_{\text{MO}}^{21}(\psi, \varphi, 1)/[12P_{211}(\psi, \varphi)]$$

$$+ S_0(\sigma_{11} - \sigma_{22}) \sin 2\varphi \cos \psi$$

$$\times S_{0211}(\psi, \varphi, 2)/[24P_{211}(\psi, \varphi)]$$

$$+ S_0^{21/2}(\sigma_{11} - \sigma_{22}) \sin 2\varphi \sin \psi$$

$$\times S_{0211}(\psi, \varphi, 1)/[12P_{211}(\psi, \varphi)].$$ (48)

Again, non-linear behaviour can be expected and it can be seen from (40) and (41) that $\psi$ splitting is predicted now, substituting $\pi + \varphi$ for $\varphi$. Note that $\psi$ splitting still could be due to non-zero $\sigma_3$ and/or $\sigma_{23}$.

5.4. The 310 reflection

This reflection is used for the general case of the $hko$ reflection.

The most convenient choice for the vector parallel to $L_3$ is $[031]$. In this case one has: $\varphi = \arccos 10^{-1/2}$; $\beta = \pi/2$ and the equivalent of (36) now reads

$$S(l, \mu, j, \arccos(10^{-1/2}), \pi/2) = \sum_{m=-t}^{t} \Delta^m \mu^{r/m}(10^{-1/2}).$$

5.4.1. Orthorhombic specimen symmetry. Analogous to (43) and (45),

$$\langle \epsilon_{zz} \rangle = (\sigma_{11} + \sigma_{22}) S_l(310) + \frac{1}{2} \sigma_{66} \sin^2 \psi S_2(310)$$

$$+ 9S_0[(\sigma_{11} - \sigma_{22}) \cos 2\varphi - \sigma_{66} \sin^2 \psi]$$

$$\times C_{\text{GR}}^{11}(\psi, \varphi, 1)/[25P_{310}(\psi, \varphi)]$$

$$- 3S_0(\sigma_{11} - \sigma_{22}) \sin 2\varphi \cos \psi$$

$$\times S_{0210}(\psi, \varphi, 2)/[200P_{310}(\psi, \varphi)]$$

$$+ 9S_0^{21}(\sigma_{11} - \sigma_{22}) \sin 2\varphi \sin \psi$$

$$\times S_{0210}(\psi, \varphi, 1)/[25P_{310}(\psi, \varphi)].$$ (49)

The same conclusions as were given for the 211 reflection in § 5.3.2 can be drawn.

5.4.2. Monoclinic specimen symmetry. Here the final expression is equal to (49) except that $S_{0210}$ and $C_{\text{GR}}^{21}$ should be replaced by $S_{0210}^{\text{MO}}$ and $C_{\text{MO}}^{21}$.

For the 310 reflection the same conclusions with
regard to non-linearity and $\psi$ splitting can be drawn as were given for the 211 reflection.

The coefficients $S_{\text{OR}}^{211}(\psi, \varphi, j)$ and $C_{\text{OR}}^{310}(\psi, \varphi, j)$ are always real.

5.5. Some considerations concerning f.c.c. crystals

A treatment analogous to that for the b.c.c. case can be applied. The results can be indicated as follows.

(i) The $hhh$ and $2h00$ reflections yield exactly the same formulee as have been given for the 222 and 200 b.c.c. reflections, respectively.

(ii) The case of the $2h2h0$ f.c.c. reflections can be directly inferred from the formulee given for the 110 b.c.c. reflection.

(iii) The 311 and 331 reflections can be dealt with in the same way as the 211 b.c.c. reflection. One can choose here $\beta_\mu$ equal to $\pi/4$ as well. The constants differ, but for the rest the resulting expressions are analogous.

Note that the compliance tensor $S_{\text{magn}}$ for f.c.c. crystals [and as a consequence $S_{\text{p}}$ in (7)] can differ strongly from the one for the b.c.c. case.

6. Considerations with reference to the shear stresses

$\sigma_{12}, \sigma_{13}, \sigma_{23}$ and the normal stress $\sigma_{33}$

As has been indicated in § 5, $\psi$ splitting and/or non-linearity could be due to these stresses being non-zero for both the orthorhombic and the monoclinic specimen symmetry case. In this section restrictions on these stresses are obtained as a result of physical symmetry requirements. The influence of non-zero values for stresses escaping from these restrictions is discussed as well. For general treatment of the problem the 211 reflection is used.

6.1. Orthorhombic specimen symmetry

In this case the following physical requirements should be met:

$$\langle \epsilon'_{12}(\psi, \varphi) \rangle = \langle \epsilon'_{12}(\psi, \pi - \varphi) \rangle = \langle \epsilon'_{12}(\psi, \pi + \varphi) \rangle = \langle \epsilon'_{23}(\psi, 2\pi - \varphi) \rangle.$$  (50)

For these cases the corresponding texture functions $C_{\text{OR}}^{211}$ and $S_{\text{OR}}^{211}$ are readily found.*

It can be shown, taking all stress-tensor elements into account that (47) in this case reads:

the expression for $\langle \epsilon'_{12} \rangle$ given in (47)

$$\epsilon'_{12}(\psi, \varphi) = \epsilon'_{12}(\psi, \pi - \varphi)$$  (53)

For the expressions for $C_{\text{MO}}^{211}$ and $S_{\text{MO}}^{211}$ the equations given in the previous footnote can be used after substituting the symbols MO for OR.

From an expression analogous to (51) and using (48) it is found that

$$\sigma_{12} = \sigma_{23} = 0.$$  (54)

No conclusions with respect to $\sigma_{13}$ and $\sigma_{33}$ are obtained.

6.3. Discussion

For the orthorhombic specimen symmetry case it seems very unlikely that a non-zero $\sigma_{33}$ could exist while $\sigma_{13}$ and $\sigma_{23}$ should be equal to zero. Gradients in $\sigma_{12}$, $\sigma_{13}$ or $\sigma_{23}$ cannot occur and non-linearity or

* i.e.: $C_{\text{OR}}^{211}(\psi, \pi \pm \varphi, j) = C_{\text{OR}}^{211}(\psi, \varphi, j)$

$S_{\text{OR}}^{211}(\psi, \pi \pm \varphi, j) = \pm S_{\text{OR}}^{211}(\psi, \varphi, j)$

$C_{\text{OR}}^{211}(\pi - \psi, \pi + \varphi, j) = -1C_{\text{OR}}^{211}(\psi, \varphi, j)$

$S_{\text{OR}}^{211}(\pi - \psi, \pi + \varphi, j) = -1S_{\text{OR}}^{211}(\psi, \varphi, j)$

$C_{\text{OR}}^{310}(\psi, 2\pi - \varphi, j) = C_{\text{OR}}^{310}(\psi, \varphi, j)$

$S_{\text{OR}}^{310}(\psi, 2\pi - \varphi, j) = -S_{\text{OR}}^{310}(\psi, \varphi, j)$.

†Note that an orthorhombic specimen 'monoclinically' machined in a direction not coincident with a principal direction of symmetry would exhibit a non-zero $\sigma_{12}$. 19
curvature in this case can be attributed to the influence of $\sigma_{11}$ and $\sigma_{22}$ in connection with texture phenomena. Gradients in $\sigma_{11}$ and $\sigma_{22}$ could occur.

For the monoclinic specimen symmetry case the $\psi$ splitting cannot be attributed to a non-zero $\sigma_{33}$ or a gradient in $\sigma_{23}$. In view of the special features of a 'monoclinic' machining treatment (shearing of a surface layer in the machining direction), it could be imagined that a non-zero gradient in $\sigma_{13}$ exists. However, for both cases the point made in the introduction remains valid: $\sigma_{13}(z)=\sigma_{23}(z)=\sigma_{33}(z)=0$ for $z=0$. If the components of the stress tensor and the strain tensor depend on $z$ only, the gradients in $\sigma_{13}$ and $\sigma_{23}$ should satisfy the condition

$$\frac{\partial \sigma_{13}(z)}{\partial z} = \frac{\partial \sigma_{23}(z)}{\partial z} = 0.$$ 

Furthermore, in the absence of body forces the gradient in $\sigma_{33}$ with respect to $z$ should be equal to zero then too, owing to the equations of mechanical equilibrium (Timoshenko & Goodier, 1970).

Hence, both $\psi$ splitting and non-linearity should be explained using $\sigma_{11}$ and $\sigma_{22}$ (or gradients in them) connected to texture phenomena.

7. Discussion of experimental data

7.1. $\psi$ splitting

7.1.1. Orthorhombic specimen symmetry. Orthorhombic specimen symmetry can be found after rolling and also after axisymmetric deformation, simple tensile plastic deformation, extrusion, sheet or strip drawing, etc.

In agreement with the theoretical prediction (§§ 5.1, 5.2.1, 5.3.1 and 5.4.1), in this case no $\psi$ splitting has been found in general (Hauk, Krug & Vaessen, 1981; Dölle, 1979; James & Cohen, 1980; Cohen, Dölle & James, 1979; Marion & Cohen, 1975, 1977). Only the results shown by Hauk, Krug & Vaessen (1981) in their Fig. 11 display a $\psi$ splitting after an orthorhombic deformation history (cold rolling + tensile plastic loading). In this case the specimen appears to be drawn up to near the ultimate tensile strength (UTS) point in the stress-strain diagram and it could have been possible that shear-band formation (Mathur & Backofen, 1973) disturbed the orthorhombic texture.

From the absence of $\psi$ splitting in the general orthorhombic case the following can be concluded: Substituting $\varphi = \pi$ for $\varphi$ in (51) and because $P_{M}(\varphi, \varphi + \pi) = P_{M}(\varphi, \varphi)$ here, it is immediately found from the absence of $\psi$ splitting for all $\varphi$ that $\sigma_{13} = \sigma_{23} = 0$. Hence, from the absence of $\psi$ splitting no conclusions can be drawn other than those derived in § 6.1, where it was found that $\sigma_{13}, \sigma_{23}$ and $\sigma_{11}$ should be equal to zero. No conclusion about $\sigma_{33}$ can be drawn.

7.1.2. Monoclinic specimen symmetry. This may be found after a shear-like deformation such as occurs in grinding, milling, wear, etc.

In agreement with the theoretical prediction (§§ 5.2.2, 5.3.2 and 5.4.2), $\psi$ splitting is generally observed. It is frequently reported that the amount of $\psi$ splitting, $\Delta(\varepsilon'_{23})$, decreases with increasing $\varphi$ (Hauk, Krug & Vaessen, 1981; Dölle, Hauk & Neubauer, 1978; Dölle & Cohen, 1980a; Cohen, Dölle & James, 1979). The expression

$$\Delta(\varepsilon'_{23}) = \langle \varepsilon'_{23}(\varphi, \varphi) \rangle - \langle \varepsilon'_{23}(\varphi, \pi + \varphi) \rangle - \langle \varepsilon'_{23}(\varphi, \varphi) \rangle$$

cannot be treated generally because $C_{MO}^{M}(\varphi, \varphi + \pi, j)$, $S_{MO}^{M}(\varphi, \varphi + \pi, j)$ and $P_{M}(\varphi, \varphi + \pi)$ are not equal to $C_{MO}^{M}(\varphi, \varphi, j)$, $S_{MO}^{M}(\varphi, \varphi, j)$ and $P_{M}(\varphi, \varphi)$ respectively. There is an exception, however:

$$C_{MO}^{M}(\varphi, 3\pi/2, j) = C_{MO}^{M}(\varphi, \pi/2, j)$$

(56)

$$S_{MO}^{M}(\varphi, 3\pi/2, j) = -S_{MO}^{M}(\varphi, \pi/2, j)$$

(57)

$$P_{M}(\varphi, 3\pi/2) = P_{M}(\varphi, \pi/2).$$

(58)

Hence, for a quantitative treatment one is restricted to the situation for $\varphi = \pi/2$ but there the $\psi$ splitting is reported to be small or negligible within the limits of accuracy. In that case

$$\langle \varepsilon'_{23}(\varphi, \pi/2) \rangle - \langle \varepsilon'_{23}(\varphi, \pi/2) \rangle = \langle \varepsilon'_{23}(\varphi, 3\pi/2) \rangle$$

(59)

From this, it is immediately found, using the monoclinic equivalent of (51) and (56)–(58), that $\sigma_{12}$ and $\sigma_{23}$ should be equal to zero. This is not surprising because the situation is analogous to the one corresponding to (54) in § 6.2 where the same conclusion was reached. It is suggested by Dölle, Hauk & Neubauer (1978) and Dölle & Cohen (1980) that their specimens were random even after the final treatment of milling and grinding. If this is true, it is found from the monoclinic equivalent of (51), using the 310 reflection employed by Dölle et al. (1978), that the amount of $\psi$ splitting is (for $\varphi = 0$)

$$\Delta(\varepsilon'_{23}) = [\varepsilon'_{23}(\psi, \pi) - \varepsilon'_{23}(\psi, 0)]$$

$$= -4S_{1212} - (73/50)S_{0}\sigma_{13}sin (2\varphi).$$

(60)

Furthermore, it can be proven, using the monoclinic equivalent of (51), that for $\varphi = 0$, $\Delta(\varepsilon'_{23}) = 0$ for the textured case also. Thus, $\Delta(\varepsilon'_{23})$ would not depend on $\sigma_{13}$ (residual or applied). This is demonstrated by Fig. 2 from the paper by Krause & Jühe (1980) and also to some extent by Fig. 6 from the paper by Dölle, Hauk & Neubauer (1978). Although no pole figures are given, both Dölle (1982) and Hauk (1982) report that no significant textures were present before grinding.
their (steel) specimens. However, in that case one needs a residual $\sigma_{13}$ to account for the $\psi$ splitting as indicated by (60). But it has been shown in § 6.3 that neither $\sigma_{13}$ nor gradients (with respect to $Z$) in $\sigma_{13}$ can occur. However, a totally different point of view is suggested by the following observations: In carbon steels, $(\alpha + \beta)$-brass and $(\alpha + \beta)$-titanium it has been found by Hauk, Oudelhoven & Vaessen (1981) and Hauk (1982) that the plus and minus branches in the graphs of $\langle \epsilon_{yy} \rangle$ vs $\sin^2 \psi$ are reversed for both (metallurgical) phases. This suggests that residual shear stresses $\sigma_{13}$ having opposite signs occur in both phases, whereas on a macro scale the residual $\sigma_{13}$ still could be equal to zero due to compensation. This point of view is supported by the experimental evidence given by Dölle & Cohen (1980a) where absence of any $\psi$ splitting after grinding of Armco iron (no second phase) is reported.

Furthermore, Wakabayashi, Nakayama & Nagata (1977) found an increasing amount of $\psi$ splitting $\Delta \langle \epsilon_{yy} \rangle$ with increasing carbon content in their steel specimens. This, however, could be due to increasing texture development in the ferrite. In addition to this, Wakabayashi et al. (1977) and Hauk (1982) report that for the 200 reflection measured for ground steel specimens $\psi$ splitting was observed. According to § 5.1.1 this can (within the context of the Reuss model) only be due to residual $\sigma_{13}$ whether there is any texture development or not. Again, this could only be possible if compensation due to a second phase were present.

Hence it cannot be excluded (with respect to the present 'state of the art') that on a micro scale residual stresses $\sigma_{13}$ could exist (not to be confused with residual microstresses, i.e. stresses associated with structural broadening). That grinding can be associated with a change of texture (however weak) may be seen from Figs. 4(a) to (d) from the paper by Hauk, Krug & Vaessen (1981). Furthermore, it may be seen that in the case of rolling friction as indicated in the paper by Krause & Demirci (1978b) the development of the monoclinic texture is rather strong in steel. This should also be the case in Fig. 4 from the paper by Krause & Jühe (1980).

Since it is attempted here to deal with the possible influence of crystallographic texture on the $\psi$ splitting the treatment will be restricted to texture dependency in all that follows.

It should be realized that using (40), (41) and (48) it follows that even a weak texture could contribute to the $\psi$ splitting because the (large) residual stresses $\sigma_{11}$ and $\sigma_{22}$ are coupled to the o.d.f. expansion coefficients. Owing to texture, non-zero coefficients $C_{14}^{\text{tr}}$, $C_{44}^{\text{tr}}$, etc. occur. Hence, the texture functions $C_{14}^{\text{tot}}$ and $C_{44}^{\text{tot}}$ will be non-zero as well. Because they differ for both $\varphi$ and $\varphi + \pi$ [even $\sigma$ in (49) and (50)] the residual $\sigma_{11}$ and $\sigma_{22}$ can contribute to the $\psi$ splitting (58) or the 310 equivalent of (58). Furthermore, all authors report values of the residual stresses $\sigma_{11}$ and $\sigma_{22}$ after grinding to be much larger than the residual stress $\sigma_{13}$. Hence, generally speaking, the texture-dependent part of the $\psi$-splitting problem should be explained using residual $\sigma_{11}$ and $\sigma_{22}$ in connection with the orientation distribution function. Consider, for instance, Figs. 4(a) and 6 from the paper by Hauk, Krug & Vaessen (1981). It is seen that the monoclinic part of the texture after grinding is very small and subsequently the amount of $\psi$ splitting is very small. However, Figs. 4(c) and 9 from the same paper exhibit a texture with a stronger monoclinic part and subsequently the amount of $\psi$ splitting is larger.

The reversal in $\psi$ splitting behaviour when the direction of final grinding is reversed, as has been reported by Dölle & Cohen (1980a) and Cohen, Dölle & James (1979), can be explained as follows: After a reversal of the final direction of grinding one finds the same physical properties in the direction $(\psi, \varphi + \pi)$ as were found in the direction $(\psi, \varphi)$ before the reversal. Hence, for the situation with positive $\psi$ after the reversal, one should substitute $\varphi + \pi$ for $\varphi$. This is, of course, equal to the situation with positive $\psi$ before the reversal. Consequently, the entire situation with respect to $\psi$ splitting is reversed.

Note, however, that it follows from (51) using $C_{44}^{\text{tr}} = C_{14}^{\text{tr}} = 0$ that if there were no texture the observed reversal reported by Dölle & Cohen (1980a) could also be explained using a residual $\sigma_{13}$, Hence, nothing conclusive concerning this point can be said here and further experiments are needed.

7.2. Curvature in the graph of $\langle \epsilon_{xx} \rangle$ vs $\sin^2 \psi$

7.2.1. Orthorhombic specimen symmetry. There is an appreciable amount of experimental data for the case of cold-rolling (Hauk, Krug & Vaessen, 1981; James & Cohen, 1980; Dölle & Cohen, 1980; Marion & Cohen, 1975, 1977) displaying a strong curvature in the graph of $\langle \epsilon_{xx} \rangle$ vs $\sin^2 \psi$ for $\varphi = 0$, whereas for $\varphi = \pi/2$ linear behaviour is found. Both these effects will be shown to be in agreement with theoretical predictions: In general, (47) predicts a non-linear behaviour in the presence of texture. Marion & Cohen (1975, 1977) showed that the oscillations (of $\epsilon_{xx}$ vs $\sin^2 \psi$) follow closely the variation in peak intensity due to texture.

Some useful attempts at explaining these non-linearities using 'ideal orientations' may be found in the papers by Dölle & Hauk (1978), Dölle, Hauk & Zeegers (1978), Dölle (1979) and Dölle & Cohen (1980b). However, from the paper by Schläfer & Bunge (1974) it may be seen that the cold-rolling texture of

*Gradients (with respect to $Z$) in $\sigma_{13}$ and $\sigma_{11}$ cannot be excluded. They should be subject, however, to the compatibility conditions for the stresses, the conditions of equilibrium and Hooke's law.
iron or low-carbon steel consists of a whole 'orientation tube' in Euler space. Hence, it follows that ideal orientations cannot be used to explain the observed oscillations quantitatively. Instead, o.d.f. methods will be used in what follows.

Of course, using ideal orientations could perform quite well in the case of transformer steel sheet where only a few orientations occur.

The following two (general) kinds of oscillations may be distinguished:

'Normal curvature,' e.g., for the 211 reflection, is found (for \( \varphi = 0 \)):

\[
\langle \epsilon^{\prime}_{zz}(\psi, \varphi = \pi/2) \rangle = (\sigma_{11} + \sigma_{22})S_{1}(211) + \frac{1}{2} \sigma_{11}S_{2}(211)\sin^{2}\psi + S_{0}2^{1/2}C_{011}^{211}(\psi, \varphi, \pi/2, 1)\sigma_{22} \times \sin 2\psi/[12P_{211}(\psi, \varphi/2)] + S_{0}C_{011}^{211}(\psi, \varphi, \pi/2, 2)(-\sigma_{11}) + \sigma_{11}\cos^{2}\psi/[24P_{211}(\psi, \pi/2)].
\]

(62)

From (61) and (62) it is seen [using (37) and the fact that the Jacobi polynomial \( P_{n}^{c}(\psi = 0) = \delta_{b,c} \) that \( \langle \epsilon^{\prime}_{zz}(\psi, 0, 0) \rangle = \langle \epsilon^{\prime}_{zz}(\psi, \pi/2, 0) \rangle \), as required because the same diffracting lattice planes are irradiated. This can be shown to be true for all \( \varphi \) while \( \psi = 0 \). In the experimental data this is never encountered (Hauk, Krug & Vaessen, 1981).

Owing to the complicated expressions for the \( C_{ijkl}^{011}(\psi, \varphi, \rho, j) \) in (37) no quantitative conclusion concerning curvature can be obtained but it is seen from (61) that changing the sign of \( \sigma_{11} \) from compressive to tensile (due, for instance, to tensile elastic stress acting on a stress-free specimen or compensating a compressive residual stress) reverses the sign of the two 'anisotropic' (i.e. non-linear texture-depending) parts of (61) as well.

About the curvature behavior the following can be said: in the texture functions \( C_{ijkl}^{011} \) or \( C_{ijkl}^{011} \) ([37] and [38]) there appear coefficients like \( P_{1}^{2i-1}(\cos \psi) \pm P_{1}^{2i-1}(\cos \psi) \). Generally speaking, these behave like an \( i \)-th degree polynomial in \( \cos \psi \). That these oscillations can be observed experimentally depends on the o.d.f. coefficients \( C_{ijkl}^{011} \). Consider the 211 reflection and the cases of \( \varphi = 0 \) (strong curvature) and \( \varphi = \pi/2 \) (approximately linear behaviour). Equations (61) and (62) are used, hence only non-zero \( \sigma_{11} \) and \( \sigma_{22} \) are taken into account. From the curves of \( \langle \epsilon^{\prime}_{zz} \rangle \) vs \( \sin^{2}\psi \) in Fig. 8 of the paper by Hauk, Krug & Vaessen (1981) and Fig. 15 of the paper by James & Cohen (1980) and Fig. 6 of the paper by Dölle & Cohen (1980b), it follows that the graph for \( \varphi = 0 \) behaves like, say, sin \( 8\psi \), whereas for \( \varphi = \pi/2 \) the graph looks like a straight line with a negative first derivative with respect to \( \sin^{2}\psi \). In all cases this derivative is negative for \( \sin^{2}\psi = 0 \). Note that for compressive \( \sigma_{11} \) and \( \sigma_{22} \) the isotropic part of (61) yields a negative first derivative with respect to \( \sin^{2}\psi = 0 \). Furthermore, numerical calculations show that the anisotropic parts of (61) should have a negative first derivative in \( \sin^{2}\psi = 0 \) as well in order to account for the experimental data. It follows that the sum over \( \nu \) in \( C_{ijkl}^{011}(\psi, 0, j) \) in (37) alternates due to the factor \((-1)^{-1}\), whereas in \( C_{ijkl}^{011}(\psi, \pi/2, j) \) the alternating behaviour disappears.

From experimental data (Schläfer & Bunge, 1974;
Brakman, 1978) it is obtained that for 76% cold-rolled steel the most predominant o.d.f. coefficients are those with \( l = 6 \) and \( l = 12 \) (i.e. \( C_{6}^{1} = +3.30 \), \( C_{6}^{1} = -2.77 \) and \( C_{12}^{2} = 2.12 \), \( C_{12}^{2} = 2.50 \)), whereas the other coefficients (including \( C_{1}^{2} \), \( C_{1}^{2} \) and \( C_{3}^{2} \)) are relatively small. Hence, the most important o.d.f. coefficients alternate. In addition to this it can be shown that for \( l = 6 \) and \( v = 1 \) and \( v = 2 \) in the \( \psi \)-dependent parts of (61) and (62) the coefficients of equal powers of \( \sin^{2} \psi \) all have the same sign. Hence, it is argued that, owing to the coupling with the o.d.f. coefficients, for \( \phi = \pi/2 \) the various powers of \( \sin^{2} \psi \) more or less cancel, whereas for \( \phi = 0 \) they tend to reinforce each other owing to the coefficient \((-1)^{-1}\). Although \( C_{12}^{1} \) and \( C_{12}^{2} \) are relatively large as well, it is believed that this kind of high-order oscillations cannot account for the experimental data because the coefficients \( P_{12}^{2(1)-1}(\cos \psi) \pm P_{12}^{2(2)-1}(\cos \psi) \) oscillate very rapidly then.

7.2.2. Monoclinic specimen symmetry. As predicted \([48], \S 5.3.2]\), curvature in the graph of \( \langle \epsilon_{zz} \rangle \) vs \( \sin^{2} \psi \) is frequently observed in practice (Dödle & Cohen, 1980a; Krause & Jühe, 1976; Dödle, Hauk & Neubauer, 1978).

In general it can be expected that the coefficients \( P_{\mu}^{1} \varphi \sigma_{\mu}^{-1}(\cos \psi) \pm P_{\mu}^{-1} \varphi \sigma_{\mu}^{-1}(\cos \psi) \) as they occur for the textured case in (48), will cause the behaviour of \( \langle \epsilon_{zz} \rangle \) vs \( \sin^{2} \psi \) to be non-linear. However, since very little is known about cubic–monoclinic o.d.f.'s, a detailed qualitative discussion of the experimental data cannot be given.

From (48) for the 211 reflection and \( \psi = 0 \):

\[ \langle \epsilon_{zz} \rangle(0, \varphi) = (S_{1122} + 2 S_{0})(\sigma_{11} + \sigma_{22}) \]

\[ + S_{2112}^{1/2}(-\sigma_{11} + \sigma_{22}) \]

\[ + 24 P_{1111}(0, \varphi) \]

\[ \times \sum_{\mu} S_{\mu}(1, \mu, 2, \arccos(2/3)^{1/2}, 2 \pi/4) C_{1}^{\mu} \]  

(63)

Equation (63) yields the same value for all \( \varphi \) because for \( \psi = 0 \) the X-ray intensities \( P_{2111}(0, \varphi) \) have the same value for all \( \varphi \) (centre of the pole figure). This is in agreement with the experimental data found in the literature.

8. Final remarks

(i) In § 5.1.1 and 5.1.2 it has been argued that for the \( 2h2h2h \) and \( 2h00 \) b.c.c. reflections (and, implicitly, for the \( \{hkh \) and \( 2h00 \) f.c.c. reflections also) \( \psi \) splitting and non-linearity would occur if \( \sigma_{13} \) and/or \( \sigma_{23} \) were non-zero. In that case the non-linearity or the amount of \( \psi \) splitting for any specimen would behave like \( \sin 2 \psi \) as follows from (51).

(ii) The X-ray elastic constants \( R_{ij} \) as defined by Dölle (1979) or Dölle & Hauk (1978) in the expression

\[ \langle \epsilon_{zz} \rangle = R_{ij} \sigma_{ij} = \langle F_{ij}(\psi, \varphi, R_{ij}) \sigma_{ij} \rangle \]  

(64)

can be redefined using the present analysis. The coefficient \( F_{ij} \) could be taken, for instance, from (47) and (48). Note that the functions \( S(l, \mu, j, \varphi, R_{ij}) \) \([37, 38, 40, 41]\) need to be calculated only once for a given \( hki \) reflection. The sums over \( l \) in these equations can be truncated for the technological materials under discussion at \( l_{max} = 22 \) or even less, as experience shows (Bunge, 1969, p. 120).

(iii) It seems highly profitable to develop a small number of standard o.d.f.'s for both orthorhombic and monoclinic specimen symmetry cases. This should prove very helpful for in situ stress measurements where no pole figures can be obtained. For quite a number of cases (i.e. grinding, milling, rolling of, for instance, low-carbon steel) textures develop systematically and as a consequence the o.d.f. coefficients for a specific deformation history do not show much variation.

(iv) More accurate results can be obtained using for the elastic constants the mean of the Reuss and Voigt approximations (Hill, 1952) or applying the treatment due to Kröner (1958, 1967).

(v) It could be worthwhile to test the equations given using a material with \( S_{6} \approx 0 \). Then, it should become clear whether \( \psi \) splitting is due to texture or residual \( \sigma_{13} \) because it follows from (for instance) (48) and (51) that all texture influence disappears in that case. Note that texturess (i.e. random) materials exist consisting of crystals exhibiting a large value of \( S_{6} \). Elastically isotropic materials exhibit \( S_{6} = 0 \), whereas isotropic materials in the texture sense exhibit \( C_{66}^{\mu} = S_{66}^{\mu \mu} = 0 \) (or their monoclinic counterparts).

(vi) Owing to its inherent simplicity the case of axisymmetric deformation (wire-drawing or rod-extrusion) may be very well suited to test the present analysis. For this special case of orthorhombic specimen symmetry it may be expected that \( \sigma_{11} = \sigma_{22} \). Also, the case of electrodeposited (e.g. chromium) or nitrided layers could be studied. A rotationally symmetric texture (with reference to the surface normal) and high internal stresses occur in most cases.

(vii) In the paper by Dietze & Leibfried (1963) the stress fields of single dislocations are treated. Although \( \sigma_{13}(z) = 0 \) for \( z = 0 \) gradients in \( \sigma_{13} \) with respect to \( z \) occur then. However, these stresses only operate on a micro scale and they can only contribute to line broadening. At least it is difficult to see how a 'macro' \( \sigma_{13} \) could result from all 'micro' \( \sigma_{13} \) contributions for the case of a textureless (Dölle, Hauk & Neubauer, 1978; Dölle & Cohen, 1980a; Dölle, 1982; Hauk, 1982) specimen because then the dislocation distribution should be random also.
9. Conclusions

(i) From physical symmetry considerations only it follows that: (i) for orthorhombic specimen symmetry the residual stresses $\sigma_{12}$, $\sigma_{13}$ and $\sigma_{23}$ should be equal to zero; (ii) for monoclinic specimen symmetry the residual stresses $\sigma_{12}$ and $\sigma_{23}$ should be equal to zero. From elasticity theoretical considerations it follows that gradients of the residual stresses $\sigma_{13}$, $\sigma_{23}$ and $\sigma_{33}$ with respect to Z (direction of the surface normal) should be equal to zero for all kinds of specimen symmetry. A gradient with respect to Z in $\sigma_{33}$ can only occur in the presence of body forces. At the surface of the specimen these stresses themselves should be equal to zero and consequently they should be equal to zero everywhere in a specimen of which the dimensions in the X and Y directions are large as compared to the one in the Z direction. Gradients in $\sigma_{11}$ and $\sigma_{22}$ with respect to Z can occur.

(2) Assuming only non-zero $\sigma_{11}$ and $\sigma_{22}$ a quantitative expression can be obtained for the relationship between the mean strain measured by means of X-ray diffraction in a direction determined by the angles $\psi$ and $\varphi$ with reference to the specimen frame and the residual stresses present in the surface layers of a polycrystalline specimen of cubic material exhibiting a texture of orthorhombic or monoclinic symmetry. Results for both b.c.c. and f.c.c. crystal symmetry are derived and are summarized in Table 3.

(3) Using non-zero $\sigma_{11}$ and $\sigma_{22}$ only, the so-called $\psi$ splitting reported in the literature (Dölle, Hauk & Neubauer, 1978; Hauk, Krug & Vaessen, 1981; Dölle & Cohen, 1980a) can be explained qualitatively as a result of crystallographic texture. Even weak textures could contribute to the $\psi$ splitting because they are connected to the (relatively) large residual stresses $\sigma_{11}$ and $\sigma_{22}$. The texture-dependent part of the $\psi$ splitting can be taken into account quantitatively.

(4) In quite a number of cases $\psi$ splitting seems to originate from non-zero residual $\sigma_{13}$ (Wakabayashi, Nakayama & Nagata, 1977; Krause & Jühle, 1980; Hauk, Oudelhoven & Vaessen, 1981; Dölle, 1982; Hauk, 1982). In these reports residual shear stresses $\sigma_{13}$ are shown to be very likely after grinding of materials consisting of two phases. The $\sigma_{13}$ (having opposite sign in both phases) on a macro scale still can be equal to zero due to compensation. At least $\psi$ splitting cannot be due to texture only in these cases (§ 7.1.2). Further experiments are needed to obtain a clear distinction between the texture explanation and the residual $\sigma_{13}$ explanation.

(5) Using a non-zero $\sigma_{11}$ and $\sigma_{22}$ only, a semi-quantitative explanation can be given for the 'snake-like' curves found after heavy cold-rolling for the graph of the measured lattice strain vs $\sin^2\psi$ (Hauk, Krug & Vaessen, 1981; James & Cohen, 1980) in the case of $\varphi = 0$. The absence of non-linearity for

<table>
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<th>B.c.c. reflection</th>
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<td>$F.c.c. reflection$</td>
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$\varphi = \pi/2$ can be explained in a similar way.

The author wishes to express his gratitude to Dr Ir E. H. Mittemeijer for critically reading the manuscript and to Professor Dr Ir P. Penning for many stimulating discussions.

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APPENDIX I

The stress tensor with reference to the measurement $(L)$ frame

For the transformation from the specimen $(P)$ frame into the measurement $(L)$ frame use is made of matrix $g_1$ (8). Because the orientation of the axis $L_3$ is prescribed by the angles $\psi$ and $\varphi$, one parameter remains free to choose in fixing the orientation of the measurement $(L)$ frame. This is the angle $\varphi_2$. Defining the stress tensor with reference to the specimen $(P)$ frame as $\sigma_{kl}$, the stress tensor with reference to the measurement $(L)$ frame is $\sigma_{ij} = C_{ik}C_{lj}\sigma_{kl}$, where summation should be carried out over the repeated indices and the $C_{ij}$ are the elements of matrix $g_1$ (8).

In the most general case one finds for $\sigma_{ij}$

\[\sigma_{ij} = (\sin^2\varphi \cos^2\varphi_2 + \cos^2\varphi \cos^2\psi \sin^2\varphi_2)
\ + \frac{1}{2} \sin 2\varphi \cos \psi \sin 2\varphi_2 \sigma_{11}
\ + (\cos^2\varphi \cos^2\varphi_2 + \sin^2\varphi \cos^2\psi \sin^2\varphi_2)
\ - \frac{1}{2} \sin 2\varphi \cos \psi \sin 2\varphi_2 \sigma_{22}
\ + \sin^2\psi \sin^2\varphi_2 \sigma_{33} + (-\sin 2\varphi \cos^2\varphi_2)\]
\[\begin{align*}
-sin \ 2\phi & \cos \psi \sin 2\phi_2 \\
+sin \ 2\phi & \cos^2 \psi \sin^2 \phi_1 \sigma_{12} \\
-(sin \ \phi \ \sin \ \psi & \ \sin 2\phi_2) \sigma_{11} \\
+cos \ \psi \ \sin 2\phi & \sin^2 \phi_2 \sigma_{13} \\
+(cos \ \phi \ \sin \ \psi & \ \sin 2\phi_2) \sigma_{22} \\
-sin \ \phi & \ \sin 2\phi \ sin^2 \phi_2 \sigma_{23} \\
\end{align*}\]

\[\begin{align*}
\sigma'_{x'} &= (sin^2 \ \phi \ \sin^2 \ \phi_2 + cos^2 \ \phi \ \cos^2 \ \psi \ \cos^2 \ \phi_2) \\
-sin \ \phi & \ \sin 2\phi \ \cos \ \cos \ \psi \ \sin 2\phi_2 \\
+cos \ \phi & \ \sin 2\phi \ \cos \ \psi \ \cos 2\phi_2 \\
-sin \ \phi & \ \sin 2\phi \ \cos \ \psi \ \sin 2\phi_2 \\
\end{align*}\]

\[\begin{align*}
\sigma'_{y'} &= cos^2 \ \phi \ \sin^2 \ \psi \ \sigma_{11} + sin^2 \ \psi \ \sin^2 \ \psi \ \sigma_{22} \\
+cos \ \psi \ \sigma_{33} + sin \ 2\phi \ \sin^2 \ \psi \ \sigma_{12} \\
+cos \ \phi & \ \sin 2\psi \ \sigma_{13} + sin \ \psi \ \sin 2\psi \ \sigma_{23} \\
\end{align*}\]

\[\begin{align*}
\sigma'_{x'y'} &= (-sin \ \psi \ \sin \ \phi \ \sin 2\phi_2 + \frac{1}{2} \ \cos \ \psi \ \sin \ \phi \ \sin 2\phi_2 \\
+\frac{1}{2} & \ \cos \ \psi \ \sin \ \phi \ \sin 2\phi_2 \ \sigma_{11} \\
+(-\frac{1}{2} \ \cos \ \phi & \ \sin 2\phi \ \sin 2\phi_2 - \frac{1}{2} \ \sin \ \phi \ \cos \ \psi \ \cos 2\phi_2 \\
+\frac{1}{2} & \ \sin \ \phi \ \cos \ \psi \ \sin 2\phi_2 \ \sigma_{22} \\
+\frac{1}{2} \ \sin \ \phi & \ \sin 2\phi_2 \ \sigma_{33} \\
+\frac{1}{2} \ \sin \ \phi \ \sin 2\phi_2 - \cos \ \phi \ \cos \ \psi \ \cos 2\phi_2 \\
+\frac{1}{2} & \ \cos \ \phi \ \cos \ \psi \ \sin 2\phi_2 \ \sigma_{12} \\
+(-sin \ \phi & \ \sin \ \psi \ \cos \ \phi \ \sigma_{13} \\
-\frac{1}{2} & \ \cos \ \phi \ \sin 2\phi \ \sigma_{13} \\
+cos \ \phi \ \sin \ \psi \ \cos \ \phi_2 \\
-\frac{1}{2} & \ \sin \ \phi \ \sin 2\phi_2 \ \sigma_{23} \\
\end{align*}\]

\[\begin{align*}
\sigma'_{y'x'} &= -\frac{1}{2} \ \sin \ \phi \ \sin 2\phi \ \sin \ \phi \ \sigma_{11} \\
+\frac{1}{2} & \ \cos \ \phi \ \sin 2\phi \ \sin \ \phi_1 \ \sigma_{11} \\
+\frac{1}{2} \ \sin \ \phi \ \cos \ \psi \ \cos \ \phi_2 \\
-sin^2 \ \phi \ \sin 2\psi \ \sigma_{12} \\
+\frac{1}{2} & \ \sin \ \phi \ \sin 2\phi \ \sigma_{33} \\
+(cos \ \phi & \ \sin \ \psi \ \cos \ \phi_2 \\
-\frac{1}{2} & \ \sin \ \phi \ \sin 2\phi \ \sigma_{23} \\
\end{align*}\]
RESIDUAL STRESSES IN CUBIC MATERIALS

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3. DIFFRACTION ELASTIC CONSTANTS OF TEXTURED CUBIC MATERIALS. THE VOIGT MODEL CASE.
Diffraction elastic constants of textured cubic materials

The Voigt model case

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ABSTRACT

Diffraction elastic constants connect residual or applied macro-stresses to measured diffraction elastic line-shift strains. They have the dimension of compliance and supply a means of determining unknown macro-stresses from measured strain data.

For texture-free materials the diffraction elastic constants can be calculated for the Reuss, Voigt or Kröner models of elasticity. The latter model yields results very close to physical reality. The Reuss and Voigt models lead to two extreme solutions. The Kröner solution is in most cases very close to the arithmetic mean of the Reuss and Voigt solutions which conforms to the Hill approximation. For textured materials, use of the Kröner model (based on a self-consistent method) is not (yet) feasible.

The diffraction elastic constants for textured materials according to the Voigt model are derived in this paper. It is shown that only three orientation distribution function (o.d.f.) series-expansion coefficients are necessary for the calculations conforming to earlier derivations.

The Hill approximation can also be applied to the case of textured materials. The Reuss-model diffraction elastic constants have been derived earlier for these materials. Averaged with the Voigt-model data obtained in this paper they may lead to a realistic approximation of the diffraction elastic constants. Consequently, determination of unknown macro-stresses in textured materials may be performed to a higher degree of accuracy.

§ 1. INTRODUCTION

1.1. General theory

The so-called quasi-isotropic diffraction elastic constants $s_1$ and $\frac{1}{2}s_2$ (Dölle 1979) for texture-free materials occur in the equation relating the measured elastic diffraction line-shift strain $\langle \epsilon_{zz} \rangle$ and the stresses

$$\frac{(d_{\psi, \Phi} - d_0)}{d_0} = \langle \epsilon_{zz}(\psi, \Phi) \rangle = s_1(hkl)[\hat{\sigma}_{11} + \hat{\sigma}_{22} + \hat{\sigma}_{33}]$$

$$+ \frac{1}{2}s_2(hkl)[\hat{\sigma}_{11} \cos^2 \Phi + \hat{\sigma}_{22} \sin^2 \Phi + \hat{\sigma}_{12} \sin 2\Phi \sin \psi]$$

$$+ \frac{1}{2}s_2(hkl)\hat{\sigma}_{33} \cos^2 \psi + \frac{1}{2}s_2(hkl)[\hat{\sigma}_{13} \cos \Phi + \hat{\sigma}_{23} \sin \Phi] \sin 2\psi,$$

where $d_{\psi, \Phi}$ is the $hkl$ interplanar spacing measured in the direction determined by the angles $\psi$ and $\Phi$, which define the direction of measurement with respect to the specimen's reference frame (fig. 1); and $d_0$ the $hkl$ interplanar spacing of a stress-free specimen of the same material.
Experimental arrangement in diffraction strain analysis. The specimen (P-) frame coincides with the specimen's axes of symmetry. RD, SD, TD and ND stand for rolling direction, shear direction, transverse direction, and normal direction, respectively. The diffraction strain is measured in the Z-direction of the laboratory (L-) frame. The orientation relationship between the P- and the L-frame is given (in terms of Euler angles) in Brakman (1983).

Usually, the angle $\psi$ is varied at constant $\Phi$; it may be changed in two different ways: (i) by rotation of the specimen about the direction (in the specimen's surface) perpendicular to the diffraction plane, i.e. in the $\theta'$-direction' ($\Omega$-dilectrometer, situation drawn); or (ii) by rotation of the specimen about the bisecting line of the specimen's surface and the diffraction plane ($\Psi$-dilectrometer). The latter method clearly allows larger values of $\psi$-tilt.

The stresses are taken as averaged values over the volume of the material irradiated, indicated by a tilde. The angular brackets in eqn. (1) denote averaging over all diffracting crystallites. Use of these two different levels of averaging in one equation is not self-evident. It will be shown that for the Reuss-model case (eqn. (8)) and the Voigt-model case (eqn. (14)) it is justified. The procedure is subject to the condition that all crystallite orientations are represented in the volume of material irradiated. For the case of the Kröner model it can be written (subject to the same condition as mentioned above) as

$$\langle \varepsilon_{zz} \rangle = [S'_{zzij} + \langle t'_{zzij} \rangle] \sigma_{ij} \tag{1a}$$

where $t'_{zzij}$ is the orientation-dependent elastic polarization tensor as introduced by Kröner (1958), it should hold here that $t'_{zzij} \equiv 0$; and $S'_{zzij}$ the specimen's macroscopic compliance tensor.

Equation (1a) leads, after elaboration, to an expression similar to eqn. (1) (Bollenrath, Hauk and Müller 1967). Equation (1) shows that, if $\bar{\sigma}_{13} = \bar{\sigma}_{23} \equiv 0$, $\langle \varepsilon_{zz} \rangle$ should behave linearly with respect to $\sin^2 \psi$ for the case of texture-free materials.

The diffraction elastic constants (in most cases termed X-ray elastic constants, XEC) $s_1$ and $s_2$ can be written according to the Reuss, Voigt or Kröner models of elastic polycrystal coupling. The relevant equations are given in Dölle (1979).
Bollenrath et al. (1967) and also in Möller and Martin (1939). For texture-free materials the XEC do not depend on \( \psi \) and \( \Phi \). If they are taken according to the Voigt model they depend on the single-crystal elastic constants but not on hkl. For textured materials eqn. (1) can be written (Dölle and Hauk 1978) more generally as

\[
\langle \varepsilon^{zz}(\psi, \Phi) \rangle = (d_v - d_0)/d_0 = R'_{ij} \bar{\varepsilon}_{ij}
\]

(summation over repeated indices). The \( R'_{ij} \) are general XEC defined with respect to the laboratory (L-) frame (fig. 1). In most cases one wishes to obtain the stresses with respect to the specimen (P-) frame; hence, it is written (Dölle 1979)

\[
\langle \varepsilon^{zz}(\psi, \Phi) \rangle = F_{ij}(\psi, \Phi, R'_{ij}) \bar{\varepsilon}_{ij}.
\]

(3)

Since the new XEC, i.e. the \( F_{ij} \), connect quantities \( \bar{\varepsilon}_{ij} \) defined with respect to the P-frame to those defined with respect to the L-frame (\( \langle \varepsilon^{zz} \rangle \)) they are not the elements of a tensor. The \( F_{ij} \) depend on the single-crystal elastic constants, hkl, \( \psi \) and \( \Phi \) and the texture.

In this paper primes indicate quantities defined with respect to the L-frame, while their unprimed counterparts refer to the P-frame unless indicated otherwise. The single-crystal elastic constants are denoted by a lower-case letter, for instance \( s_{ijkl} \). Generally, \( s_{ijkl} \) (lower case or capital \( s \)) stands for a compliance. The macroscopic elastic constants of the specimen as a whole are given by a capital letter, for instance \( C_{ijkl} \). Generally, \( c_{ijkl} \) (lower case or capital \( c \)) stands for a stiffness. Mean values obtained from averaging over all crystallite orientations in the specimen are indicated by a bar, for instance \( \bar{c}_{ijkl} \). Such an averaging may be written for instance as

\[
\bar{\varepsilon}_{ijkl} = \int \varepsilon_{ijkl}(g) f(g) \, dg,
\]

(3a)

where \( \bar{\varepsilon}_{ijkl} \) is defined with respect to the P-frame just like the orientation distribution function (o.d.f.), i.e. \( f(g) \), which occurs here as a weight function. \( c_{ijkl}(g) \) is transformed from cubic fourfold axes in the crystallite’s orientation \( g \) to the P-frame. The integral comprises all crystallite orientations in the specimen. This procedure is equivalent to the treatment by Kröner (1958). Mean values obtained from averaging over all diffraacting crystallite orientations are indicated by angular brackets. Mean values obtained from averaging over all crystallite orientations in the irradiated volume are indicated by a tilde.

It generally holds that (Kröner 1958)

\[
\bar{\varepsilon}_{ijkl} = C_{klij} \bar{\varepsilon}_{ij} \text{ (and } \bar{\varepsilon}_{ij} = S_{ijkl} \bar{\varepsilon}_{kl}).
\]

(4)

1.2. Mean stresses obtained in the diffraction experiment in (fictive) textured specimens obeying the Reuss or Voigt models and the case of a real, textured specimen

Owing to the specific nature of the diffraction experiment, one always measures a mean strain \( \langle \varepsilon_{ij} \rangle \) regardless of the model used in the calculation. In this section only stresses and strains defined with respect to the P-frame are considered.

1.2.1. (Fictive) specimen obeying the Reuss model of elastic polycrystal coupling

For this model (see fig. 2(a)) it holds that the stresses (with respect to a common basis) everywhere in the specimen should be equal to one another, so

\[
\sigma_{kl}(g) = \langle \sigma_{kl} \rangle = \bar{\sigma}_{kl} = \bar{\sigma}_{kh}
\]

(5)
(a) Fictive case of a specimen obeying the Reuss model of elastic polycrystal coupling. The shaded area represents the volume irradiated. The Reuss model assumes that the weighted mean value of the single-crystal compliances is equal to the specimen’s compliance: \( \bar{\epsilon}_{ijkl} = S_{ijkl} \). Then, stress tensors everywhere in the specimen should be equal (with respect to a common basis) to one another (Kröner 1958), see eqn. (5). If a sufficient number of crystallite orientations are present in the volume irradiated, it can be shown that \( \bar{\epsilon}_{ij} = \bar{\epsilon}_{ij} \), where \( \bar{\epsilon}_{ij} = S_{ijkl} \bar{\delta}_{kl} \) similarly to eqns. (7a) and (4) respectively. The diffraction experiment only determines the strain averaged over the crystallites, \( \langle \epsilon_{ij} \rangle \). The unknown stress \( \bar{\delta}_{kl} \) can be obtained from this measurement using \( \langle \epsilon_{ij} \rangle = \langle S_{ijkl} \sigma_{kl} \rangle = \langle S_{ijkl} \rangle \bar{\delta}_{kl} \). After Bunge (1982, p. 322).

(b) Fictive case of a specimen obeying the Voigt model of elastic polycrystal coupling. The shaded area represents the volume irradiated. The Voigt model assumes that the (weighted mean value of the single-crystal stiffness is equal to the specimen’s stiffness: \( \bar{\epsilon}_{ijkl} = C_{ijkl} \). Then the stress tensors everywhere in the specimen should be equal (with respect to a common basis) to one another (Kröner 1958), see eqn. (9). Only a small number of crystallites are indicated. If a sufficient number of crystallite orientations are present in the volume irradiated it can be shown that \( \bar{\delta}_{kl} = \bar{\delta}_{kl} \), similarly to eqn. (13) where \( \bar{\delta}_{kl} = C_{ijkl} \bar{\epsilon}_{ij} \) and eqn. (4). Generally the latter equation holds. The diffraction experiment only determines the strain averaged over the crystallites, \( \langle \epsilon_{ij} \rangle \). The unknown stress \( \bar{\delta}_{kl} \) can be calculated from this measurement using \( \langle \sigma_{ij} \rangle = \bar{\epsilon}_{ij} = \bar{\epsilon}_{ij} = S_{ijkl} \bar{\sigma}_{kl} = S_{ijkl} \bar{\delta}_{kl} \) as in eqn. (14). After Bunge (1982, p. 322).

\[
\bar{\epsilon}_{ij} = \frac{\sigma_{ij}(g)}{C_{ijkl}}
\]

where \( \sigma_{ij}(g) \) stands for the stress in the crystallite with orientation \( g \) defined with respect to the P-frame. In general it can be expected that

\[
e_{ij}(g) \neq \langle \epsilon_{ij} \rangle \neq \bar{\epsilon}_{ij} \neq \bar{\epsilon}_{ij}.
\]

Since \( \bar{\epsilon}_{ij} \) is the mean stress obtained on averaging over the entire specimen, it follows that a non-trivial 'Reuss stress-state' never can be attained without an externally applied stress. For a specimen at rest in the absence of external forces (body-forces not considered), it should always hold that \( \bar{\delta}_{kl} = 0 \).
Diffraction elastic constants of textured cubic materials

Equation (5) is the consequence of the essential Reuss assumption, i.e.

\[ \bar{s}_{ijkl} = S_{ijkl}. \]  

(6)

\( S_{ijkl} \) and \( \bar{s}_{ijkl} \) are defined with respect to the \( P \)-frame. This model does not allow elastic polarization (Kröner 1958). The strain \( \varepsilon_{ij}(g) \) in a crystallite is equal to \( s_{ijkl}(g) \bar{\sigma}_{kl} \). This strain may differ from grain to grain, the difference depending on the orientation difference between them. If the volume irradiated (approximately) comprises all crystallite orientations representing the texture of the specimen it may be assumed, in addition to eqn. (6) that

\[ \bar{s}_{ijkl} = S_{ijkl}. \]  

(7)

It then follows (since \( \bar{\varepsilon}_{ij} = s_{ijkl} \bar{\sigma}_{kl} = \bar{s}_{ijkl} \bar{\sigma}_{kl} \) for the Reuss model) that

\[ \bar{\varepsilon}_{ij} \approx \bar{\varepsilon}_{ij}. \]  

(7a)

Consequently, gradients of \( \bar{\varepsilon}_{ij} \) with respect to the coordinates cannot occur. Equation (7a) imposes a restriction upon eqn. (5a). The expression relating the diffraction strains \( \langle \varepsilon_{ij} \rangle \) to the mean stresses \( \bar{\sigma}_{kl} \) reads:

\[ \langle \varepsilon_{ij} \rangle = \langle s_{ijkl} \rangle \bar{\sigma}_{kl}. \]  

(8)

1.2.2. (Fictive) specimen obeying the Voigt model of elastic polycrystal coupling

For this model (see fig. 2(b)) it holds that strains (with respect to a common basis) everywhere in the specimen should be equal to one another:

\[ \varepsilon_{ij}(g) = \langle \varepsilon_{ij} \rangle = \bar{\varepsilon}_{ij} = \bar{\varepsilon}_{ij}. \]  

(9)

In general it is expected that

\[ \sigma_{kl}(g) \neq \langle \sigma_{kl} \rangle \neq \bar{\sigma}_{kl} \neq \bar{\sigma}_{kl}. \]  

(10)

The mean strain \( \bar{\varepsilon}_{ij} \) is obtained by averaging over the entire specimen. It follows that a non-trivial 'Voigt strain-state' can never be attained without an applied, external strain. Equation (9) is a consequence of the essential Voigt assumption that

\[ \bar{\varepsilon}_{ijkl} = C_{ijkl}, \]  

(11)

where \( C_{ijkl} \) is the stiffness tensor of the specimen and \( \bar{\varepsilon}_{ijkl} \) has been defined in eqn. (3a). The model does not allow elastic polarization.

The stress \( \sigma_{kl}(g) \) in a crystal is equal to \( c_{klij}(g) \bar{\varepsilon}_{ij} \). This stress may again differ from grain to grain depending on the orientation difference between them. If the volume irradiated (approximately) comprises all crystallite orientations representing the texture of the specimen it may be assumed, in addition to eqn. (10) that

\[ \bar{\varepsilon}_{ijkl} \approx C_{ijkl}. \]  

(12)

It then follows (since \( \bar{\sigma}_{kl} = c_{klij} \bar{\varepsilon}_{ij} = \bar{c}_{klij} \bar{\varepsilon}_{ij} \) for the Voigt model), that

\[ \bar{\sigma}_{kl} \approx \bar{\sigma}_{kl}. \]  

(13)

† Note that the irradiated volume, although much smaller than the specimen's volume in most cases, may easily contain all texture-representing crystallite orientations. This may be especially true for a fine-grained material. The volumes exhibiting such behaviour may be thought of as being connected in regular three-dimensional order.
which imposes a restriction upon eqn. (10). The expression relating the diffraction strains $\langle \varepsilon_{ij} \rangle$ to the mean stresses $\bar{\sigma}_{kl}$ then reads

$$
\langle \varepsilon_{ij} \rangle = \bar{\varepsilon}_{ij} = S_{ijkl} \bar{\sigma}_{kl}.
$$

(14)

It follows from eqn. (13) that gradients of $\bar{\sigma}_{kl}$ with respect to the coordinates cannot occur. Equation (14) predicts a diffraction strain equivalent to a mechanical strain measurement. As such, it predicts the same strain for every hkl reflection used in the diffraction experiment.

1.2.3. Case of a real, textured specimen

In this case, equations (5) and (9) generally do not hold. Elastic polarization occurs and gradients of $\bar{\sigma}_{kl}$ and $\bar{\varepsilon}_{ij}$ with respect to the coordinates frequently occur. Even the case of uniformly applied, external stress does not lead to realization of a 'Reuss' stress-state. Consequently, diffraction experiments conducted on a real specimen can only give information about the mean stress in the volume irradiated, i.e. $\bar{\sigma}_{kl}$, at most. Applying the Reuss and Voigt models of eqns. (8) and (14) to a real specimen may still yield useful results for the stresses $\bar{\sigma}_{kl}$. Elastic polarization must then be neglected.

For the case of specimens only exhibiting residual stresses (i.e. not externally loaded) it is required that $\bar{\sigma}_{kl} \equiv 0$. Then, gradients of $\bar{\sigma}_{kl}$ and/or $\bar{\varepsilon}_{ij}$ with respect to the coordinates must occur. The irradiated volume can be considered as a specimen itself as far as residual stress analysis is concerned. If one wishes to apply the Reuss model to this specimen, $\bar{\sigma}_{kl}$ and (due to eqn. (4)) $\bar{\varepsilon}_{ij}$ should be removed from eqns. (5) and (9). Equations (6) and (7) can still be used but the strain in a crystallite is equal to $S_{ijkl}(g) \bar{\sigma}_{kl}$. Equation (7a) does not hold. For this model it may be written that

$$
\bar{\varepsilon}_{ij} = S_{ijkl} \bar{\sigma}_{kl} = S_{ijkl} \bar{\sigma}_{kl} = S_{ijkl} \bar{\sigma}_{kl},
$$

(14a)

and, as a consequence,

$$
\langle \sigma_{kl} \rangle = \bar{\sigma}_{kl} = C_{klji} \bar{\varepsilon}_{ij}.
$$

(14b)

Equation (8) still holds:

$$
\langle \varepsilon_{ij} \rangle = \langle S_{ijkl} \sigma_{kl} \rangle = \langle S_{ijkl} \bar{\sigma}_{kl} \rangle.
$$

(14c)

If one wishes to apply the Voigt model to a textured specimen exhibiting residual stresses only, eqns. (11) and (12) are still valid. Again $\bar{\sigma}_{kl}$ and $\bar{\varepsilon}_{ij}$ must be equal to zero. Equation (13) does not hold but it can be written that

$$
\bar{\sigma}_{kl} = C_{klji} \bar{\varepsilon}_{ij} = C_{klji} \bar{\varepsilon}_{ij} = C_{klji} \bar{\varepsilon}_{ij},
$$

(14d)

and, as a consequence, $\langle \varepsilon_{ij} \rangle = \bar{\varepsilon}_{ij} = S_{ijkl} \bar{\sigma}_{kl}$ and hence eqn. (14) still holds.

1.2.4. Hill's approximation

The measured strain $\langle \varepsilon_{ij} \rangle$ only represents the averaged strains of the diffracting crystallites. However, a good approximation of the stresses $\bar{\sigma}_{kl}$ in a real (textured) specimen can be obtained by averaging the Reuss and Voigt model predictions of Hill's (1952) approximation:

$$
\langle \varepsilon_{ij} \rangle = \frac{1}{2} [\langle S_{ijkl} \sigma_{kl} \rangle_v + \langle S_{ijkl} \sigma_{kl} \rangle_r] = \frac{1}{2} [S_{ijkl} + \langle S_{ijkl} \rangle] \bar{\sigma}_{kl},
$$

(15)

where, on the right-hand side, use has been made of eqns. (8) and (14). Equation (15) also holds for the case of a specimen only exhibiting residual stresses as can be inferred from §1.2.3.
The Reuss model in connection with diffraction experiments on textured materials, and the subsequent derivation of $\langle s_{ijkl} \rangle$ as a function of the single-crystal elastic constants, the texture and the used $hkl$ reflection, has been the subject of work by Brakman (1983) and Sayers (1984). In the latter paper, the case of axi-symmetric textures was studied where only fourth-order o.d.f. series-expansion coefficients were used. However, the Reuss model requires all o.d.f. coefficients for the calculation of the XEC.

It is the purpose of this paper to derive general expressions for the $s_{ijkl}$ (and hence, the XEC) for textured specimens according to the Voigt model. Expressions for the XEC connected to $\sigma_{11}$ and $\sigma_{22}$, i.e. $F_{11}$ and $F_{22}$ according to eqn. (3) as a function of $\sin^2 \psi$ are derived for the two (often used) $\Phi$-angles: 0 and $\pi/2$. Two practical examples are given of materials exhibiting a rolling texture, i.e. an orthorhombic specimen symmetry. Equations determining the XEC, $F_{33}$, $F_{12}$, $F_{13}$ and $F_{23}$ are also given.

§ 2. Stress–strain relationships for the Voigt model applied to textured materials

Equation (9) also holds of course, for quantities defined with respect to the L-frame. Then, it can be written that

$$\langle \tilde{e}_{zz}(\psi, \Phi) \rangle = \tilde{e}_{zz}(\psi, \Phi).$$

(16)

Tensor transformation from the P-frame to the L-frame yields

$$\tilde{e}_{zz}(\psi, \Phi) = (\tilde{e}_{11} \cos^2 \Phi + \tilde{e}_{22} \sin^2 \Phi + \tilde{e}_{12} \sin 2\Phi) \sin^2 \psi + \tilde{e}_{33} \cos^2 \psi$$

$$+ (\tilde{e}_{13} \cos \Phi + \tilde{e}_{23} \sin \Phi) \sin 2\psi. \quad (17)$$

It is unimportant (in this model) whether one measures the strain by diffraction, involving a limited number of crystallites, or by mechanical methods involving the entire specimen. Equation (17) is useless for the determination of the stresses but it states that, if the shears $\tilde{e}_{13}$ and $\tilde{e}_{23}$ are absent, $\tilde{e}_{zz}(\psi, \Phi)$ should behave linearly with respect to $\sin^2 \psi$ for both texture-free and textured materials.

The Voigt model does not impose constraints upon the stresses. The stress-state may vary from crystal to crystal. Consequently, in a stress–strain relationship within the context of the Voigt model the stresses occur as mean values. In view of the practical application of the model to real specimens it is the mean stress $\sigma_{ij}$ one is looking for.

Consider the diffraction strain $\langle \tilde{e}_{zz}(\psi, \Phi) \rangle$ written in terms of compliances and stresses with respect to the L-frame. Dropping the tilde from now on it follows that, similarly to eqn. (14),

$$\langle \tilde{e}_{zz}(\psi, \Phi) \rangle = S_{zzkl} \sigma_{kl}. \quad (18)$$

Tensor transformation yields expressions for $S_{zzkl}$ in terms of the specimen's compliance tensor elements defined with respect to the P-frame. Using the expressions
for \( \sigma_{kl} \) as given in Brakman (1983) (letting \( \phi_2 = 0 \)) it follows that

\[
\langle \epsilon'_{zz}(\psi, \Phi) \rangle = \sigma_{11} S_{1133} + \sigma_{22} S_{2233} + \frac{1}{2} \sigma_{33} (S_{1133} + S_{2233}) \\
+ [\sigma_{11}(S_{1122} - S_{1133}) + \sigma_{22}(S_{1122} - S_{2233})] \sin^2 \psi \\
+ [\sigma_{11}(S_{1111} - S_{1122}) \cos^2 \Phi + \sigma_{22}(S_{2222} - S_{1122}) \sin^2 \Phi] \\
+ \frac{1}{2} \sigma_{33} (S_{1313} - S_{2323}) \cos 2\Phi \\
+ 2 \sigma_{12} S_{1212} \sin 2\Phi \sin^2 \psi + \sigma_{33} [S_{3333} - \frac{1}{2}(S_{1133} + S_{2233})] \cos^2 \psi \\
+ 2[\sigma_{13} S_{1313} \cos \Phi + \sigma_{23} S_{2323} \sin \Phi] \sin 2\psi,
\]

(19)

where the stresses and the compliances are defined with respect to the P-frame. Note that the right-hand side of eqn. (19) is not specific for the Voigt model. If one writes \( C_{zz}(\psi, \Phi) \) instead of \( \langle \epsilon'_{zz}(\psi, \Phi) \rangle \), eqn. (19) becomes Hooke's law for a macroscopic stress–strain relationship due to eqn. (13). The Voigt model is only introduced after (i) the \( S_{ijkl} \) are written in terms of the \( C_{ijkl} \) and subsequently it is taken that \( C_{ijkl} = C_{ijkl} \) and (ii) the macroscopic strain is taken to be equal to the diffraction strain. Note that eqn. (19) does not exhibit any \( hkl \)-dependence.

In analogy with eqns. (1) and (17), it follows that, if \( \sigma_{13} \) and \( \sigma_{23} \) are equal to zero, the predicted strain \( \langle \epsilon'_{zz} \rangle \) is linear with respect to \( \sin^2 \psi \). Texture-dependence enters into eqn. (19) through the compliances \( S_{ijkl} \). They can be inverted for say, the orthorhombic specimen symmetry case as indicated in Appendix B.

2.1. Check for a texture-free specimen

This case can be considered as a special condition for eqn. (19). It should hold that

\[
S_{1122} = S_{1133} = S_{2233} \\
S_{1111} = S_{2222} = S_{3333} \\
S_{1212} = S_{1313} = S_{2323} \\
2 S_{1212} = S_{1111} - S_{1122}.
\]

(20)

Writing formally,

\[
s_{1} = S_{1122} = -\nu/E = -C_{1122}/(C_{1111} + 2 C_{1122})(C_{1111} - C_{1122})
\]

(20c)

and

\[
\frac{1}{2} s_{2} = S_{1111} - S_{1122} = (1 + \nu)/E = 1/(C_{1111} - C_{1122}),(20d)
\]

it follows for eqn. (19) that

\[
\langle \epsilon'_{zz}(\psi, \Phi) \rangle = s_{1} [\sigma_{11} + \sigma_{22} + \sigma_{33}] \\
+ \frac{1}{2} s_{2} [\sigma_{11} \sin^2 \psi + \sigma_{12} \sin 2\Phi \sin^2 \psi + \sigma_{33} \cos^2 \psi] \\
+ \frac{1}{2} s_{2} [\sigma_{13} \cos \Phi + \sigma_{23} \sin \Phi] \sin 2\psi,
\]

(21)

where \( \sigma_{\Phi} = \sigma_{11} \cos^2 \Phi + \sigma_{22} \sin^2 \Phi \).

Applying \( C_{ijkl} = \tilde{c}_{ijkl} \) for the Voigt model, eqn. (20c) can be written as

\[
s_{1}^{*} = (5c_{1122} - c_{0})/(c_{1111} + 2c_{1122})(10c_{1212} + 2c_{0}),
\]

(22a)

and eqn. (20d) as

\[
\frac{1}{2} s_{2}^{*} = 1/2G' = 1/(2c_{1212} + 2/5c_{0}),
\]

(22b)

where the \( c_{ijkl} \) denote the single-crystal stiffnesses with respect to cubic fourfold axes and \( c_{0} \) is defined in eqn. (A.10a) (see Appendix A).
Equations (22 a) and (22 b) are identical to eqn. (28) from Møller and Martin (1939) as may be immediately found by expressing the stiffnesses in terms of cubic-crystal compliances. Substituting \( s_1' \) and \( \frac{1}{2} s_2' \) for \( s_1 \) and \( \frac{1}{2} s_2 \) respectively in eqn. (21) yields the Voigt equation for the stress–strain relationship for a texture-free material. It predicts linear behaviour with respect to \( \sin^2 \psi \) if the stresses \( \sigma_{13} \) and \( \sigma_{23} \) are equal to zero.

2.2. Specimens exhibiting orthorhombic symmetry, i.e. rolling or extrusion textures

The \( S \)-tensor elements in eqn. (19) according to the Voigt model are obtained from Appendix B. The XEC can then be immediately derived from eqn. (19). Restricting the treatment to \( F_{11} \) and \( F_{22} \) of eqn. (3) it can be found for \( \Phi = 0 \) that

\[
F_{11}(\psi, 0) = D^{-1}\left\{ -2(c_{1122} + 1/5c_0)(c_{1212} + 1/5c_0) \\
+ \frac{c_0}{15\sqrt{21}}(c_{1111} + 2c_{1122})(2C^1_{41} - C^1_{42}/\sqrt{5}) - \frac{c_0}{15\sqrt{3}}(c_{1122} + 1/5c_0)(C^1_{44} \sqrt{7} + C^1_{43} \sqrt{5}) \\
+ \frac{c_0^2}{4725}(2[C^1_{41}]^2 - 5[C^1_{42}]^2 + 2C^1_{44}C^1_{43} \sqrt{35}) \right\} + D^{-1}(c_{1111} + 2c_{1122}) \left\{ 2(c_{1212} + 1/5c_0) \\
+ \frac{c_0}{30\sqrt{21}}(7C^1_{44} + 4C^1_{42} \sqrt{5} + C^1_{43} \sqrt{35}) \right\} \sin^2 \psi,
\]

(23)

where \( C^1_{41}, C^1_{42} \) and \( C^1_{43} \) stand for the three fourth-order o.d.f. series-expansion coefficients.

\[
F_{22}(\psi, 0) = D^{-1}\left\{ -2(c_{1122} + 1/5c_0)(c_{1212} + 1/5c_0) \\
+ \frac{c_0}{15\sqrt{21}}(c_{1111} + 2c_{1122})(2C^1_{41} + C^1_{42} \sqrt{5}) - \frac{c_0}{15\sqrt{3}}(c_{1122} + 1/5c_0) \\
\times (C^1_{44} \sqrt{7} + C^1_{43} \sqrt{5}) + \frac{c_0^2}{4725}(2[C^1_{41}]^2 - 5[C^1_{42}]^2 + 2C^1_{44}C^1_{43} \sqrt{35}) \right\} \\
+ D^{-1}\frac{c_0}{6\sqrt{105}}(c_{1111} + 2c_{1122})(-C^1_{44} \sqrt{5} - 2C^1_{42} + C^1_{43} \sqrt{7}) \sin^2 \psi,
\]

(24)

where \( D \) has been defined in eqn. (B 11).

It can be inferred that \( F_{11}(\pi/2) = F_{22}(0) \) except that the sign of \( C^1_{42} \) is reversed. It also can be shown that \( F_{22}(\pi/2) = F_{11}(0) \), subject to the same restriction. From eqns. (23) and (24) it follows that indeed the general XEC \( F_{11} \) and \( F_{22} \) of eqn. (3) exhibit linear behaviour with respect to \( \sin^2 \psi \). It can be shown that this is also the case for the other XEC. However, \( F_{13} \) and \( F_{23} \) depend linearly on \( \sin 2\psi \).

For the XEC \( F_{33}, F_{12}, F_{13} \) and \( F_{23} \) it follows that

\[
F_{33}(\psi, \Phi) = S_{3333} + \left[ \frac{1}{2}(S_{1133} - S_{2233}) \cos 2\Phi + \frac{1}{2}(S_{1133} + S_{2233} - 2S_{3333}) \right] \sin^2 \psi,
\]

(25 a)

\[
F_{12}(\psi, \Phi) = 2S_{1212} \sin 2\Phi \sin^2 \psi,
\]

(25 b)

\[
F_{13}(\psi, \Phi) = 2S_{1313} \cos \Phi \sin \psi,
\]

(25 c)

and

\[
F_{23}(\psi, \Phi) = 2S_{2323} \sin \Phi \sin \psi.
\]

(25 d)
Using eqns. (B 3) and (B 7) to (B 9) in combination with eqns. (A 2) to (A 10) leads directly to the expressions for $F_{33}$ to $F_{23}$.

The XEC depend on (i) the single-crystal stiffness tensor elements $c_{ijkl}$, and (ii) the orientation distribution function (o.d.f.) series-expansion coefficients $C_4^{11}$, $C_4^{12}$ and $C_4^{13}$. A complete treatment of the o.d.f. and its series-expansion coefficients is given by Bunge (1982). The case of diffraction line-shift strains in conjunction with the Voigt model has been treated by Sayers (1984) for the case of axi-symmetric textures ($C_4^{12} = C_4^{13} = 0$).

§ 3. Results and Discussion

Figures 3–6 show the XEC $F_{11}$ and $F_{22}$ as a function of $\sin^2 \psi$ for two $\Phi$-angles of a rolled steel sheet specimen. The details of this specimen are given in the table. The solid straight lines represent the XEC $F_{11}(\psi, 0)$ through $F_{22}(\psi, \pi/2)$ for this textured specimen for the Voigt model. The dashed lines depict their counterparts for a texture-free specimen. The curved solid lines exhibit the Reuss-model XEC for this textured material as it is obtained from Brakman (1983) for the supposedly used 211 measuring reflection. For the texture-free case, the XEC for the Reuss model in combination with

Fig. 3

![Graph showing XEC values as a function of $\sin^2 \psi$]

Predicted diffraction elastic constant $F_{11}$ plotted against $\sin^2 \psi$ for $\Phi = 0$ and the 211 reflection calculated for the steel specimen of the table. Solid straight line, Voigt model in conjunction with crystallographic texture calculated according to eqn. (23); solid curved line, Reuss model in conjunction with crystallographic texture calculated according to Brakman (1983); dashed straight line, Voigt model for texture-free iron specimen. Note that the Voigt model predicts the same XEC for all $hkl$ measuring reflections whereas the Reuss model does not. The mean value of the Reuss and Voigt models (in conjunction with crystallographic texture) according to Hill's (1952) approximation may lead to a practicable solution for the determination of the XEC of textured materials.
**Diffraction elastic constants of textured cubic materials**

**Fig. 4**

As for fig. 3, but for $F_{22}$ plotted against $\sin^2 \psi$, $\Phi = 0$.

**Fig. 5**

As for fig. 3, but for $F_{11}$ plotted against $\sin^2 \psi$, $\Phi = \pi/2$.  

39
Fourth-order orientation distribution function (o.d.f.) series-expansion coefficients for the materials covered in figs. (3)-(6) and figs. (7)-(10). Data for the steel sheet specimen from unpublished research, those for the copper sheet specimen from Bunge and Tobisch (1968).

<table>
<thead>
<tr>
<th>Specimen</th>
<th>O.d.f. series expansion coefficients</th>
<th>Chemical composition</th>
<th>Specimen thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel sheet</td>
<td>$C_4^{11} = -1.51$</td>
<td>0.058% C</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$C_4^{12} = -0.15$</td>
<td>0.33% Mn</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$C_4^{13} = +0.81$</td>
<td>0.009% P</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.020% S</td>
<td>1.45</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.043% N</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.054% Al</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.013% Si</td>
<td></td>
</tr>
<tr>
<td>Cold-rolled copper sheet</td>
<td>$C_4^{11} = -1.02$</td>
<td>Not given</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$C_4^{12} = -0.48$</td>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td>$C_4^{13} = -1.60$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Diffraction elastic constants of textured cubic materials

the b.c.c. 211 reflection and those for the Voigt model almost coincide (Bollenrath et al. 1967). It can be seen (figs. 3–6) that this is not the case for a textured material.

Figures 7–10 exhibit the same XEC for a copper sheet specimen, reduced by 90% by cold-rolling, taken from the literature (Bunge and Tobisch 1968). It follows (figs. 3–10) that the differences between the predicted Voigt-XEC for these textured materials do not differ very much from the texture-free Voigt-XEC. However, the difference is significant and can be of practical importance. Note that the difference between the textured and the texture-free material case is largest for the Reuss model. For a texture-free material, the Reuss model predicts a straight line and the ‘oscillations’, i.e. departures from linearity, for the textured material case in figs. 3–10 can be quite large. Indeed, the averaged Voigt and Reuss XEC of textured materials similarly to the Hill approximation as indicated in eqn. (15) of this paper may lead to a better determination of unknown stresses in these materials.

There is no physical justification for the Hill approximation but its practical results may fall to within a few per cent of the (iterative) Kröner prediction for textured materials (Bunge 1982, p. 327). Note that the Kröner model cannot be used in its explicit form for the case of textured materials. An improvement with respect to the Hill approximation could be obtained by taking into account a minimal (elastic) energy

![Fig. 7](image_url)

Predicted diffraction elastic constant $F_{11}$ plotted against $\sin^2 \psi$ for $\Phi = 0$, calculated for a Cu specimen reduced by 90% by cold-rolling as given in the literature by Bunge and Tobisch (1968). See also the table. Solid straight line, Voigt model in conjunction with crystallographic texture calculated according to eqn. (23). Dashed straight line, Voigt model for texture-free copper specimen. The Reuss model prediction is not shown but since the texture is much sharper than the steel specimen’s texture of figs. (3)–(6) stronger ‘oscillations’ may be expected.
Fig. 8

As for fig. 7, but for $F_{22}$ plotted against $\sin^2 \psi$, $\Phi = 0$.

Fig. 9

As for fig. 7, but for $F_{11}$ plotted against $\sin^2 \psi$, $\Phi = \pi/2$. 
requirement. This method has been proposed for textured materials by Bunge (1974) but it still is not exact (as the author states) because granular interaction is neglected.

§4. CONCLUSIONS

(i) Expressions for the diffraction elastic constants of textured materials for the Voigt model of elastic polycrystal coupling have been derived.

(ii) Averaging according to the Hill approximation of these Voigt-model results, with the diffraction elastic constants of textured materials according to the Reuss model obtained earlier, may lead to a better determination of unknown stresses in textured materials.

(iii) hkl reflections where the Voigt and Reuss XEC (almost) coincide for texture-free materials exhibit significant differences for the textured materials case as far as the XEC are concerned.

ACKNOWLEDGMENTS

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APPENDIX A

The mean stiffness tensor elements $c_{ijkl}$

The quantities are the mean values of the single-crystal stiffnesses $c_{ijkl}$ obtained upon averaging over all crystallite orientations present in the specimen (similarly to
eqn. (3 a)). It is assumed that the specimen exhibits orthorhombic symmetry. The $c_{ijkl}$ are defined with respect to the P-frame (fig. 1). In eqn. (3 a) the orientation distribution function (o.d.f.), i.e. the symbol $f(g)$, is written as a weight function. The o.d.f. is normalized such that

$$
\int f(g) \, dg = 1.
$$

(A 1)

The o.d.f. (and consequently, its set of series-expansion coefficients $C_{ij}^E$) according to Bunge (1982, p. 47) is defined with respect to the P-frame. After elaboration it is found that

$$
c_{1111} = c_{1111} - 2/5c_0 + \frac{c_0}{10\sqrt{21}} C_4^{11} - \frac{c_0}{3\sqrt{105}} C_4^{12} + \frac{c_0}{6\sqrt{15}} C_4^{13},
$$

(A 2)

$$
c_{2222} = c_{1111} - 2/5c_0 + \frac{4c_0}{15\sqrt{21}} C_4^{11} - \frac{c_0}{6\sqrt{15}} C_4^{13},
$$

(A 3)

$$
c_{3333} = c_{1111} - 2/5c_0 + \frac{4c_0}{15\sqrt{21}} C_4^{11} - \frac{c_0}{6\sqrt{15}} C_4^{13},
$$

(A 4)

$$
c_{1122} = c_{1122} + 1/5c_0 - \frac{c_0}{6\sqrt{15}} C_4^{13},
$$

(A 5)

$$
c_{1133} = c_{1122} + 1/5c_0 - \frac{2c_0}{15\sqrt{21}} C_4^{11} + \frac{c_0}{3\sqrt{105}} C_4^{12},
$$

(A 6)

$$
c_{2233} = c_{1122} + 1/5c_0 - \frac{2c_0}{15\sqrt{21}} C_4^{11} - \frac{c_0}{3\sqrt{105}} C_4^{12},
$$

(A 7)

$$
c_{1122} = c_{1212} + 1/5c_0 + \frac{c_0}{30\sqrt{21}} C_4^{11} - \frac{c_0}{6\sqrt{15}} C_4^{13},
$$

(A 8)

$$
c_{1313} = c_{1212} + 1/5c_0 - \frac{2c_0}{15\sqrt{21}} C_4^{11} + \frac{c_0}{3\sqrt{105}} C_4^{12},
$$

(A 9)

$$
c_{2323} = c_{1212} + 1/5c_0 - \frac{2c_0}{15\sqrt{21}} C_4^{11} - \frac{c_0}{3\sqrt{105}} C_4^{12},
$$

(A 10)

where

$$
c_0 = c_{1111} - c_{1122} - 2c_{1212}.
$$

(A 10 a)

Note that the single-crystal stiffnesses $c_{1111}$, $c_{1122}$ and $c_{1212}$ are defined with respect to the crystallites' reference axes, whereas the $c_{ijkl}$ are defined with respect to the P-frame. In the analysis it has been assumed that the reference axes of the specimen-frame coincide with the specimen's axes of symmetry (RD, TD and ND). Consequently, $c_{ijkl}$ reflects the nature of the stiffness tensor on principal axes of an orthorhombic crystal (Nye 1985) (i) $c_{1111} \neq c_{2222} \neq c_{3333}$, $c_{1122} \neq c_{1133} \neq c_{2233}$; (ii) $c_{ijkl} = 0$ ($k \neq j$, $k$ and $j \neq i$; no implied summation); and (iii) $c_{ijij} = 0$ ($j \neq i$; no implied summation).†

† For every symmetric fourth-rank tensor, general expressions such as $c_{ijkl} = c_{ijkl} = c_{kijl} = c_{klij}$ must hold.
Diffraction elastic constants of textured cubic materials

In eqns. (A 2) to (A 10) the o.d.f. series-expansion coefficients occur only up to the fourth order. Since the integration of eqn. (3 a) is extended to all orientations, orthogonality conditions of generalized spherical harmonics (Bunge 1982, p. 368) apply. These harmonics are functions of three rotation (Euler) angles. The calculated macroscopic elastic constants only depend on the fourth-order o.d.f. coefficients. This has been shown earlier by Pursey and Cox (1954) and by Bunge (1968).

The single-crystal stiffnesses \( c_{ijk} \) only depend on (at most) a fourfold of these angles. Then, only zero-order (\( C_i^0 \)), second-order (\( C_i^1 \) and \( C_i^2 \)) and fourth-order (\( C_i^4 \), \( C_i^4 \) and \( C_i^4 \)) o.d.f. series-expansion coefficients remain after the integration. The coefficient \( C_i^1 \) is, by definition equal to unity, while the coefficients \( C_i^1 \) and \( C_i^2 \) are "forbidden" for cubic materials (Bunge 1982, p. 80) and hence, are taken to be equal to zero.†

In eqns. (A 2) to (A 10) the first two terms of the right-hand side represent the random (texture-free) contributions: if no crystallographic texture were present at all it would hold: \( C_i^4 = C_i^4 = C_i^4 = 0 \). It follows that the numerical coefficients of \( C_i^1 \), \( C_i^4 \) and \( C_i^4 \) in eqns. (A 2) to (A 10) are identical with those given in another form by Bunge (1982, p. 324). Using the expression (Bunge 1982, p. 97)

\[
W_{4mn} = 2^{1/2}(24\pi)^{-1} C_i^{mn} \quad \text{and} \quad C_i^{mn} = \sum_{v=1}^{3} \tilde{A}_v^{n} C_i^{m},
\]

it follows that the expressions (A 2) to (A 10) are equivalent to eqn. (10) of Sayers (1982) where the tensor \( \bar{C}_{ijk} \) for orthorhombic specimen symmetry is also treated.

Equations (A 2) to (A 10) also lead to

\[
\bar{c}_{114} = \bar{c}_{1111} + \bar{c}_{1122} + \bar{c}_{1133} = \bar{c}_{224} = \bar{c}_{334} = \bar{c}_{1111} + 2\bar{c}_{1122}
\]

(A 11)

and as a consequence

\[
\bar{c}_{i4k} = 3(\bar{c}_{1111} + 2\bar{c}_{1122}) = \bar{c}_{i4k}.
\]

(Summation convention of repeated indices.) And

\[
\bar{c}_{i4k} = \bar{c}_{i4k}.
\]

(A 11 a)

Note that these observations are general, they are not specific for the Voigt model. Equation (A 12) exhibits the invariants of the first degree of the 9 × 9 matrices representing these tensors. It can be shown that the eigenvalues constituting the invariant of the cubic single-crystal tensor are: \( \bar{c}_{1111} - 2\bar{c}_{2222} \) (twofold), \( \bar{c}_{1111} + 2\bar{c}_{1122} \) and \( 2\bar{c}_{1122} \) (threefold).

The sums in eqn. (A 12) represent the sums of the main diagonal elements of the 9 × 9 matrices representing the respective tensors. Apparently, \( \bar{c}_{ijk} \) and \( \bar{c}_{i4k} \) are independent of texture. Equations (A 11 a) and (A 12) are identical with those for texture-free

† The difference between the Voigt and Reuss models used for stress analysis from diffraction strain data is striking. For the Voigt model, only the fourth-order o.d.f. series-expansion coefficients occur whereas for the Reuss-model application (Brakman 1983) all o.d.f. series-expansion coefficients are needed. In the latter case this should be expected since the diffracting crystallites only comprise a small subset of the orientations representing the texture of the specimen. As a consequence, orthogonality conditions of generalized spherical harmonics (Bunge 1982, p. 368) do not apply.
materials (Kröner 1958). It does not follow, however, that the tensor $\mathbf{C}_{ijkl}$ is equal to the true macroscopic-stiffness tensor $\mathbf{C}_{ijkl}$ of the specimen as a whole. The Voigt model assumes that $\mathbf{C}_{ijkl} = C_{ijkl}$. In that case

$$\mathbf{c}_{ijk} = \mathbf{C}_{ijkl} = c_{ijk}. \quad (A\ 13)$$

It can be shown that $\mathbf{C}_{ijkl}$ is an invariant (with respect to rotation of the reference frame) for materials of even triclinic symmetry, but it can only generally be proven (using Kröner’s (1958) elastic-polarization concept) for the case of a texture-free material that $\mathbf{C}_{ijkl} = c_{ijk}$ without use of the Voigt or Reuss model. It also holds for the Voigt model for the case of both texture-free and textured materials

$$\mathbf{c}_{ijk} = \mathbf{C}_{ijkl} = c_{ijk}. \quad (A\ 14)$$

The o.d.f. series-expansion coefficients $C_{ijkl}^1$, $C_{ijkl}^2$ and $C_{ijkl}^3$ can be determined from elastic measurements (Bunge 1982, p. 324). For the case of orthorhombic specimen symmetry only three coefficients occur, whereas monoclinic specimen symmetry exhibits five.

---

**APPENDIX B**

**Inversion of the macroscopic S-tensor**

**Dependency on the texture for the case of the Voigt model**

In order to apply Voigt’s model the (macroscopic) S-tensor elements of eqn. (19) are written in terms of the (macroscopic) C-tensor elements of the specimen after which the Voigt model according to eqn. (11) can be applied. The $S_{ijkl}$ read (Borik and Aler 1965)

\[
S_{1111} = (C_{2222}C_{3333} - C_{2333}^2)D^{-1}, \quad (B\ 1)
\]

\[
S_{2222} = (C_{1111}C_{3333} - C_{1133}^2)D^{-1}, \quad (B\ 2)
\]

\[
S_{3333} = (C_{1111}C_{2222} - C_{1122}^2)D^{-1}, \quad (B\ 3)
\]

\[
S_{1122} = (C_{1133}C_{2233} - C_{1122}C_{3333})D^{-1}, \quad (B\ 4)
\]

\[
S_{1133} = (C_{1122}C_{2233} - C_{1133}C_{2222})D^{-1}, \quad (B\ 5)
\]

\[
S_{2233} = (C_{1122}C_{1133} - C_{2233}C_{1111})D^{-1}, \quad (B\ 6)
\]

\[
S_{1212} = 1/(4C_{1212}), \quad (B\ 7)
\]

\[
S_{1313} = 1/(4C_{1313}) \quad (B\ 8)
\]

and

\[
S_{2223} = 1/(4C_{2223}), \quad (B\ 9)
\]

where

\[
D = C_{1111}(C_{2222}C_{3333} - C_{2333}^2)
- C_{1122}(C_{1122}C_{3333} - C_{2233}C_{1133})
+ C_{1133}(C_{1122}C_{2233} - C_{2222}C_{1133}). \quad (B\ 10)
\]
Putting eqn. (11) into effect if follows, after elaboration, that
\[
D = (c_{1111} + 2c_{1122}) \left[ 4(c_{1212} + 1/5c_0)^2 + \frac{2c_0}{15\sqrt{3}} (c_{1212} + 1/5c_0)(C_{4}^{11}/\sqrt{7} + C_{4}^{13}/\sqrt{5}) 
+ \frac{c_0^2}{1575} (2[C_{4}^{11}]^2 - 5[C_{4}^{12}]^2 + 2C_{4}^{11}C_{4}^{13}/35) \right], \quad (B\ 11)
\]
where the first term on the right-hand side stands for the texture-free contribution:
\[
S_{1133} = \left[ -2(c_{1212} + 1/5c_0)(c_{1122} + 1/5c_0) 
+ \frac{c_0}{15\sqrt{21}} (c_{1111} + 2c_{1122})(2C_{4}^{11} - C_{4}^{12}/\sqrt{5}) 
- \frac{c_0}{15\sqrt{3}} (c_{1122} + 1/5c_0)(C_{4}^{11}/\sqrt{7} + C_{4}^{13}/\sqrt{5}) 
+ \frac{c_0^2}{4725} (2[C_{4}^{11}]^2 - 5[C_{4}^{12}]^2 + 2C_{4}^{11}C_{4}^{13}/35) \right] D^{-1}; \quad (B\ 12)
\]
(for $S_{2233}$ the same expression is obtained except that the sign of $C_{4}^{12}$ is reversed):
\[
S_{1122} - S_{1133} = \frac{c_0}{6\sqrt{105}} (c_{1111} + 2c_{1122})(-C_{4}^{11}/\sqrt{5} + 2C_{4}^{12} + C_{4}^{13}/\sqrt{7}) D^{-1}; \quad (B\ 13)
\]
\[
S_{1122} - S_{2233} = \frac{c_0}{6\sqrt{105}} (c_{1111} + 2c_{1122})(-C_{4}^{11}/\sqrt{5} - 2C_{4}^{12} + C_{4}^{13}/\sqrt{7}) D^{-1}; \quad (B\ 14)
\]
\[
S_{1111} - S_{1122} = (c_{1111} + 2c_{1122}) \left[ 2(c_{1212} + 1/5c_0) + \frac{c_0}{15\sqrt{21}} (6C_{4}^{11} + C_{4}^{12}/\sqrt{5}) \right] D^{-1}; \quad (B\ 15)
\]
\[
S_{2222} - S_{1122} = (c_{1111} + 2c_{1122}) \left[ 2(c_{1212} + 1/5c_0) + \frac{c_0}{15\sqrt{21}} (6C_{4}^{11} - C_{4}^{12}/\sqrt{5}) \right] D^{-1}; \quad (B\ 16)
\]
\[
S_{3333} = \left\{ 2(c_{1111} + c_{1122} - 1/5c_0)(c_{1212} + 1/5c_0) 
+ \frac{4c_0}{15\sqrt{21}} (c_{1212} + 1/5c_0)C_{4}^{11} + \frac{c_0}{15\sqrt{21}} (c_{1111} + c_{1122} - 1/5c_0) 
\times (C_{4}^{11} + C_{4}^{13}/35) + \frac{c_0^2}{4725} (2[C_{4}^{11}]^2 - 5[C_{4}^{12}]^2 + 2C_{4}^{11}C_{4}^{13}/35) \right\} D^{-1}. \quad (B\ 17)
\]
Using $C_{1212} = \overline{c_{1212}}$, $C_{1313} = \overline{c_{1313}}$ and $C_{2323} = \overline{c_{2323}}$, eqns. (B 7) to (B 9) can readily be evaluated with the aid of eqns. (A 8) to (A 10). It can be shown that, for this (Voigt) model, it follows from eqns. (B 12) to (B 17) that
\[
S_{1111} + S_{1122} + S_{1133} = S_{1111} + S_{2233} = S_{1111} + 2s_{1122} \quad (B\ 18)
\]
and, as a consequence,

\[ S_{i\ell k} = s_{i\ell k} = 3(s_{1111} + 2s_{1122}) \]  \( \dagger \)  

(B 18a)

Note that this may not be the case for the true S-tensor of the specimen. Furthermore, it follows that

\[ S_{i\ell k} \neq 3(s_{1111} + 2s_{1122}) \]  

(B 19)

The latter inequality also holds for texture-free material (and the Voigt model applied to it). (Equation (B 19) exhibits an equals sign for the case of the Reuss model applied to both texture-free and textured materials.)

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\[ \dagger \] This equation can also be derived, of course, for the case of a texture-free material without using the Voigt or Reuss model. The equation also holds for the Reuss model case where it is assumed \( s_{i\ell k} = \overline{s}_{i\ell k} \) for both the textured and texture-free case. Then, the relevant equations in analogy to eqns. (A 2) to (A 10) yield \( \overline{s}_{i\ell k} = s_{i\ell k} \) independent of texture.
4. SURFACE SHERICAL HARMONICS AND INTENSITY AND STRAIN POLE FIGURES OF CUBIC TEXTURED MATERIALS.
Surface Spherical Harmonics and Intensity and Strain Pole Figures of Cubic Textured Materials

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Abstract

The equations for diffraction strain pole figures measured on textured cubic materials exhibit an hkl-dependence. This is expressed by an hkl-permutation-invariant 'surface' spherical harmonic. Four types of new harmonics are defined. These harmonics differ in essence from those for the hkl-dependent expression obtained for diffraction intensity pole figures. In the latter case associated Legendre polynomials arise whereas in the former (Jacobi type) generalizations of these polynomials occur. Equations exhibiting diffraction intensity and diffraction strain expressions are given for all cubic point groups. Structure factors arise in the expressions. The treatment is given for both anomalous and normal scattering modes. Surface spherical harmonics do not satisfy Laplace's equation. This only occurs upon conversion into 'solid spherical harmonics'. Then the harmonics associated with intensity pole figures satisfy Laplace's equation. The 'diffraction strain harmonics' do not, however. Orthonormalization is also different from the case of conventional hkl-permutation-invariant surface spherical harmonics. Stereographic projections are given for a few examples of harmonics.

1. Introduction

Spherical harmonics occur in (among others) quantum mechanics, electromagnetism, geodesics and crystal physics. The present treatment deals with spherical surface harmonics in conjunction with crystal physics and, more specifically, residual stress analysis of textured cubic materials.

The new harmonics occur in the hkl-dependent part of the expression for diffraction line-shift strain pole figures obtained on textured materials for the general \{hkl\} reflection case. Diffraction strain may be defined as the averaged strain of the crystals engaged in the diffraction experiment. It depends on hkl, the loading of the specimen and the orientation of the scattering vector \( Q \) with respect to the specimen's reference axes [definition of \( Q \) according to Sayers (1984)]. It is determined from the shift of the diffraction line's profile with respect to some initial condition. Crystals exhibit different strains depending on their orientation, when subject to an even uniform stress system. If the specimen exhibits crystallographic texture some orientations may occur frequently, others may be absent. Consequently the texture enters in the diffraction strain equations (Brakman, 1983; Sayers, 1984). Since the diffraction strain depends on the orientation of \( Q \) it can be represented in terms of a pole figure. Like the conventional diffraction intensity pole figure, it can be depicted in a stereographic projection with respect to specimen axes. By contrast with the intensity pole figure the strain pole figure depends on the stress state (residual or externally applied) of the volume of material irradiated. If the texture is homogeneous over the specimen, the intensity pole figure does not depend on the size of the volume irradiated provided grain statistics are adequately retained. The intensity pole figure is therefore an intensive quantity. Although stress and strain are also intensive quantities, the strain pole figure is an extensive quantity.

For instance, the case of neutron diffraction (Sayers, 1984; Pintschovius & Macherauch, 1982) could yield a totally different strain pole figure from that obtained using X-rays. In the case of X-ray diffraction the strain pole figure represents a very local average of the specimen strains due to the strong attenuation of the radiation. In the neutron diffraction experiment the specimen as a whole may be irritated. For each specimen the conditions of mechanical equilibrium must be satisfied. Then the strains due to macrostresses (assumed to be constant over distances large compared with the grain size) compensate. This does not occur in the X-ray experiment.

The intensity pole figure presents data in a (normalized) compact form allowing visual interpretation and presentation. The texture type can be determined from one or more pole figures. The strain pole figure may serve a similar purpose. If the texture is known the approximate stress state can be determined from the strain pole figure. Practical examples are given by Hoffmann, Neff, Scholtes & Macherauch (1984) and Hauk, Vaessen & Weber (1985). The orientation distribution function (o.d.f.) of the crystals of a textured specimen is usually expanded in a series

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(Bunge, 1982, p. 47). The expansion coefficients can be calculated from intensity pole figures. However, these pole figures only allow even-order (Bunge, 1982, pp. 100-107) expansion coefficients. The strain pole figures also exhibit odd-order expansion coefficients (Brakman, 1985). Consequently they provide a means of determining the complete o.d.f.

For point group 432 the expression for the diffraction strain pole figure (according to the Reuss model of elasticity), for the hkl reflection contribution only, is given in Brakman (1986). It reads (only stress-tensor elements \(\sigma_{ij}\) and \(\sigma_{ij}\) are taken non-zero, the expression can easily be extended to the full stress tensor):

\[
\langle e'_{2z}(\psi, \alpha) \rangle = s_1(hkl)(\sigma_{11} + \sigma_{22}) + \frac{1}{2} s_2(hkl)\sigma_6 \sin^2 \psi
+ [-s_0/2P_{hkl}(\psi, \alpha)] \\
\times [(\sigma_{11} - \sigma_{22}) \cos 2\alpha - \sigma_6 \sin^2 \psi] \\
\times \sum_{j=1}^{4} \sum_{\mu=1}^{4} [F_j(hkl, j, \mu)B_{j}^{\psi}(\psi, \alpha) \\
+ F_2(hkl, j, \mu)C_{j}^{\psi}(\psi, \alpha)] \\
+ [s_0/2P_{hkl}(\psi, \alpha)] \\
\times (\sigma_{11} - \sigma_{22}) \sin 2\alpha \cos \psi \\
\times \sum_{j=1}^{4} \sum_{\mu=1}^{4} [-F_j(hkl, j, \mu)C_{j}^{\psi}(\psi, \alpha) \\
+ F_2(hkl, j, \mu)B_{j}^{\psi}(\psi, \alpha)] \\
+ [s_0/2P_{hkl}(\psi, \alpha)] \\
\times (\sigma_{11} - \sigma_{22}) \sin 2\alpha \sin \psi \\
\times \sum_{j=1}^{4} \sum_{\mu=1}^{4} [F_j(hkl, j, \mu)E_{j}^{\psi}(\psi, \alpha) \\
- F_2(hkl, j, \mu)D_{j}^{\psi}(\psi, \alpha)] \\
+ [s_0/2P_{hkl}(\psi, \alpha)]\sigma_6 \sin 2\psi \\
\times \sum_{j=1}^{4} \sum_{\mu=1}^{4} [F_j(hkl, j, \mu)D_{j}^{\psi}(\psi, \alpha) \\
+ F_2(hkl, j, \mu)E_{j}^{\psi}(\psi, \alpha)],
\]

where \(s_1(hkl)\) and \(\frac{1}{2} s_2(hkl)\) are the so-called quasi-isotropic diffraction elastic constants (Dölle, 1979). \(P_{hkl}\) is defined in equation (15c). Apart from its corresponding structure factor and a proportionality factor, it is equal to the single hkl reflection’s scattered intensity.

Functions \(B_{j}^{\psi}(\psi, \alpha)\) , \(C_{j}^{\psi}(\psi, \alpha)\), \(D_{j}^{\psi}(\psi, \alpha)\), \(E_{j}^{\psi}(\psi, \alpha)\) are defined in Brakman (1986). They depend on the texture and need not be discussed here. \(s_0\) stands for single cubic crystal elastic anisotropy:

\[
s_0 = s_{1111} - s_{1122} - 2s_{1212}
\]

\[
\sigma_a = \sigma_{11} \cos^2 \alpha + \sigma_{22} \sin^2 \alpha.
\]

The stresses \(\sigma_{11}\) and \(\sigma_{22}\) are taken to operate parallel to the specimen’s axes of symmetry. They are assumed to be macrostresses. It is the purpose of this paper to deal with the harmonics denoted by the symbols \(F_1, F_2, F_3\) and \(F_4\) in (1). They depend on \(hkl\), \(j\) and \(\mu\) similar to the \(K_{j}^{p}\) harmonics defined in (6) and (18) to (20). An example of a diffraction strain pole figure of a cold-rolled steel specimen calculated for an assumed stress state of \(\eta = \sigma_{22}/\sigma_{11} = 10\) is given in Fig. 1.

In the calculation use of the \([211]\) b.c.c. reflection has been assumed and expressions involving functions \(F_2\) and \(F_4\) were omitted.

2. Definitions

Spherical harmonics are usually divided into three classes:

(i) Zonal spherical harmonics: the ‘normal’ Legendre polynomials \(P_{\ell}(\cos \Phi)\) and tesseral spherical harmonics: the ‘associated’ Legendre polynomials \(P_{\ell}^{m}(\cos \Phi)\).

* Equation (1) represents the Reuss model of elasticity. For the Voigt model an \([hkl]\)-independent diffraction strain pole figure results. The Kröner model is not (yet) feasible for textured materials. Expression (1) averaged with the Voigt model prediction allows calculation of the stress state of the irradiated volume according to the well known ‘sin’ \(\psi\) method’ (Dölle, 1979; Hauk, 1984; Hauk & Macherauh, 1984; James & Cohen, 1980).

Fig. 1. Calculated \([211]\) diffraction strain for a textured cold-rolled steel sheet sample. Stress state assumed: \(\eta = \sigma_{22}/\sigma_{11} = 10\). All other stresses taken equal to zero. \(\sigma_{11}\) operates parallel to RD (rolling direction). Diffraction strain \(\langle e'_{2z}(\psi, \alpha) \rangle\) divided by \(s_0\sigma_{11}\). Isostrain values: \(\Delta = -1.60, + -2.20, \times -0.80, \square -0.40, \bigcirc 0.00, \bigodot +0.40, \star +0.80, \asem \+1.20, \blacklozenge +1.60\). Angle \(\psi\) measured in the plane of RD and TD (transverse direction). Angle \(\psi\) is the deviation angle from ND (normal direction). The orientation of the scattering vector with respect to the specimen axes is indicated by \(\psi, \alpha\).
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(ii) Surface spherical harmonics:

\[ K^m_j(\Phi, \beta) = P^m_j(\cos \Phi) \exp(i m \beta) \]  \hspace{1cm} (2)

(angles \( \Phi \) and \( \beta \) according to Fig. 2). These functions are often used in normalized form:

\[ K^m_j(\Phi, \beta) = (2\pi)^{-1/2} P^m_j(\cos \Phi) \exp(i m \beta). \] \hspace{1cm} (2a)

If we use a definition of the associated Legendre polynomials such that (Bunge, 1982, p. 356)

\[ \int_0^\pi P^m_j(\cos \Phi) P^n_j(\cos \Phi) \sin \Phi \, d\Phi = \delta_{jn}, \] \hspace{1cm} (3)

it follows that

\[ \int \frac{1}{2} K^m_j(\Phi, \beta) K^n_j(\Phi, \beta)^* \sin \Phi \, d\Phi \, d\beta = \delta_{jm} \delta_{mn}. \] \hspace{1cm} (4)

(In what follows the spherical surface element \( \sin \Phi \, d\Phi \, d\beta \) will be denoted by \( dA \).) These functions occur (apart from a factor) as eigenfunctions of the squared angular momentum operator of a single particle in quantum mechanics (Landau & Lifshitz, 1974, p. 54) and also as eigenfunctions of the squared differential operator for infinitesimal rotations (Gel'fand, Minlos & Shapiro, 1963, p. 41).

(iii) Solid spherical harmonics:

\[ u = r^l K^m_j(\Phi, \beta) \] or \[ u = r^{-j-1} K^m_j(\Phi, \beta). \] \hspace{1cm} (5)

These functions are particular solutions of Laplace's equation \( \Delta u = 0 \) (case of \( m = 0 \) included) and \( r \) is a radius vector.

The \( K^m_j \) satisfy mathematical constraints:

(i) They are continuous in the poles of the sphere, i.e. they exhibit the same value for all \( \beta \) if \( \Phi = 0 \) or \( \Phi = \pi \).

(ii) They exhibit the same value if \( \beta \) is replaced by \( \beta + 2\pi \); 'cyclic behaviour'.

(iii) They satisfy the orthonormalization condition of (4).

(iv) Upon multiplication by \( r^l \) or \( r^{-j-1} \) they satisfy Laplace's equation. However, for the physics discussed in this paper Laplace's equation does not need to be satisfied.

For the application to crystal physics one often needs harmonics satisfying the symmetry of the point group of the crystal under consideration (Bettis, Bhatia & Wyman, 1956; Von der Lage & Bethe, 1947; Meyer, 1954; Fox & Krohn, 1977; Kara & Kurki-Suonio, 1981).

2.1. Symmetrized harmonics

The symmetry elements of a crystal point group can be seen as transformations of crystal reference axes. They operate on orientations. For such orientations, the parent and product crystal orientations are physically indistinguishable. In texture analysis, the symbol \( g \) is commonly used for orientations and transformations of orientations. \( g \) can be written as a \( 3 \times 3 \) matrix.

There are three types of crystal point-group symmetry elements:

(i) Pure rotations of which the determinant of \( g \) is equal to +1, 'proper rotations'.

(ii) Mirror-like operations without an explicit centre of inversion.

(iii) Centres of inversion.

In the two latter cases \( \det (g) \) is equal to \(-1\). The harmonics treated in this paper are all defined with respect to crystal reference axes.

For the construction of harmonics satisfying point-group symmetry one can proceed in two different ways:

(a) Construct linear combinations of harmonics \( K^m_j \) and impose the symmetry elements upon them. This method can be applied for the case of cubic harmonics associated with diffraction intensity pole figures:

\[ K^m_j(\Phi, \beta) = \sum_{m=\pm j} A_{m \mu}^j K_{m \mu}^j(\Phi, \beta). \] \hspace{1cm} (6)

The coefficients can be chosen real (Bunge, 1982, p. 267) and they can be made to satisfy the symmetry requirements of the point group. Equation (6) represents a linear combination of the normal harmonics \( K^m_j \) and \( \mu \) enumerates the number of possible linearly independent constructions \( K^m_j \).

It is required that

\[ \int \frac{1}{2} K^m_j(\Phi, \beta) K^n_j(\Phi, \beta)^* \, dA = \delta_{jn} \delta_{\mu \mu'}. \] \hspace{1cm} (7)

and

\[ \sum_{m=\pm j} A_{m \mu}^j A_{m' \mu'}^j = \delta_{\mu \mu'}. \] \hspace{1cm} (8)

The total number of possible linearly independent constructions according to (6), i.e. \( \mu_{\max} \), has been given by Bunge (1982, pp. 62 and 365) for even \( j \) and
odd \( j \), respectively. \( \mu_{\text{max}} \) depends on the point group. For non-cubic point groups the coefficients \( A_{j}^{\mu} \) take a very simple form (Bunge, 1982, p. 383). For the cubic point groups the full series expansion [cf. (6)] is needed owing to the threefold axis. The coefficients\(^*\) cannot be written in a simple form; they have been tabulated by Bunge (1982, p. 501) for point group 432.

(b) For both intensity and strain pole figures the \( hkl \)-dependent harmonics arise as a consequence of the physics of the problem. For both types of pole figure the value of the function in the direction of \( Q \) is obtained as an average over the crystal orientations engaged in the diffraction. For textured materials, the orientation distribution function (o.d.f.)\(^+\) of the crystals then occurs in the equations for the averaging procedure.

The o.d.f. is a function of orientations. It is defined for orientations obtained via rotations only. The rotational symmetry elements of the crystal's point group can be imposed upon the o.d.f. with the cubic symmetry coefficients \( A_{j}^{\mu} \) treated in § 3. See also Bunge (1982, p. 384).

In the eventual equations for both types of pole figure, harmonics arise satisfying the rotational symmetry elements of the point group considered. However, in some cases the harmonics satisfy additional symmetry elements not imposed on the o.d.f. This may be due to:

(i) The physical nature of the diffraction experiment. Expressions for the contributions from crystal orientations exhibiting \( [hkl] \) parallel to \( Q \) and \( [hk\ell] \) parallel to \( Q \) have to be added. Harmonics satisfying only point group 432 are then cancelled whereas harmonics satisfying \( m3m \) are retained. The same holds for point group 23 with respect to \( m3 \).

(ii) The value of both intensity and strain in the direction of the scattering vector \( Q \) is an average over basically the two orientation types mentioned above. The averaging covers \( 2\pi \) rad rotation about \( Q \) [angle \( \varphi_{2} \) in Brakman (1985)]. The o.d.f. is a function of three independent (Euler) rotation angles for fixed orientation of \( Q \). The three angles determine the crystal's orientation with respect to the laboratory frame. The harmonics can be seen as a result of integration of the o.d.f. with respect to one (Euler) angle, i.e. \( \varphi_{2} \). For the diffraction strain the same holds

but the o.d.f. times the single-crystal strain\(^*\) is averaged with respect to \( \varphi_{2} \). As a consequence of the averaging with respect to this angle, the behaviour with respect to symmetry of both harmonic types may be different from that of the o.d.f.

In this paper method (b) is used since the harmonics associated with the strain pole figures cannot be derived using method (a).

2.2. Symmetry

A clear distinction must be made between the symmetry exhibited by the o.d.f. and by the harmonics. The symmetry of the o.d.f. may be defined as follows. Consider a crystal symmetry element leaving the value of the o.d.f. unchanged in the crystal’s product orientation with respect to the parent orientation. These orientations are physically equivalent. Then the o.d.f. may be said to exhibit symmetry with respect to the crystal symmetry element. The symmetry of the o.d.f. is defined with respect to orientations. The symmetry the harmonics satisfy may be defined as follows. The harmonic is some continuous function of two independent angles defined with respect to crystal reference axes. The harmonic is a function of directions. If a crystal symmetry element is applied to crystal reference axes, the behaviour of the harmonic’s function may be left unchanged. That is, the (curved) surface representing the function (plotted, for instance, with respect to a reference sphere) coincides exactly in the product and parent orientations of the crystal reference axes. However, this only occurs for the pure rotational symmetry elements (cf. Figs. 3 to 8). Therefore it is better to define the symmetry of the harmonics with respect to directions. The symmetry definition then reads: apply a crystal symmetry element to the crystal reference axes. The same vector fixed in space exhibits different elements in the parent and product orientations. The harmonic’s function value may be left unchanged in the direction of the vector in the parent and product orientation. Then the harmonic exhibits symmetry with respect to the crystal symmetry element.

\(^*\) In Bunge’s formalism the cubic symmetry coefficients \( A_{j}^{\mu} \) and also the harmonics \( K_{j}^{\mu} \) are usually written with two dots \( A_{j}^{\mu} \) etc. In this paper only cubic point groups are treated and since no confusion is to be expected the quantities are written without dots.

\(^+\) The o.d.f. may be defined as follows: consider the volume fraction \( dV/V \) of the crystals (of one metallurgical phase) with orientations in the interval between \( g \) and \( g + \text{dg} \). The proportionality factor is the o.d.f., \( f(g): \text{d}V/V = f(g) \text{d}g \). Evidently it is normalized such that the integral over all orientations yields unity.
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This definition allows all possible symmetry elements, those of the 'second kind'\(^*\) (changing a right-handed frame of reference into a left-handed one), included. Examples are given in Table 7 and Figs. 3 to 8.

2.3. The o.d.f. vs crystal point-group symmetry elements of the second kind

Crystals belonging to one metallurgical phase may exhibit right-handed or left-handed behaviour (Bunge, 1982, p. 100). They may occur in different fractions and exhibit different o.d.f.’s. Consequently, a distinction has to be made between the left-handed\(^†\) and right-handed o.d.f.’s (Bunge, 1982, p. 103) indicated by \(f^L(g)\) and \(f^R(g)\). If the crystal’s point group only exhibits pure rotations, these two o.d.f.’s are not related. They both enter in the eventual scattered intensity expression (Bunge, 1982). Consequently, the fractions of left- and right-handed crystals then have to be known.

If the point group exhibits a centre of inversion the crystals can be seen as left- and right-handed at the same time (Bunge, 1982, p. 105). Then \(f^L\) and \(f^R\) are identical.

For the point groups exhibiting mirror-like symmetry elements but not an explicit centre of inversion (for instance, 43m) a similar condition follows. Then \(f^L\) and \(f^R\) are one-to-one correlated.\(^‡\) From this it follows that for all three possible crystal point-group symmetry cases treatment of the pure rotation elements is sufficient. For the rotational point groups, the treatment of \(f^L\) is self-evident (Bunge, 1982). Only \(f^R\) is used in what follows.

3. The cubic symmetry coefficients \(A_j^{nu}\)

The purpose of these coefficients is to render the value of the o.d.f. invariant with respect to (rotational) point-group symmetry elements (Bunge, 1982, pp. 363–369). In the expressions for diffraction intensity and diffraction strain pole figures the same cubic symmetry coefficients \(A_j^{nu}\) occur. In this section they are studied for the lowest possible cubic symmetry, i.e. point group 23. The coefficients \(A_j^{nu}\) for the higher-symmetry point groups are shown to be a subset of these.

3.1. Point group 23

With an expression given by Esling, Bechler-Ferry & Bunge (1981) it can be shown that

\[
\mu_{\text{max}}(j) = \frac{1}{12} \left( (2j+1) \frac{8}{3} \frac{\sin \left( \frac{\pi}{3} \right)}{\sin \left( \frac{\pi}{3} \right)} + 3(-1)^j \right)
\]

\(\mu_{\text{max}}\) determines the number of linearly independent \(A_j^{nu}\) solution vectors for a given \(j\), from which it follows that

\[
\mu_{\text{max}} = \begin{cases} 
0 & \text{for } j = 1, 2, 5, \\
1 & \text{for } j = 0, 3, 4,
\end{cases}
\]

and

\[
\mu_{\text{max}}(j+6) = \mu_{\text{max}}(j) + 1.
\]

It can be shown that the symmetry elements of this (pure rotation) point group yield (via the o.d.f.) the following 'selection rules':

(i) Twofold axis in [001]:

\[
m = \text{multiple of } 2.
\]

(ii) Twofold axis in [100]:

\[
A_j^{nu} = (-1)^j A_{j-2}^{nu}.
\]

The twofold axis in [010] does not lead to anything new.

(iii) Threefold axis in [111]:

\[
A_j^{nu} = \sum_{m=-j}^{j} (-1)^{m/2} A_{j-m}^{nu} P_{j}^{nu}(\cos \pi/2)
\]

for a rotation of \(2\pi/3\) about [111];

\[
A_j^{nu} = (-1)^{j/2} \sum_{m=-j}^{j} A_{j+m}^{nu} P_{j}^{nu}(\cos \pi/2)
\]

for a rotation of \(4\pi/3\) about [111] (in both cases \(s = \text{multiple of } 2\)).

It is suggested by (14a) and (14b) that two series of possible solutions exist for the coefficients \(A_j^{nu}\). However, it can be shown for both even and odd \(j\) that (14a) and (14b) lead to the same solution.

Two kinds of solutions for both equations are alternately obtained [using (14a) or (14b) and (8)]:

(i) A solution vector (consisting of all \(A_j^{nu}\) with \(m = -j(2)j\) for a given value of \(j\)) where the \(A_j^{nu}\) for both even and odd \(j\) are only significantly different from zero if \(m = \text{multiple of } 2\). Then (14a) and (14b) are identical. On inspection (Bunge, 1982, p. 501) it is seen that the \(A_j^{nu}\) coefficients for point group 432 are obtained. This is logical since the higher symmetry (432) also satisfies the lower (23).

\(^*\) Terminology due to Bunge, Esling & Muller (1981). The determinant of the matrices of these elements is equal to \(-1\).

\(^†\) The left-handed o.d.f. is also a function of rotations only.

\(^‡\) The o.d.f. series-expansion coefficients of the left- and right-handed o.d.f.’s can be expressed in each other, accordingly: see equation (79) of Bunge, Esling & Muller (1981). Note that for this point group one physical crystal is right- and left-handed at the same time (Bunge, 1982, equation (25)), like the centrosymmetric crystal case.

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(ii) A solution vector where the $A^m_j$ are only significantly different from zero for even $m$ or a multiple of 4 for both even and odd $j$. Then, (14a) and (14b) are also identical. These $A^m_j$ are the 'pure' point-group 23 cubic symmetry coefficients. Computer outputs exhibiting these coefficients for $j = 4(2)52$ and $j = 3(2)51$ can be obtained from the author.

Upon analysis, the solutions are alternately obtained, the index $\mu$ enumerating them in systematic order. For instance, $\mu = 1$ yields a '432' solution, $\mu = 2$ stands for a 'pure 23' solution etc. This choice is purely arbitrary and could lead to confusion among different laboratories.

3.2. The other cubic point groups

The coefficients $A^m_j$ for point group 432 are contained within the solutions obtained for the 23 case as indicated in § 3.1. The $A^m_j$ coefficients for point groups $m3$ and $43m$ are identical to those of 23. The $A^m_j$ coefficients for point group $m3m$ are identical to those of 432.

However, a difficulty now arises. The symmetry elements of the second kind $[\det(g) = -1]$ of these point groups could be taken as imposing additional restrictions on the $A^m_j$. For instance:

(i) It could be taken from the $K_j^u$ harmonics that the $A^m_j$ should be equal to zero for odd $j$ for point groups $m3$ and $m3m$ using their centre of inversion. The same holds with respect to their $h00$ mirror planes.

(ii) The $\{hkl\}$ mirror planes occurring in point groups $m3m$ and $43m$ could lead to the condition that $A^m_j = (-1)^{m/2} A^m_j$ for the $K_j^u$ harmonics (Bunge, 1982, p. 385) in addition to (13).

However, these restrictions do not lead to fulfillment of the same symmetry elements in harmonics $F_1, \ldots, F_4$.

If one starts from the harmonics $F_1, \ldots, F_4$ the imposed symmetry is not satisfied in the $K_j^u$ harmonics. From a principal point of view there is no preference for one type of harmonic. Therefore:

(i) The cubic symmetry coefficients should be defined using the rotational symmetry elements of the crystal point group considered. The symmetry elements should be taken as transformations of orientations.

(ii) The coefficients generate the symmetry of the o.d.f. with respect to (rotational) crystal point-group symmetry elements (Bunge, 1982, pp. 48 and 366). They should be derived via expressions obtained from the o.d.f. (Bunge, 1982, pp. 363–369). They should not be derived from the harmonics $K_j^u$ or $F_1, \ldots, F_4$.

(iii) Fulfillment of symmetry elements of the second kind in the harmonics $K_j^u$ and $F_1, \ldots, F_4$ is obtained by imposing selection rules on $j$ and $m$ as indicated in Table 7. No additional restrictions on the $A^m_j$ are necessary.

4. The polycrystalline diffraction experiment performed on textured materials

According to § 2.3 only point groups 23 and 432 are necessary for the mathematical treatment of the diffraction experiment for all cubic point groups. This holds whether crystals belong to $m3$ or $43m$ (as compared to 23) or $m3m$ (as compared to 432).

Only the right-handed o.d.f. is taken into account. Upon diffraction, all crystal orientations exhibiting an $(hhk)$ vector parallel to the scattering vector $Q$ contribute. The number of physically equivalent crystal orientations contributing is determined by the number of symmetry elements of the point group considered.

Use of the rotation elements of the point group leads to an expression for the diffracted intensity and the diffraction strain via the o.d.f. For the mathematical treatment of the $(hhk)$ diffraction experiment only the expressions for the $hk1$ and $h1k$ reflections have to be considered for the 432 case (Brakman, 1985). Multiplied by their appropriate weight factors, their sum represents physical reality.

Point group 23 does not exhibit fourfold rotation symmetry elements. Consequently, the treatment of, say, the $hkl$ and $hkl$ reflections in addition to those mentioned is necessary for this point group. The structure factors for the $hkl$ and $hkl$ reflections are different for point group 23. For the case of normal scattering the structure factors of $hkl$ and $hkl$ reflections are equal (all point groups, Friedel's law). The same holds for the $hkl$ with respect to the $hkl$ reflection. In the case of anomalous scattering the structure factors are unequal and Friedel's law does not hold.

For all cubic point groups it holds that 48 permutations of $h, k$ and $l$ leading to 48 $(hkl)$ lattice planes diffract at the same $2\theta$, equal structure factors or not.

The relationships between the structure factors for the various cubic crystal classes in conjunction with both anomalous and normal scattering are summarized in Table 1.

4.1. Diffraction intensity pole figures

It can be shown that the $(hkl)$ intensity pole figure exhibits the following expression for the case of

* This corresponds to two physically different orientation types contributing at the same time: (i) Crystal orientations exhibiting $(hkl)$ parallel to $Q$. All orientations obtained from this one using a (point-group allowed) rotational symmetry element are physically equivalent and hence not treated. (ii) Crystal orientations exhibiting $(hkl)$ parallel to $Q$. For the general $hkl$ case the latter orientation cannot be obtained from the former by a rotation (Brakman, 1985) nor does it imply an inversion of the crystal's reference axes. Generally, the o.d.f. differs in these two orientation types. Consequently, the $hkl$ and $hkl$ intensities are different, too.

† i.e. $S_{hkl}/(S_{hkl} + S_{hkl})$ and $S_{hkl}/(S_{hkl} + S_{hkl})$, where $S_{hkl}$ is the geometric structure factor. See also Bunge & Esling (1981).
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Table 1. Relationships between squares of geometric structure factors for cubic point groups in conjunction with anomalous scattering and normal scattering (note the use of Laue indices)

<table>
<thead>
<tr>
<th>Cubic pointer group</th>
<th>Anomalous scattering (a.s.)</th>
<th>Normal scattering (n.s.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>Four structure factors all different from each other; no relationships</td>
<td>$S_{hkl}^2 = S_{hk}^2$</td>
</tr>
<tr>
<td>$m$</td>
<td>$S_{hkl}^2 = S_{hk}^2$</td>
<td>$S_{hkl}^2 = S_{hk}^2$</td>
</tr>
<tr>
<td>$43m$</td>
<td>As left-hand column +</td>
<td>$S_{hkl}^2 = S_{hk}^2$</td>
</tr>
<tr>
<td></td>
<td>$S_{hkl}^2 = S_{hk}^2$</td>
<td>As above</td>
</tr>
<tr>
<td>$32$</td>
<td>As left-hand column +</td>
<td>$S_{hkl}^2 = S_{hk}^2$</td>
</tr>
<tr>
<td></td>
<td>$S_{hkl}^2 = S_{hk}^2$</td>
<td>As above</td>
</tr>
</tbody>
</table>

Crystals belonging to point group 23 in conjunction with anomalous scattering:

$$
\hat{P}_{hkl}(\psi, \alpha) = \sum_{j=1}^{4} C_{j}^{*} \sum_{n} A_{j}^{n}(-1)^{n/2} \exp(i\alpha)P_{j}^{n}(\cos \psi)
$$

$$
\times \sum_{m=-j}^{j} (-1)^{m/2} A_{j}^{m} \exp(-im\beta)P_{j}^{m}(\cos \Phi)
$$

$$
\times \left[ 12S_{HKL}^2 + 12(-1)^{m/2}S_{KRL}^2 
+ 12(-1)^{l}S_{HKL}^2 + 12(-1)^{l+m/2}S_{KRL}^2 
+ 12S_{HKL}^2 + 12S_{KRL}^2 + 12S_{HKL}^2 + 12S_{KRL}^2 \right]^{-1},
$$

(15a)

where $\psi, \alpha$ is the direction of the scattering vector $\mathbf{Q}$ with respect to specimen reference axes. The $C_{j}^{*}$ are the well known o.d.f. series-expansion coefficients. $S_{HKL}^2$ stands for $S_{HKL}$ times its complex conjugate.

A clear distinction is made between the quantities $P_{hk}$ and $\hat{P}_{hkl}$. $P_{hk}$ stands for the (structure-factor) weighted $(hk)$ scattered intensity constituted by the reflections according to the physically different permutations of $h$, $k$, and $l$; Apart from a proportionality factor, it is equal to the measured scattered intensity. The denominator in (15a) serves as a normalization with respect to the structure factors. As a consequence, the integral

$$
\frac{1}{4\pi} \hat{P}_{hkl}(\psi, \alpha) \sin \psi \, d\psi \, d\alpha = 4\pi
$$

(15b)

as required.

The quantity $P_{hk}$ is defined via the o.d.f:

$$
P_{hk}(\psi, \alpha) = (2\pi)^{-1} \int_{0}^{2\pi} \text{O.D.F.} \left( \psi, \alpha, [hkl], \varphi_{j} \right) \, d\varphi_{j}.
$$

(15c)

The equation is written for the single $hkl$ reflection. It may occur that the structure factor of the reflection is equal to zero whereas the o.d.f. is non-zero. Therefore, it should be written

$$
I_{HKL} = AS_{HKL}^2 P_{hkl}
$$

(15d)

where $HKL$ are Laue indices. $I_{HKL}$ is the integrated (with respect to $2\theta$) intensity of the $HKL$ reflection and $A$ is a proportionality factor. $P_{hkl}$ is written using Miller indices since it does not depend on the order of the reflection. The relationship between $P_{hk}$ and $P_{hkl}$ is given in Table 2.

The harmonics of interest are given by the $m$ sum in (15a).

Although the equations given may look complicated, essentially only one type of $hkl$-dependent harmonic emerges:

$$
K_{j}^{m}(\Phi, \beta) = \sum_{m=-j}^{j} (-1)^{m/2} A_{j}^{m} P_{j}^{m}(\cos \Phi) \exp(-im\beta).
$$

(16)

$P_{j}^{m0}(x)$ in (15a) can be reduced to $P_{j}^{m}(x)$ using

$$
P_{j}^{m0}(x) = (-1)^{m/2} \left[ 2/(2j+1) \right]^{1/2} P_{j}^{m}(x).
$$

(17)

The factor $(-1)^{m/2}$ in (15a) can then be omitted ($m$ is multiple of 2 in all cases). Evidently, on some occasions [15(a)] an additional factor $(-1)^{m/2}$ is introduced. It seems that an additional type of harmonic arises, different from (16) in that the factor $(-1)^{m/2}$ is absent:

$$
K_{j}^{m}(\Phi, \beta) = \sum_{m=-j}^{j} A_{j}^{m} P_{j}^{m}(\cos \Phi) \exp(-im\beta).
$$

(18)

However, for the 432 and $3m$ case ($m$ only equal to a multiple of 4) (16) and (18) are identical.

Exactly the same holds for the 23, 3$3$, and 43$3$ cases if the '432 solution' for the $A_{j}^{m}$ coefficients is used. And it follows from the 'pure 23 solution' (§3.1) for these coefficients that (16) and (18) then differ only by a minus sign.

Consequently, (16) is taken as the definition of the harmonics associated with intensity pole figures. Note the similarity of (16) to (6). It also follows that in all cases (16) reduces to

$$
K_{j}^{m}(\Phi, \beta) = \sum_{m=-j}^{j} (-1)^{m/2} A_{j}^{m} P_{j}^{m}(\cos \Phi) \cos m\beta
$$

for even $j$

$$
K_{j}^{m}(\Phi, \beta) = \sum_{m=-j}^{j} (-1)^{m/2} A_{j}^{m} P_{j}^{m}(\cos \Phi) \sin m\beta
$$

(20)

for odd $j$ [a factor $(-1)^{1/2}$ has been omitted in (20)].

In Table 3 the other cubic point groups in conjunction with both anomalous and normal scattering are dealt with. The intensity expression is similar to (15a).

The quotient involving the structure factors, however,
C. M. Brakman

Table 2. \(\{hkl\}\) intensity expression \(\tilde{P}_{hkl}\) (cf. equation (15a)) for combinations of cubic point groups and scattering modes

For point group 23, four physically different \(hkl\) reflections occur (same 2\(\beta\)). The quantities \(P_{AB}\) etc. are defined in equation (15e). Weighted with their structure-factor squares, they constitute \(P_{hkl}\). The denominator \(D\) normalizes the expression with respect to structure factors. Apart from a proportionality factor, \(P_{hkl}\) stands for the measured intensity. It depends on \(\phi, \alpha\) (i.e., the orientation of the scattering vector with respect to specimen axis). It is equal to the \(\{hkl\}\) intensity pole figure. The expressions for the pure-rotation point groups do not exhibit the left-handed crystal contributions. Their treatment is not essentially different (Bunge, 1982, p. 102)

<table>
<thead>
<tr>
<th>Point group and scattering case</th>
<th>Constitution of (hkl) scattered intensity expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>23 and a.s.</td>
<td>([S_{hkl}^2P_{hkl} + S_{hkl}^{22}P_{2hkl} + S_{hkl}^{2g}P_{gkhl}] D^{-1})</td>
</tr>
<tr>
<td>23 and n.a.</td>
<td>([S_{hkl}^2P_{hkl} + S_{hkl}^{2g}P_{gkhl}] D^{-1})</td>
</tr>
<tr>
<td>43m and a.a.</td>
<td>([S_{hkl}^2P_{hkl} + S_{hkl}^{2g}P_{gkhl}] D^{-1})</td>
</tr>
<tr>
<td>43m and n.a.</td>
<td>([S_{hkl}^2P_{hkl}] D^{-1})</td>
</tr>
<tr>
<td>43m and g.a.</td>
<td>([S_{hkl}^{22}P_{hkl} + S_{hkl}^{2g}P_{gkhl}] D^{-1})</td>
</tr>
<tr>
<td>43m and g.n.a.</td>
<td>([S_{hkl}^{22}P_{hkl}] D^{-1})</td>
</tr>
</tbody>
</table>

\[
D = \frac{S_{hkl}^2 + S_{hkl}^{22} + S_{hkl}^{2g} + S_{hkl}^{2g}}{2} \\
= \frac{S_{hkl}^2 + S_{hkl}^{2g}}{4} \\
= \frac{S_{hkl}^{22}}{2} 
\]

Table 3. Elaboration of scattered intensity expression \(\tilde{P}_{hkl}\)

The quotient in equation (15a) should be replaced by the second-column expression. The symmetry satisfied by the \(hkl\)-dependent part of the intensity expression is displayed in the fourth column. On some occasions this expression satisfies symmetries other than those introduced into the point group (cf. §2.2). An entry \(m3\) in the fourth column signifies that all cubic point groups are satisfied. The data of the third column lead to the so-called ghosts (Ealing, 1981; Bunge, 1982, p. 116). Left-handed crystal contributions not shown.

<table>
<thead>
<tr>
<th>Point group and scattering case</th>
<th>Expression instead of the quotient in equation (15a)</th>
<th>Values of (j) and (m)</th>
<th>Symmetry satisfied by (hkl)-dependent part of intensity expression (cf. Table ?)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23 and n.s.</td>
<td>(\sum \left[\frac{1}{2} \left(1 + \frac{1}{2} \right) S_{hkl}^2 \right] )</td>
<td>(j = \text{odd})</td>
<td>(23\ and\ m3)</td>
</tr>
<tr>
<td>or m3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>43m and a.s.</td>
<td>(\sum \left[\frac{1}{2} \left(1 + \frac{1}{2} \right) S_{hkl}^2 \right] )</td>
<td>(j = \text{even}) m = 0, 2, 4, …</td>
<td>(m3)</td>
</tr>
<tr>
<td>or m3</td>
<td></td>
<td>(j = \text{odd}) m = 0, 2, 4, …</td>
<td></td>
</tr>
<tr>
<td>43m and g.a.</td>
<td>(\sum \left[\frac{1}{2} \left(1 + \frac{1}{2} \right) S_{hkl}^2 \right] )</td>
<td>(j = \text{odd}) m = 0, 2, 4, …</td>
<td>(m3)</td>
</tr>
<tr>
<td>or m3</td>
<td></td>
<td>(j = \text{even}) m = 0, 2, 4, …</td>
<td></td>
</tr>
</tbody>
</table>

should be replaced by the corresponding second-column entry of Table 3. Except for the 23+ anomalous scattering case a certain amount of harmonics does not arise in the final intensity expression (third column of Table 3). This represents the so-called ‘ghost’ phenomenon well known in texture analysis.

4.2. Diffraction strain pole figures

Instead of the harmonics \(K_p\) of § 4.1 the harmonics \(F\) etc. (cf. equation (1)) arise as the \(hkl\)-dependent part in the theoretical expression for diffraction strain pole figures (Brakman, 1986). They can be seen as surface spherical harmonics, but their properties differ from those of the \(K_p\). These harmonics can only be arrived at via the o.d.f. Hence, they cannot be constructed using method (a) of § 2.1. In Appendix I they are defined as a function of \(hkl, j\) and \(\mu\). However, use of (1-14) and (1-15) allows them to be expressed generally in \(\Phi\) and \(\beta\). The definitions

\[
A(\Phi, \beta) = \frac{1}{8} \left[2 \sin^2 \Phi \sin^2 2\beta - (2 - \frac{1}{2} \sin^2 2\beta) \sin^2 2\Phi \right] \tag{21}
\]

and

\[
B(\Phi, \beta) = \frac{1}{8} \sin 4\beta \cos \Phi \sin^2 \Phi \tag{22}
\]

*Appendices I-III, which give further details of complex mathematical expressions, have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43428 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
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From the definition
\[
g(hkl) = \sum_{\phi} [\text{o.d.f.}(\psi, \alpha, [hkl], \varphi'_l)] \
\times \text{compliance} ([hkl], \varphi'_l) \
\times \text{stress} (\varphi'_l) \, d\varphi'_l, \tag{29a}
\]

it follows that the expression for the \(hkl\) reflection diffraction strain [equation (1)] is the consequence of
\[
\langle \varepsilon'_l(\psi, \alpha) \rangle = g(hkl) \sum_{\phi} [\text{o.d.f.}(\psi, \alpha, [hkl], \varphi'_l)] \
\times d\varphi'_l. \tag{29b}
\]

The strain is determined in the direction of the \(Z\) axis of a laboratory frame. This \(Z\) axis is parallel to \(Q\) and consequently parallel to the diffracting lattice plane normal \([hkl]\). The integration only includes those crystals with \([hkl]\) parallel to \(Q\). The denominator is a normalization factor, and is defined in (15c). In the numerator, the o.d.f. expression depends on \(\psi\) and \(\alpha\) and the orientations of the single crystals with \([hkl]\) parallel to \(Q\). The numerator comprises a summation over products of compliance and stress-tensor elements. For the Reuss model, the stresses are taken out of the integration.

Equation (29) is written for the \(hkl\) reflection only. However, the \(hkl\) reflection also contributes at the same time. A similar expression to (29) can then be written.

The question arises of how the ‘measured’ diffraction strain (i.e. the composition of the weighted contributions of the various reflections) expression is constituted. The \(2\theta\) shifts of the centroids of the \(hkl\) and \(hkl\) line profiles can be shown (via Bragg’s law) to lead to an expression:
\[
\langle \varepsilon'_l \rangle = [S_{hkl} \cdot g(hkl) + S_{\bar{h}k\bar{l}} \cdot g(h\bar{h}\bar{l})] \
\times [2\pi (S_{hkl} + S_{\bar{h}k\bar{l}})P_{\text{mean}}]^{-1} \tag{30}
\]

[the factor \(\pi\) is cancelled upon integration of (29a)].

The procedure can be extended to all combinations of crystal point groups and scattering modes. The result is shown in Table 4, which exhibits a close analogy to Table 2.

It can be seen from (1) that four different expressions occur involving the stresses \(\sigma_{11}\) and \(\sigma_{22}\) in conjunction with the functions \(F_1, \ldots, F_4\). They are a part of the \(g(hkl)\) function.

All four of them are displayed in Tables 5 and 6 together with the coefficients they exhibit in the evaluated Table 4’ expressions. The texture-free terms \(s_1(hkl)[\sigma_{11} + \sigma_{22}]\) and \(\frac{1}{2}s_2(hkl)\sigma_{11} \sin^2 \psi\) are not written. They are independent of the permutation of \(h, k\) and \(l\) and these two terms remain unchanged in the eventual equation. The complete \(\{hkl\}\) diffraction strain equation is obtained as follows:

(i) Start with the \(s_1\) and \(\frac{1}{2}s_2\) expressions.

For \(n = 0\) the ‘normal’ Legendre differential equation is obtained. 

lead to
\[
F_1(\Phi, \beta, j, \mu) = A(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \cos m\beta
\]
\[
- B(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \sin m\beta
\tag{23}
\]
\[
F_2(\Phi, \beta, j, \mu) = A(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \sin m\beta
\]
\[
+ B(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \cos m\beta
\tag{24}
\]
The definitions
\[
C(\Phi, \beta) = \frac{1}{2}(\sin 4\Phi + \sin 2\Phi \sin^2 \Phi \sin^2 2\beta) \tag{25}
\]
and
\[
D(\Phi, \beta) = \frac{1}{2} \sin^3 \Phi \sin 4\beta \tag{26}
\]
lead to
\[
F_3(\Phi, \beta, j, \mu) = C(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \cos m\beta
\]
\[
- D(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \sin m\beta,
\tag{27}
\]
\[
F_4(\Phi, \beta, j, \mu) = C(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \sin m\beta
\]
\[
+ D(\Phi, \beta) \sum_{m=-j(2)}^{j} (-1)^{m/2} A_{j}^{m}\mu \\
\times P_{j}^{m}(\cos \Phi) \cos m\beta.
\tag{28}
\]
The expressions for \(A, \ldots, D\) arise as a consequence of cubic-crystal compliance or stiffness-tensor transformations (Brakman, 1983, Appendix II). Functions \(F_1\) and \(F_2\) are purely real whereas \(F_3\) and \(F_4\) are purely imaginary. These functions behave as (symmetrized) harmonics.* The symmetries these harmonics satisfy are summarized in Table 7.

* The definition of functions \(P_{i}^{m}\) is given by Geiľlicant, Minlos & Shapiro (1963, p. 85) and by Bunge (1982, p. 351). The general differential equation these functions obey reads (Geiľlicant, Minlos & Shapiro, 1963, p. 82):
\[
\alpha^2 P_{i}^{m}(\cos \Phi) / \partial \Phi^2 + \cot(\Phi) \alpha P_{i}^{m}(\cos \Phi) / \partial \Phi \\
+(j + 1) - (n^2 - 2m \cos \Phi + m^2) / \sin^2 \Phi ) \alpha P_{j}^{m}(\cos \Phi) = 0.
\]

For \(n = 0\) the ‘normal’ Legendre differential equation is obtained.
Table 4. Diffraction strain pole figure expression \(\{e_{ij}\}\) in terms of structure factors, the function \(g(hkl)\) defined in equation (29a) and the quantity \(\hat{P}_{hkl}\) defined in equation (15a) and Table 2.

No elasticity model has yet been used since \(g(hkl)\) is written for the general case. Function \(g(hkl)\) is basically the numerator of the RHS of equation (1). \(\{e_{ij}\}\) represents the \((hkl)\) measured diffraction strain. In equation (1) only the \((hkl)\) reflection is treated. Even in the most symmetric case (bottom row of this table and equation (30)) the additional treatment of the \((hkl)\) reflection is required. For point groups not exhibiting fourfold axes, four reflections according to four physically different permutations of \(h, k, l\) constitute the \(\{e_{ij}\}\) expression. Through \(g(hkl)\) and \(\hat{P}_{hkl}\), the diffraction strain depends on \(\phi\) and \(\alpha\). \(\{e_{ij}\}\) can be seen as a diffraction strain pole figure. Left-handed crystal contributions not shown.

<table>
<thead>
<tr>
<th>Point group and scattering case</th>
<th>Constitution of ((hkl)) diffraction strain ({e_{ij}})</th>
<th>(D[\hat{P}_{hkl}]) according to equation (15a) and Table 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>23 and a.s.</td>
<td>({S_{hkl}(g(hkl)) + S_{hkl}(g(hkl)) + S_{hkl}(g(hkl))}D^{-1})</td>
<td>({S_{hkl}(g(hkl)) + S_{hkl}(g(hkl))}D^{-1})</td>
</tr>
<tr>
<td>23 and n.s. or m(_3)</td>
<td>({S_{hkl}(g(hkl)) + g(hkl)}D^{-1})</td>
<td>({S_{hkl}(g(hkl)) + S_{hkl}(g(hkl))}D^{-1})</td>
</tr>
<tr>
<td>43m and a.s.</td>
<td>({S_{hkl}(g(hkl)) + g(hkl)}D^{-1})</td>
<td>({S_{hkl}(g(hkl)) + S_{hkl}(g(hkl))}D^{-1})</td>
</tr>
<tr>
<td>432 and a.s.</td>
<td>({S_{hkl}(g(hkl)) + g(hkl)}D^{-1})</td>
<td>({S_{hkl}(g(hkl)) + S_{hkl}(g(hkl))}D^{-1})</td>
</tr>
<tr>
<td>432 and n.s. or m(_3m)</td>
<td>({S_{hkl}(g(hkl)) + g(hkl)}D^{-1})</td>
<td>({S_{hkl}(g(hkl)) + S_{hkl}(g(hkl))}D^{-1})</td>
</tr>
</tbody>
</table>

Table 5. Elaboration of \((hkl)\) diffraction strain expression (cf. Table 4) for point groups 23, m3, 432 and m\(_3m\)

Functions \(B_j^m(\phi, \alpha, \ldots, E^m_j(\phi, \alpha)\) defined in Brakman (1986). Functions \(F_1, \ldots, F_8\) (depending on \(hkl\) and \(\mu\)) defined in equations (21) to (28). For point groups 23, m3 and 43m the \(\{e_{ij}\}\) expression is evaluated by multiplying alternately the second or third column by the stress expressions in the left-hand column. The resulting four expressions are multiplied by \(S_0(2\hat{P}_{hkl})^{-1}\) and added. The texture-free contribution \(s(hkl)[\sigma_{11} + \sigma_{22} + \sigma_{33}]/3\) is not shown since it does not depend on the point group or the scattering mode. Only stresses \(\sigma_{11}\) and \(\sigma_{22}\) are taken into account. Coefficients \(c_1, \ldots, c_8\) depend on the structure factors. They are defined in equations (31a) to (31e). Note the vanishing of the non-centrosymmetric functions \(F_2\) and \(F_8\) upon changing from the anomalous to the normal scattering mode. The symmetries to which the functions \(F_1, \ldots, F_8\) are subject are given in Table 7. In Tables 2 to 5 the cases of 23 + n.s. and 432 + n.s. have been taken equivalent to m3 and m3m, respectively. However, although normal scattering renders \(S_{hkl}^{\text{NL}}\) and \(S_{hkl}^{\text{REC}}\) equal, an essential difference remains. For m3 and m3m the left-handed o.d.f. does not have to be treated. For 23 and 432 the right-handed o.d.f. may be essentially different from the right-handed one. This fact is not changed in normal scattering.

<table>
<thead>
<tr>
<th>Coefficients of left-hand column in ((e_{ij})<em>x) expression for (A</em>{m}^m) coefficients</th>
<th>Coefficients of left-hand column in ((e_{ij})<em>y) expression for (A</em>{m}^m) coefficients</th>
<th>Coefficients of left-hand column in ((e_{ij})<em>z) expression for (A</em>{m}^m) coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>23 and n.s. (-(\sigma_{11} - \sigma_{22})\cos 2\alpha - \sigma_{33}\sin^2 \phi)</td>
<td>(\sum_{x} C_{x} B_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
<td>(\sum_{x} B_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
</tr>
<tr>
<td>(-(\sigma_{11} - \sigma_{22})\cos 2\alpha - \sigma_{33}\sin^2 \phi)</td>
<td>(\sum_{x} C_{x} B_{x} F_{x} - c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
<td>(\sum_{x} B_{x} F_{x} - c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
</tr>
<tr>
<td>(-(\sigma_{11} - \sigma_{22})\cos 2\alpha - \sigma_{33}\sin^2 \phi)</td>
<td>(\sum_{x} C_{x} B_{x} F_{x} - c_{x} C_{x} F_{x} - c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
<td>(\sum_{x} B_{x} F_{x} - c_{x} C_{x} F_{x} - c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
</tr>
<tr>
<td>(\sigma_{11} \sin 2\phi)</td>
<td>(\sum_{x} C_{x} D_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
<td>(\sum_{x} D_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
</tr>
<tr>
<td>432 and n.s. or m(<em>3m) (-(\sigma</em>{11} - \sigma_{22})\cos 2\alpha - \sigma_{33}\sin^2 \phi)</td>
<td>(\sum_{x} c_{x} B_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
<td>(\sum_{x} B_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
</tr>
<tr>
<td>(-(\sigma_{11} - \sigma_{22})\cos 2\alpha - \sigma_{33}\sin^2 \phi)</td>
<td>(\sum_{x} c_{x} C_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
<td>(\sum_{x} B_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
</tr>
<tr>
<td>(\sigma_{11} \sin 2\phi)</td>
<td>(\sum_{x} c_{x} D_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
<td>(\sum_{x} D_{x} F_{x} + c_{x} C_{x} F_{x} + c_{y} C_{y} F_{y} + c_{z} C_{z} F_{z})</td>
</tr>
</tbody>
</table>

(ii) For the 23, m3 and 43m (whatever the scattering mode) cases the summations over \(\mu\) comprise both odd and even \(\mu\) values. As \(\mu\) steadily increases, 'pure 23 solutions' and '432 solutions' for the \(A_{m}^m\) coefficients occur alternately. Then the left-hand expressions of Tables 5 and 6 must be alternately multiplied by the second- or third-column expressions. For the 432 and m\(_3m\) (whatever the scattering mode) cases only the '432 solution' for the \(A_{m}^m\) can exist. Consequently, only one column persists.

(iii) The completed \(j, \mu\) sums are multiplied by \(s_0\) [not shown in Tables 5 and 6 but also a factor of \(g(hkl)\)].

(iv) The four \(j, \mu\) sums are added and divided by the quantity \(D\) of Table 4.
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Table 6. As Table 5 but point group 43m treated

Left-handed crystal contributions not shown in Tables 5 and 6. In both tables the Reuss model of elasticity has been used. Note that in Tables 5 and 6 no 'ghost' expressions arise by contrast to those given in Table 3, third column, for the intensity expression case.

Coefficients

Table 7. Symmetry satisfied by the harmonics $K_j^+$ and $F_1, \ldots, F_4$

Definition of symmetry: § 2.2. Definition of $K_j^+$ harmonics: equation (16). Definition of $F_1, \ldots, F_4$ harmonics: equations (21) to (28). For an entry 'm3m' it is understood that all lower cubic symmetries are also satisfied. An entry '3m' or '432' implies the same with respect to 23. The 'pure 23' and '432' solutions for the cubic symmetry coefficients $A_{nm}$ are dealt with in § 3.

Harmonic $j = \text{even}$ $j = \text{odd}$

<table>
<thead>
<tr>
<th>Harmonic $K_j^+$</th>
<th>$m = \pm 2, \pm 6, \pm 10, \ldots$</th>
<th>$j = \text{even}$</th>
<th>$j = \text{odd}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m = 3$ or 43m</td>
<td>$m = 3$ or 43m</td>
<td>$j = \text{even}$</td>
<td>$j = \text{odd}$</td>
</tr>
<tr>
<td>$F_1$ and $F_2$</td>
<td>$m3$ or 43m</td>
<td>$23$</td>
<td>$43m$</td>
</tr>
<tr>
<td>$F_3$ and $F_4$</td>
<td>$m3$ or 43m</td>
<td>$23$</td>
<td>$43m$</td>
</tr>
</tbody>
</table>

Note further that by contrast with the intensity pole figure $P_{hlk}$ the diffraction strain pole figure is not normalized. This could be achieved by dividing $(\varepsilon_{\nu})$ by $s_0$ times a stress-tensor invariant (or by $s_0\alpha_{\nu}$); cf. Fig. 1. However, the normalization then still depends on the stress state.

5. Results and discussion

From the definition of symmetry of § 2.2, it can be shown that the harmonics may exhibit symmetry as displayed in Table 7. The definition of the $K_j^+$ harmonics is given by (16) whereas the definition of harmonics $F_1, \ldots, F_4$ is given by (23), (24), (27) and (28). It follows that 43m symmetry is either satisfied by a 'pure 23' harmonic or by an m3m-type harmonic. The properties of the $K_j^+$ harmonics are not considered in what follows.

5.1. Cyclic behaviour and continuity in the poles of the sphere

It can be taken from (21) to (28) that upon replacement of $\beta$ by $\beta + 2\pi$ the same expression results. It is also seen that $F_1 = F_2 = F_3 = F_4 = 0$ for $\Phi = 0$ and $\Phi = \pi$ for all $\beta$.

5.2. Behaviour with respect to Laplace's equation

If one writes $u = rF_1$, this demonstrates that Laplace's equation $\Delta u = 0$ is not satisfied. The same holds for harmonics $F_2$ to $F_4$.

5.3. Orthogonality

5.3.1. Orthogonality of types of functions. It can be shown that

\[ \frac{1}{4\pi} \int (\Phi, \beta, j, \mu) F_j^\star (\Phi, \beta, j', \mu') \, dA = 0, \]

\[ \frac{1}{4\pi} \int (\Phi, \beta, j, \mu) F_j^\star (\Phi, \beta, j', \mu) \, dA = 0, \]

\[ \frac{1}{4\pi} \int (\Phi, \beta, j, \mu) F_j^\star (\Phi, \beta, j', \mu') \, dA = 0, \]

\[ \frac{1}{4\pi} \int (\Phi, \beta, j, \mu) F_j^\star (\Phi, \beta, j', \mu') \, dA = 0. \]
These results hold in all four cases, even if \( j = j' \) and \( \mu = \mu' \). However,

\[
\delta F_1(\Phi, \beta, j, \mu) F_j^*(\Phi, \beta, j', \mu') \, dA \neq 0, \quad (36)
\]

\[
\delta F_2(\Phi, \beta, j, \mu) F_j^*(\Phi, \beta, j', \mu') \, dA \neq 0. \quad (37)
\]

The inequalities (36) and (37) both hold, even if \( j \neq j' \) or \( \mu \neq \mu' \). Obviously, if both functions in the integrand exhibit the same symmetry (cf. Table 7) orthogonality is lost.

5.3.2. Orthogonality within one type of function with respect to \( j \) and \( \mu \). It generally follows from Appendices II and III* that

\[
\delta F_1(\Phi, \beta, j, \mu) F_j^*(\Phi, \beta, j', \mu') \, dA \neq 0 \quad (38)
\]

even for \( j \neq j' \) or \( \mu \neq \mu' \). The same holds true for functions \( F_2 \) to \( F_4 \). However, a systematic behaviour can be observed (and predicted): if \( F_i(\Phi, \beta, j, \mu) \) belongs to the ‘pure 23’ column in Table 7 and \( F_i(\Phi, \beta, j', \mu') \) belongs to the ‘432’ column of Table 7, equation (38) is on all occasions equal to zero. Again, the same holds true for harmonics \( F_2 \) to \( F_4 \).

Note that the value of the index \( \mu \) (or \( \mu' \)) determines whether a harmonic belongs to the ‘pure 23’ column or the ‘432’ column of Table 7.

A certain amount of the conventional orthogonality is retained (Appendices II and III). This is reflected by the appearance in the last terms of (II-1) and (III-1) of a factor \( \delta_{\mu \nu} \delta_{\mu \nu} \). (II-1) and (III-1) may be used for the normalization of harmonics \( F_1 \) to \( F_4 \) but the use in general terms of \( j, j', \mu \) and \( \mu' \) is very cumbersome.

The integrals of equations (II-1) and (III-1) also yield contributions for \( j \neq j \) and \( \mu \neq \mu \). However, it follows from computer calculations (and also from the isodensity contours in Figs. 5 to 8) that the evaluation of the integrals yields a value small compared with unity. This is a consequence of the normalization of the \( A_{\mu}^m \) coefficients using (8) leading to the orthonormalization of the \( K_j^\mu \) harmonics [equation (7)]. The harmonics \( F_1, \ldots, F_4 \) are not normalized then. However, this condition cannot be changed since (8) follows from the normalization of the o.d.f. itself (Bunge, 1982, p. 368).

It is expected that it is possible to reduce the expressions (II-1) and (III-1) to a much simpler form (still involving \( j, j', \mu \) and \( \mu' \)). A solution of this problem has not yet been found.

5.4. Graphical representation of results

In Figs. 3 and 4 two ‘normal’ symmetrized harmonics \( K_j^\mu \) are depicted. Figs. 5 to 8 display an example of harmonics \( F_1, F_2, F_3 \) and \( F_4 \) respectively. On all occasions the threefold cubic axes are clearly exhibited.

5.5. ‘Desymmetrized’ harmonics \( F_1 \) to \( F_4 \)

These harmonics can be written (in analogy to the \( K_j^\mu \) harmonics) without the cubic symmetrization according to (6). Harmonic \( F_1 \) is then written, for instance,

\[
F_1(\Phi, \beta, j, m) = (A(\Phi, \beta) \cos m\beta - B(\Phi, \beta) \sin m\beta) \times (-1)^{m/2} P_m^j(\cos \phi)
\]

where \( A(\Phi, \beta) \) and \( B(\Phi, \beta) \) are defined in (21) and (22). The sums over \( m \) and the cubic symmetry coefficients \( A_{\mu}^m \) vanish from (II-1) and (III-1) but the resulting equations are still complicated. Of course, upon conversion to solid spherical harmonics the desymmetrized harmonics do not satisfy Laplace’s equation either.

5.6. Extension to more general concepts

The conventional harmonics \( K_j^\mu \) governing the diffracted-intensity (i.e. a scalar quantity) expression exhibit associated Legendre polynomials \( P_n^j(\cos \phi) \)

---

* See deposition footnote.

Fig. 3. Stereographic projection of ‘normal’ symmetric harmonic \( K_j^\mu(\Phi, \beta) \) satisfies point group m3 (and 23), not 43m (cf. Table 7). Isodensity symbols used: ||, \( \beta \geq 0.00, * \geq 0.20, Z \geq 0.50, \times \geq 0.80, + \geq 0.90 \). Only a quarter is shown since the mirror planes (point group m3) are perpendicular to the plane of the paper generating the entire pole figure.

Fig. 4. ‘Normal’ symmetric harmonic \( K_j^\mu(\Phi, \beta) \) satisfies point group 23 (and 43m) not m3. Isodensity symbols: according to Fig. 3. Plane of the paper is not a mirror plane. Definition of \( K_j^\mu \) in Figs. 3 and 4 according to equation (16).
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or, more generally, \( P^n_l^m(\cos \Phi) \). The new harmonics \( F_1 \) to \( F_6 \) governing the diffraction-strain (i.e., a second-rank tensor) expression exhibit generalized associated Legendre (Jacobi-type) polynomials \( P^n_l^m(\cos \Phi) \) and \( P^n_l^m(\cos \Phi) \). It is expected then that harmonics exist exhibiting Jacobi polynomials up to, say, \( P^n_l^m(\cos \Phi) \). They may arise in conjunction with physical properties whose descriptions need higher-rank tensors than required for (diffraction) elastic strain.

6. Concluding remarks

Four new types of spherical harmonics have been defined. They can be made to satisfy cubic point-group symmetry. All cubic point groups have been dealt with. The new harmonics originate in the equations for diffraction strain pole figures obtained on textured materials. They differ essentially from those occurring in diffraction intensity pole figures.

Cubic-symmetry-coefficient equations for point group 23 have been given. The coefficients allow the calculation of both even- and odd-order symmetrized harmonics. The better known cubic symmetry coefficients for point group 432 constitute half of the solutions obtained.

General equations have been given which allow calculation of the normalization factors of the new harmonics. The expressions involve Clebsch–Gordan coefficients and the cubic symmetry coefficients leading to complicated expressions.

General diffraction intensity and diffraction strain expressions for all cubic point groups, taking into account structure factors for both anomalous and normal scattering modes, have been given. By contrast with the diffraction intensity case, the diffraction strain expressions do not exhibit the so-called 'ghosts' often encountered in texture analysis from diffraction intensity pole figures.

Fig. 5. Symmetrized harmonic \( F_1(\Phi, \beta, 9, 1) \) satisfies point group m3 (and 23), not 43m (cf. Table 7). Isodensity symbols used: * +0.07, © +0.03, Z +0.10, + −0.07, × −0.03, Δ −0.10, □ 0.00. Only a quarter is shown since the mirror planes (point group m3) perpendicular to the plane of the paper generate the entire pole figure. Definition of \( F_1 \) according to equation (23).

Fig. 6. Symmetrized harmonic \( F_2(\Phi, \beta, 12, 2) \) satisfies point group 23 (and 43m) not m3. Isodensity symbols according to Fig. 5. Plane of paper is not a mirror plane. Definition of \( F_2 \) according to equation (24).

Fig. 7. Symmetrized harmonic \( F_3(\Phi, \beta, 7, 1) \) satisfies point group m3 (and 23) not 43m. Isodensity symbols according to Fig. 5. Only a quarter is shown since the mirror planes (point group m3) perpendicular to the plane of the paper generate the entire pole figure. Definition of \( F_3 \) according to equation (27).

Fig. 8. Symmetrized harmonic \( F_4(\Phi, \beta, 6, 2) \) satisfies point group 23 (and 43m) not m3. Isodensity symbols according to Fig. 5. Plane of paper is not a mirror plane. Definition of \( F_4 \) according to equation (28).
Stimulating discussions with Dr Ir R. Delhez and Professor Dr Ir E. J. Mittemeijer are gratefully acknowledged.

References


Surface spherical harmonics and intensity and strain pole figures of cubic textured materials. Erratum.
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(Received 22 March 1987)

Abstract

Expressions given in Tables 2 and 3 of Brankan [Acta Cryst. (1987), A43, 270–283] are corrected. Table 2, column 2, line 1 should read

\[ [S_{\text{HKL}} P_{\text{HKL}} + S_{\text{HKL}}^2 P_{\text{HKL}} + S_{\text{KRL}}^2 P_{\text{KRL}} + S_{\text{KRL}} P_{\text{KRL}})] D^{-1} \]

Table 3, column 2, line 2 should read

\[ \frac{1 + (-1)^{J+M/2}}{[S_{\text{HKL}}^2 + S_{\text{KRL}}^2]} \]

All relevant information is given in the Abstract.

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Appendix I: Definition of functions $P_1$ to $P_4$ in terms of $hkl$, $j$ and $\mu$

The following expressions are needed:

\[ a_1 = h(k^2 - k^2)(h^2 + k^2)^{-1} \]  \hspace{1cm} (I-1)

\[ b_1 = 1(-h^4 - k + k^2 + h^2 + l^2)(h^2 + k^2)^{-1} \]  \hspace{1cm} (I-2)

\[ a_2 = \left[ h^4(k^2 - l^2) + k^4(h^2 - l^2) \right] (h^2 + k^2)^{-1} \]  \hspace{1cm} (I-3)

\[ b_2 = hkl(h^2 - k^2)(h^2 + k^2)^{-1} \]  \hspace{1cm} (I-4)

$h$, $k$ and $l$ are normalized such that:

\[ h^2 + k^2 + l^2 = 1 \]  \hspace{1cm} (I-5)

\[ \cos[\arg z_1(hkl)] = a_1(a_1^2 + b_1^2)^{-1} \]  \hspace{1cm} (I-6)

\[ \sin[\arg z_1(hkl)] = b_1(a_1^2 + b_1^2)^{-1} \]  \hspace{1cm} (I-7)

\[ \cos[2\arg z_2(hkl)] = a_2(a_2^2 + b_2^2)^{-1} \]  \hspace{1cm} (I-8)

\[ \sin[2\arg z_2(hkl)] = b_2(a_2^2 + b_2^2)^{-1} \]  \hspace{1cm} (I-9)

Then, it can be written:

\[ P_1(hkl,j,\mu) = (a_2^2 + b_2^2)^{1/2} \sum_{m=-j}^{j} (-1)^m/2 \mu^m p^2 m^2 (\cos\phi) \]

\[ x \cos[8m + 2\arg z_2(hkl)] \]  \hspace{1cm} (I-10)

*footnote:

In Brakman (1985) the factor $(-1)^{m/2}$ was omitted since the equations were written with special view to point-group 432.
\[ F_2(hkl, j, \mu) = (a_2^2 + b_2^2)^{\frac{1}{2}} \sum_{m=-j(2)}^{j} (-1)^{m/2} A_j^m p_j^m (\cos \phi) \times \sin \left[ \beta m + 2\arg_2(hkl) \right] \] (I-11)

\[-F_3(hkl, j, \mu) = (a_1^2 + b_1^2)^{\frac{1}{2}} \sum_{m=-j(2)}^{j} (-1)^{m/2} A_j^m p_j^m (\cos \phi) \times \sin \left[ \beta m - \arg_1(hkl) \right] \] (I-12)

\[ F_4(hkl, j, \mu) = (a_1^2 + b_1^2)^{\frac{1}{2}} \sum_{m=-j(2)}^{j} (-1)^{m/2} A_j^m p_j^m (\cos \phi) \times \cos \left[ \beta m - \arg_1(hkl) \right] \] (I-13)

where:

\[ \phi = \arccos(1) \] (I-14)

\[ \beta = \arccos \left[ \frac{1}{h^2 + k^2} \right] \] (I-15)

cf. Fig. 1.
Appendix II: The integrals $F_1(\phi, \beta, j, \mu) F_1^*(\phi, \beta, j', \mu') \sin \phi \sin \beta$ and $F_2(\phi, \beta, j, \mu) F_2^*(\phi, \beta, j', \mu') \sin \phi \sin \beta$

Elaboration yields:

$$\frac{2\pi}{2j'+1} \left[ \frac{1}{3\sqrt{1430}} (8j02\|j'2) - \frac{(-1)^{j+k}}{2\sqrt{455}} (8j42\|j'2) \right]$$

$$\times \sum_{m=-j}^{j} \mathcal{A}_{j'}^{m\mu} \left[ \delta_{j-j', m-8, \mu'} (8j-8m\|j'(m-8)) + \delta_{j-j', m+8, \mu'} (8j8m\|j'(m+8)) \right]$$

$$+ \frac{2\pi}{2j'+1} \left[ \frac{\sqrt{14}}{195\sqrt{11}} (8j02\|j'2) - \frac{(-1)^{j+k}}{65} (8j42\|j'2) \right]$$

$$\times \sum_{m=-j}^{j} \mathcal{A}_{j'}^{m4, \mu} \left[ \delta_{j-j', m-4, \mu'} (8j-4m\|j'(m-4)) + \delta_{j-j', m+4, \mu'} (8j4m\|j'(m+4)) \right]$$

$$+ \frac{2\pi}{2j'+1} \left[ \frac{2}{15\sqrt{14}} (6j02\|j'2) + \frac{2(-1)^{j+k}}{55} (6j42\|j'2) \right]$$

$$\times \sum_{m=-j}^{j} \mathcal{A}_{j'}^{m4, \mu} \left[ \delta_{j-j', m-4, \mu'} (6j-4m\|j'(m-4)) + \delta_{j-j', m+4, \mu'} (6j4m\|j'(m+4)) \right]$$

$$+ \frac{2\pi}{2j'+1} \left[ \frac{1}{13\sqrt{70}} (4j02\|j'2) - \frac{3(-1)^{j+k}}{143} (4j42\|j'2) \right]$$

$$\times \sum_{m=-j}^{j} \mathcal{A}_{j'}^{m4, \mu} \left[ \delta_{j-j', m-4, \mu'} (4j-4m\|j'(m-4)) + \delta_{j-j', m+4, \mu'} (4j4m\|j'(m+4)) \right]$$

$$+ \frac{2\pi}{2j'+1} \left[ \frac{1}{65} (8j02\|j'2) - \frac{33(-1)^{j+k}}{65\sqrt{154}} (8j42\|j'2) \right]$$

$$\times \sum_{m=-j}^{j} \mathcal{A}_{j'}^{m\mu, \mu'} \left[ \delta_{j-j', m0, \mu} (8j0m\|j'm) \right]$$

$$+ \frac{2\pi}{2j'+1} \left[ \frac{2}{105} (6j02\|j'2) - \frac{4(-1)^{j+k}}{55\sqrt{14}} (6j42\|j'2) \right]$$

$$\times \sum_{m=-j}^{j} \mathcal{A}_{j'}^{m\mu, \mu'} \left[ \delta_{j-j', m0, \mu} (6j0m\|j'm) \right]$$

$$+ \frac{2\pi}{2j'+1} \left[ \frac{1}{65} (4j02\|j'2) - \frac{42(-1)^{j+k}}{143\sqrt{70}} (4j42\|j'2) \right]$$

$$\times \sum_{m=-j}^{j} \mathcal{A}_{j'}^{m\mu, \mu'} \left[ \delta_{j-j', m0, \mu} (4j0m\|j'm) \right]$$

$$+ \frac{4\pi}{105(2j'+1)} \delta_{jj', \mu}\delta_{\mu, \mu'}$$

(II-1)
For the integral involving functions $F_1$ times $F_1^*$, $K$ in eq. (II-1) is equal to 1 whereas the expression exhibits $K = 2$ for the case of functions $F_2$ times $F_2^*$. 

The expressions $(l_{1}l_{2}m_{1}m_{2}|1_{3}(m_{1}+m_{2}))$ stand for the well-known Clebsch-Gordan coefficients. A very useful and practical program for the calculation of these C.G. coefficients has been described by Schulten & Gordon (1976). 

The coefficients $A_{j}^{m\mu}$ are the cubic symmetry coefficients defined in section 3. They can be chosen according to point-groups 23 or 432. Their main purpose is to account for the cubic 3-fold axis. 

Since function $F_2$ is equal to zero for every hkl if $j = 4, \mu = 1$ or $j = 8, \mu = 1$ eq. (II-1) should be equal to zero if $K = 2$ for those $j, \mu$ combinations. A check was run letting $j = 8, \mu = 1$ and $j' = 4(1)34$. Then, eq. (II-1) should yield a zero result in all cases. On all occasions the computer output affirmed this (within the accuracy of representing a number with a finite quantity of bits).

For instance, using $K = 2$ and $j = j' = 8$ and $\mu = \mu' = 1$ the computer-output for eq. (II-1) except the last term yields: $\frac{-4\pi}{17\times105}$. 

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Appendix III: The integrals \( \phi F_3(\phi, \beta, j, \mu) F_3^*(\phi, \beta, j', \mu') \) \( \sin \phi \phi \beta \beta \)

and \( \phi F_4(\phi, \beta, j, \mu) F_4^*(\phi, \beta, j', \mu') \) \( \sin \phi \phi \beta \beta \)

Elaboration yields:

\[
\frac{2\pi}{2j' + 1} \left[ \frac{-4}{3\sqrt{1430}} (8j01 | j'1) + \frac{2(-1)^j k}{\sqrt{2002}} (8j2-1 | j'1) \right]
\]
\[
\times \sum_{m=-j}^{j} A_{j, j'}^{m\mu} \left[ A_{j', j}^{m-8, \mu'} (8j-8m | j'(m-8)) + A_{j', j}^{m+8, \mu'} (8j8m | j'(m+8)) \right]
\]

\[
\frac{2\pi}{2j' + 1} \left[ \frac{-56}{195\sqrt{154}} (8j01 | j'1) + \frac{4(-1)^j k}{13\sqrt{110}} (8j2-1 | j'1) \right]
\]
\[
\times \sum_{m=-j}^{j} A_{j, j'}^{m\mu} \left[ A_{j', j}^{m-4, \mu'} (8j-4m | j'(m-4)) + A_{j', j}^{m+4, \mu'} (8j4m | j'(m+4)) \right]
\]

\[
\frac{2\pi}{2j' + 1} \left[ \frac{2}{165\sqrt{14}} (6j01 | j'1) - \frac{4(-1)^j k}{11\sqrt{30}} (6j2-1 | j'1) \right]
\]
\[
\times \sum_{m=-j}^{j} A_{j, j'}^{m\mu} \left[ A_{j', j}^{m-4, \mu'} (6j-4m | j'(m-4)) + A_{j', j}^{m+4, \mu'} (6j4m | j'(m+4)) \right]
\]

\[
\frac{2\pi}{2j' + 1} \left[ \frac{18}{143\sqrt{70}} (4j01 | j'1) + \frac{12(-1)^j k}{143\sqrt{7}} (4j2-1 | j'1) \right]
\]
\[
\times \sum_{m=-j}^{j} A_{j, j'}^{m\mu} \left[ A_{j', j}^{m-4, \mu'} (4j-4m | j'(m-4)) + A_{j', j}^{m+4, \mu'} (4j4m | j'(m+4)) \right]
\]

\[
\frac{2\pi}{2j' + 1} \left[ \frac{-36}{585} (8j01 | j'1) + \frac{6(-1)^j k}{13\sqrt{35}} (8j2-1 | j'1) \right]
\]
\[
\times \sum_{m=-j}^{j} A_{j, j'}^{m\mu} A_{j', j}^{m\mu'} (8j0m | j' m) \]

\[
\frac{2\pi}{2j' + 1} \left[ \frac{-2}{1155} (6j01 | j'1) + \frac{4(-1)^j k}{11\sqrt{105}} (6j2-1 | j'1) \right]
\]
\[
\times \sum_{m=-j}^{j} A_{j, j'}^{m\mu} A_{j', j}^{m\mu'} (6j0m | j' m) \]

\[
\frac{2\pi}{2j' + 1} \left[ \frac{18}{715} (4j01 | j'1) + \frac{24(-1)^j k}{143\sqrt{10}} (4j2-1 | j'1) \right]
\]
\[
\times \sum_{m=-j}^{j} A_{j, j'}^{m\mu} A_{j', j}^{m\mu'} (4j0m | j' m) \]

\[
\frac{8\pi}{105(2j' + 1)} \delta_{jj'} \delta_{\mu\mu'}
\]

(III-1)
Eq. (III-1) exhibits $K = 1$ for the integral over functions $F_3$ times $F_3^*$ whereas $K = 2$ should be used for the integral over functions $F_4$ times $F_4^*$.

Since function $F_4$ is equal to zero for every hkl if $j = 4$, $u = 1$, eq. (III-1) should yield a zero result for $K = 2$.

This has been checked by computer letting $j = 4$, $u = 1$ and $j' = 4(1)34$ which in all cases confirmed the expectations.
5. RESIDUAL STRESS ANALYSIS USING OVERLAPPING DIFFRACTION PEAKS. CASE OF TEXTURED CUBIC MATERIALS.
Residual Stress Analysis Using Overlapping Diffraction Peaks. Case of Textured Cubic Materials

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Abstract

Residual stresses in polycrystalline materials can be determined from the 2θ shift of a reflection peak’s line profile. Recently, multiple reflections have been used for residual stress analysis in single-phase textured cubic materials. Analogously, residual stresses in two-phase materials could be determined from overlapping peaks of both phases. Equations are derived for residual stress analysis using partially or completely overlapping diffraction peaks. Mainly textured cubic materials are considered. It is shown that the so-called quasi-isotropic diffraction elastic constants become connected to texture-dependent quantities. In the examples treated the calculated diffraction strains of three multiple reflections exhibit only small nonlinearities although the intensities oscillate strongly.

1. Introduction

For residual stress determination from diffraction line-angle strain data the so-called \( \sin^2 \psi \) method is well established. Review papers of the method have been given by Dölle (1979), James & Cohen (1980), Hauk (1984) and Hauk & Macherauch (1984). For texture-free materials the measured diffraction strain quite often exhibits straight-line behaviour when plotted vs \( \sin^2 \psi \). The stresses can be determined from the intercepts and slopes.

For materials exhibiting preferred orientation of the crystallites (crystallographic texture) nonlinear behaviour with respect to \( \sin^2 \psi \) is often found. The \( \sin^2 \psi \) method has been extended for this case by Dölle, Hauk & Zegers (1978), Dölle & Hauk (1978, 1979), van Baal (1983), Barral (1983), Sayers (1984), Hauk, Vaessen & Weber (1985) and Brakman (1983, 1985a, b, 1986a, b). Although texture introduces cumbersome expressions and requires additional (intensity) measurements the texture-extended \( \sin^2 \psi \) method faces the same problems as does the ‘classical’ method.

In practice reflections potentially useful for residual stress analysis until recently were not often used owing to overlap with other diffraction peaks. Several authors (Hauk, Oudelhoven & Vaessen, 1981; Hauk, 1984; Stuitje, 1985) have shown the practical viability of their application. It may be expected that their use for stress analysis will increase because of the availability of synchrotron and neutron radiation and also because of the advent of the position-sensitive detector (PSD).

Examples of coinciding reflections of (cubic) single-phase materials are: the \{651 + 732\} b.c.c. reflection used on Fe and steel specimens; the \{511 + 333\} f.c.c. reflection used on Al specimens; the \{911 + 753\} f.c.c. reflection used on Ni specimens; and the (non-cubic) \{122\}, \{203\} and \{301\} reflections of \( \alpha \)-quartz. These reflections have been used in practice (Hauk, 1984; Hauk & Vaessen, 1983). For other examples of coinciding reflections see Bunge (1982, p. 67). In two-phase materials (partially) overlapping reflections frequently occur. Examples are the \{103\} h.c.p. and \{211\} b.c.c. reflections of the \( \alpha \) and \( \beta \) phases, respectively, of \((\alpha + \beta)\)-TiAl6V4, and the \{101\} b.c.t. and \{111\} f.c.c. reflections of hardened steel specimens exhibiting considerable amounts of retained austenite. An extensive investigation conducted on two-phase materials is reported by Stuitje (1985, p. 103).

It is the purpose of this paper to deal quantitatively with double or multiple reflections obtained on both single- and two-phase textured materials with a view to residual stress analysis. Equations are derived for both cases. Examples are treated for the single-phase-materials case. The treatment is restricted to the combined influence of single-crystal elastic anisotropy and crystallographic texture. The case of plastic anisotropy is not considered.* In the treatment the following assumptions are made:

(i) Line profiles can be corrected for instrumental broadening and background subtraction is feasible.
(ii) The centroid of an arbitrary number of partially or completely overlapping reflection peaks can be calculated with arbitrary accuracy.

*In the deformation history of a specimen some crystallites may have exhibited more resistance (owing to their specific orientations) in accommodating the imposed plastic strain (‘hard’ orientations) than others. After the deformation, such crystallites have more difficulties retaining intergranular coherence. As a consequence, these crystallites may exhibit different elastic strain states from those of their environment. Nonlinear diffraction strain behaviour then also results.
(iii) The strains exhibited by the diffracting crystals lead to a shift of the line profile. It is taken that the averaged strain is represented by the 2θ shift of the centroid of the line profile. The centroid is defined in a physically meaningful sense and it allows easy mathematical handling.

(iv) The orientation distribution function (o.d.f.) of the crystals is an adequate description of the specimen's texture.

We summarize here the principal conclusions that will be reached:

(i) General expressions are derived relating the 2θ shift of the centroid of an arbitrary number of coinciding or partially overlapping diffraction peaks to the stress-tensor elements generating the 2θ shift. The equations apply to textured, single-phase or two-phase cubic materials. In the expressions, the so-called ‘quasi-isotropic’ diffraction elastic constants become connected to texture-dependent quantities.

(ii) B.c.c. \{651 + 732\}, \{330 + 411\} and \{510 + 431\} multiple-reflection diffraction strains calculated for a cold-rolled low-carbon steel specimen exhibit very small nonlinearities with respect to \(\sin^2 \psi\). Practical \{651 + 732\} results reported in the literature obtained on similar steel specimens comply with the calculations.

(iii) In the equations derived, complicated texture-dependent expressions can be neglected for the three multiple reflections mentioned. However, this result depends on the texture.

2. Elastic line-shift strain and the case of overlapping diffraction peaks; cubic materials

In the treatment of the diffraction experiment it is necessary to take into account orientation types ‘a’ and ‘b’ (Fig. 1) for all crystal point groups. Some point groups may require consideration of additional orientations. In what follows these are neglected since their treatment can be deduced from the ‘a’ and ‘b’ expressions.

If specimens exhibit crystallographic texture it must be expected that the crystallographic orientation distribution function (o.d.f.) differs in the a and b orientations. Therefore, the usual symbol for the general hkl reflection, \{hkl\}, is split into two in this paper: \{hkl\} and \{hkl\}. For the 432 or m3m case both can be seen as constituted from 24 physical equivalents of the hkl and \(hkl\) reflections, respectively.

It is taken (in the 432 or m3m case) that \{hkl\} and \{hkl\} both exhibit a multiplicity of 24 indicated by \(m(hkl) = 24\) etc. Hence, the definition of multiplicity is (in all crystal point-group cases) halved with respect to the conventional one. The centroid of a diffraction peak is the logical physical quantity for representing elastic line-shift strain. In what follows the centroid of a group of reflection peaks is dealt with. The symbols for the relevant reflections, \(\{hkl\}_1, \{hkl\}_2, ..., \{hkl\}_n\) are shortened to \(h_1, -h_1, ..., h_n, -H_1, ..., -H_n\) for Miller or Laue indices, respectively.

Squares of structure factors (i.e., structure factors times their complex conjugates) are denoted by \(S^2\) (\(-H_1\)) for the general \(\{hkl\}_1\) reflection etc. (structure factors are written with Laue indices).

A more general treatment that considers all crystal point groups is given in Appendix I.*

*Appendices I–III have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44141 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
2.1. The centroid of a group of reflection peaks

The centroid of an arbitrary group of reflection peaks results from a weighted composition of the constituent single reflection peaks. From the theoretical point of view it does not matter whether the reflection peaks are a consequence of: (i) only the \{hkl\} and \{hk\} reflections according to the \(a\) and \(b\) orientations (if the textured material is strained they become shifted with respect to each other); (ii) multiple reflections obtained from a single-phase material; (iii) reflections obtained from both phases of a two-phase material; or (iv) combinations of these.

For the centroid of a single reflection peak one can write

\[
\langle 2\theta \rangle = \frac{\int_{2\theta_a}^{2\theta_b} 2\theta I(2\theta) \, d2\theta}{\int_{2\theta_a}^{2\theta_b} I(2\theta) \, d2\theta}
\]

where \(I(2\theta)\) stands for the peak’s intensity at the angle \(2\theta\). The integration boundaries \(2\theta_a\) and \(2\theta_b\) have to be taken at sufficiently large distances from the low-angle and high-angle sides of the peak. For the centroid of a group of \(n\) completely or partially overlapping peaks one can write using (1)

\[
\langle 2\theta \rangle = \frac{\sum_{j=1}^{n} \langle 2\theta \rangle_{h_j} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_h(2\theta) \, d2\theta}{\sum_{j=1}^{n} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_h(2\theta) \, d2\theta}
\]

The centroid of the combined line profile is written as a weighted sum of centroids of all contributing line profiles. This equation can also be used for reflections which do not even disturb each other on the \(2\theta\) scale.

The expression holds for all crystal classes and all metallurgical phases. The denominator is equal to the integrated intensity of the combined line profile.

However, for the textured-material case, (2) has to be rewritten as

\[
\langle 2\theta \rangle = \sum_{j=1}^{n} \int_{2\theta_{a_j}}^{2\theta_{b_j}} \langle 2\theta \rangle_{h_j} \frac{1}{\sum_{j=1}^{n} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_h(2\theta) \, d2\theta} \times \left\{ \sum_{j=1}^{n} \frac{1}{\sum_{j=1}^{n} [I_{-h_j}(2\theta) + I_{h_j}(2\theta)]} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_h(2\theta) \, d2\theta \right\}^{-1}.
\]

For some point groups both numerator and denominator have to be extended with additional terms. A completely analogous treatment applies to the centroid in some initial condition \(2\theta_0\). The denominators are identical (the group of reflections is taken to be shifted only). One can then write* [where \(D\)

represents the denominator of (3)]

\[
\langle 2\theta \rangle = \langle 2\theta \rangle_0 + \Delta \langle 2\theta \rangle
\]

\[
= D^{-1} \sum_{j=1}^{n} \left\{ \Delta \langle 2\theta \rangle_{-h_j} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_{-h_j}(2\theta) \, d2\theta + \Delta \langle 2\theta \rangle_{h_j} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_{h_j}(2\theta) \, d2\theta \right\}
\]

2.2. Line-shift strain

From Bragg’s law it follows that the shift of the centroid is given by

\[
\Delta \langle 2\theta \rangle = -2 \langle \epsilon \rangle \tan \theta
\]

where the tangents in the shifted and unshifted conditions have been taken as equal.

The centroids of the \{hkl\} and \{hk\} line profiles are very close to each other and also very close to the centroid of the total line profile:

\[
\tan \langle \theta \rangle_{-h_j} \approx \tan \langle \theta \rangle_{h_j} \approx \tan \langle \theta \rangle.
\]

As a consequence,

\[
\langle \epsilon \rangle = D^{-1} \sum_{j=1}^{n} \left\{ \langle \epsilon \rangle_{-h_j} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_{-h_j}(2\theta) \, d2\theta + \langle \epsilon \rangle_{h_j} \int_{2\theta_{a_j}}^{2\theta_{b_j}} I_{h_j}(2\theta) \, d2\theta \right\}
\]

where the left-hand side (LHS) represents the total elastic line-shift strain. This quantity is the weighted strain of all crystallites contributing to the diffraction in the direction of the scattering vector \(Q\) [definition of \(Q\) according to Sayers (1984)]. The orientation of \(Q\) with respect to specimen axes is determined by the commonly used angles \(\varphi\) and \(\psi\) (see Brakman, 1985b, Fig. 1). \(\psi\) is a tilting angle about an axis in the specimen’s surface and \(\varphi\) is a rotation angle about the specimen’s surface normal. Accordingly, \(\langle \epsilon \rangle\), depends on \(\psi, \varphi\), \(\langle \epsilon(\varphi, \psi) \rangle\), \(\langle \epsilon \rangle_{-h_j}\) stands for the elastic strain in the direction of \(Q\) of all crystallites exhibiting \([hk\ell]\), parallel to \(Q\) etc.

A similar definition holds for the \(+h_j\) reflection etc.

From the definitions given in Appendix II and with \(g(-h_j)\) for the numerator of equation (II-3) the complete line-shift strain expression is found to be

\[
\langle \epsilon(\varphi, \psi) \rangle = \frac{\sum_{j=1}^{n} \epsilon m(h_j) \left[ g(-h_j) S^2(-H_j) + g(h_j) S^2(H_j) \right]}{2\pi \sum_{j=1}^{n} \epsilon m(h_j) \left[ S^2(-H_j) P_{-h_j}(\psi, \varphi) + S^2(H_j) P_{h_j}(\psi, \varphi) \right]}.
\]

*For high \(\theta\) values this only holds if the left- and right-hand specimens of the constituent single reflections are separated from each other by not more than, say, 2° \(2\theta\).

*See deposition footnote.
Define

\[ Z = \sum_{i=1}^{n} c_i m(h_i)[S^2(-H_i) + S^2(H_i)] \quad (9) \]

and

\[ \bar{P}(\psi, \varphi) = \sum_{j=1}^{n} c_j m(h_j)[S^2(-H_j)P_{-h_j}(\psi, \varphi) + S^2(H_j)P_{h_j}(\psi, \varphi)]Z^{-1} \quad (10) \]

(see Appendix II for definition of \( P_{-h_j} \) and \( P_{h_j} \)).

It follows that

\[ \langle \sigma(\psi, \varphi) \rangle_i = \left[ 2\pi \bar{P}(\psi, \varphi) \right]^{-1} \sum_{j=1}^{n} c_j m(h_j) \times [S^2(-H_j)g(-h_j) + S^2(H_j)g(h_j)]Z^{-1}. \quad (11) \]

\( \bar{P}(\psi, \varphi) \) equals the total intensity (i.e. that from all reflections concerned) normalized in terms of 'times random'. It can be obtained from a pole-figure measurement of the multiple reflection. Note that (11) allows both normal and anomalous scattering modes.

Until now the treatment has been completely free from any assumption concerning elasticity models. For the case of the Reuss model of elasticity applied to one reflection only (\( n = 1 \)), (11) reduces to equation (9) of Brakman (1985b).

3. Multiple-reflection line-shift strain expressions

The most interesting case is the one where two or more reflections obtained on a single-phase material exhibit exactly the same (theoretical) interplanar lattice spacing and hence the same centroid of the corresponding diffraction line profiles. It can be shown in this case that the structure factors of a group of double or multiple reflections are equal. The same holds for the coefficients \( c_j \) [equation (II-2)]. Consequently, structure factors and coefficients \( c_j \) vanish from (11) for the single-phase-materials case. However, the multiplicities may differ.

Recently, practical use has been made (Hauk, Oudelhaven & Vaessen, 1981; Hauk, 1984; Hauk & Vaessen, 1984; Stuitje, 1985) of the \( 651 + 732 \) b.c.c. reflection. Here the multiplicities are equal and (11) reduces to

\[ \langle \sigma(\psi, \varphi) \rangle_i = \left[ 2\pi \bar{P}_{651}(\psi, \varphi) \right]^{-1} \times [2\pi \bar{P}_{651 + 732}(\psi, \varphi)]^{-1}. \quad (12) \]

Note that function \( g \) also depends on \( \psi \) and \( \varphi \) [numerator of (II-3)].

The Reuss model of elastic polycrystal coupling and application of equation (9) of Brakman (1985b) to (12) yields

\[ \langle \sigma(\psi, \varphi) \rangle_i = (\sigma_{11} + \sigma_{22}) \left[ \frac{1}{2} \bar{P}_{651}(\psi, \varphi) \right] s_1(651) + \frac{1}{2} \bar{P}_{732}(\psi, \varphi) s_1(732) \times \left[ \bar{P}_{651 + 732}(\psi, \varphi) \right]^{-1} + \sigma_{22} \sin^2(\psi) \left[ \frac{1}{2} \bar{P}_{651}(\psi, \varphi) \right] s_2(651) \]

\[ + \frac{1}{2} \bar{P}_{732}(\psi, \varphi) s_2(732) \times \left[ \bar{P}_{651 + 732}(\psi, \varphi) \right]^{-1} + \left[ 2 \bar{P}_{651 + 732}(\psi, \varphi) \right]^{-1} \times \sigma_0 \left( (\sigma_{11} - \sigma_{22}) \sin 2\varphi \sin \psi \right) \]

\[ \times \sum_{j=1}^{n} E_j(\psi, \varphi) \left[ \frac{1}{2} F_{3}(651, j, \mu) \right] + \frac{1}{2} F_{3}(732, j, \mu)] \]

\[ + \sigma_{22} \sin^2(\psi) \sum_{j=1}^{n} D_j(\psi, \varphi) \left[ \frac{1}{2} F_{3}(651, j, \mu) \right] + \frac{1}{2} F_{3}(732, j, \mu)] \]

\[ - \left[ (\sigma_{11} - \sigma_{22}) \cos 2\varphi - \sigma_{22} \sin^2(\psi) \right] \]

\[ \times \sum_{j=1}^{n} B_j(\psi, \varphi) \left[ \frac{1}{2} F_{1}(651, j, \mu) + \frac{1}{2} F_{1}(732, j, \mu \right) \]

\[ - \left( (\sigma_{11} - \sigma_{22}) \sin 2\varphi \cos \psi \sum_{j=1}^{n} C_j(\psi, \varphi) \right. \]

\[ \times \left[ \frac{1}{2} F_{1}(651, j, \mu) + \frac{1}{2} F_{1}(732, j, \mu) \right]. \quad (13) \]

where \( s_1(651) \) and \( s_2(732) \) are the so-called 'quasi-isotropic' diffraction elastic constants (XEC) (Dölle, 1979).

\[ \sigma_{22} = \sigma_{11} \cos^2(\varphi) + \sigma_{22} \sin^2(\varphi). \quad (14) \]

Stresses \( \sigma_{11} \) and \( \sigma_{22} \) are taken to operate along two of the specimen's reference axes (in the specimen's surface). Functions \( B_j, C_j, D_j \) and \( E_j \) depend on the texture and they have been defined by Brakman (1986b). Functions \( F_1 \) and \( F_3 \) depend on \( hkl \) and they have been defined for all cubic crystal point groups by Brakman (1987b). The symbol \( \bar{P}_{651} \) stands for the 651 pole-figure intensity in the direction of \( Q \) (normalized in terms of 'times random') if the 651 reflection could have been separately measured. Since this is impossible it has to be calculated from the o.d.f. with equation (II-1). A similar observation holds for \( \bar{P}_{732} \).

One can write

\[ \bar{P}_{651} = (S_{651}^2 P_{651} + S_{651}^2 P_{651} + S_{651}^2 P_{651} + S_{651}^2 P_{651}). \quad (15) \]

which reduces for the normal scattering case to

\[ \bar{P}_{651} = \frac{1}{2} (P_{651} + P_{651}). \quad (16) \]

(A similar expression applies to \( \bar{P}_{732} \).)

The symbol \( \bar{P}_{651 + 732} \) stands for the measured pole-figure intensity (normalized in terms of 'times random') obtained for both reflections at the same time:

\[ \bar{P}_{651 + 732} = (S_{651}^2 \bar{P}_{651} + S_{651}^2 \bar{P}_{732})/(S_{651}^2 + S_{732}^2). \quad (17) \]
which reduces to
\[ \tilde{P}_{651 + 732} = \frac{1}{2}(\tilde{P}_{651} + \tilde{P}_{732}). \]  
(18)

It is interesting to note that, in the first two terms of the RHS of (13), the quantities \( s_1 \) and \( \frac{1}{2} s_2 \) are connected to the \( \psi, \omega \)-dependent factors \( \tilde{P}_{651}(\psi, \omega) \), \( \tilde{P}_{651 + 732}(\psi, \omega) \) etc. Obviously, these factors operate as weight factors in the total measured line-shift strain. An expression similar to (13) can be derived for the \( \{510 + 431\} \) and \( \{330 + 411\} \) b.c.c. reflections. In those cases the multiplicities differ. The case of double reflections obtained on a two-phase material is treated in Appendix III.\footnote{An expression similar to (13) can be derived. The following alterations should be made:
(i) Change the divisors \( \tilde{P}_{351 + 732} \) and \( 2\tilde{P}_{651 + 732} \) to \( \tilde{P}_{510 + 432} \) and \( 2\tilde{P}_{510 + 432} \), respectively.
(ii) The quantities \( \tilde{P}_{651}(510) \) and \( \tilde{P}_{732}(510) \) should be replaced by \( \tilde{P}_{651}(510) \) and \( \tilde{P}_{432}(510) \), respectively. A completely analogous reasoning holds for the terms exhibiting \( \frac{1}{2}s_2 \).
(iii) The expressions \( \tilde{P}_5(510, \omega) \) and \( \tilde{P}_4(510, \omega) \) should be replaced by \( \tilde{P}_5(510, \omega) \) and \( \tilde{P}_4(510, \omega) \).}

4. Results and discussion

In residual stress analysis for the texture-free material case, the "quasi-isotropic" diffraction elastic constants (XEC) \( s_1(hkl) \) and \( \frac{1}{2}s_2(hkl) \) are essential. They allow the conversion of strains into stresses. They do not depend on the scattering vector's orientation with respect to specimen axes. They are independent of the angles \( \psi \) and \( \varphi \). In the equations for the texture-free cases these XEC also play a role in the single-reflection case. For the multiple-reflection case, \( s_1 \) and \( \frac{1}{2}s_2 \) become connected [equations (13) and (11–11)] to weight factors depending on the texture, i.e. \( \tilde{P}_{651}(\psi, \omega) / \tilde{P}_{651 + 732}(\psi, \omega) \) etc. As a result, the first two members of the RHS of these equations also become texture dependent. They do not exhibit the o.d.f.-dependent functions \( B_T \) or \( E_T \) [definitions of which are given by Brakman (1986b)]. The single reflection intensities \( \tilde{P}_{651} \) etc. cannot be separately measured in most cases. They have to be calculated from the o.d.f. Hence, knowledge of the o.d.f. (obtained from other single reflections) is still required.

In the examples following, the o.d.f. of a cold-rolled deep-drawing steel sheet specimen (Brakman, 1985a) has been used. The cold-rolling textures of these low-carbon steels develop almost independently of most material and deformation variables. They strongly resemble the well known b.c.c. rolling-texture type (Wassermann & Grewen, 1962). Therefore, the significance of results obtained extends beyond the scope of the steel specimens referred to (Brakman, 1985a). It allows comparison with similar cold-rolled steel results on at least a qualitative basis.

As shown in Brakman (1986a) the calculated \{211\} diffraction strain exhibits the usual "oscillations", i.e. non-linearity vs \( \sin^2 \psi \) for \( \varphi = 0 \) as frequently measured in practice (angle \( \varphi \) defined in the rolling plane, with respect to the rolling direction) (e.g. Faninger & Hauk, 1976; Marion & Cohen, 1977; Döller & Cohen, 1980; Hauk, Krieg & van Haux, 1981; Hauk, van Haux & Weber, 1985).

In what follows calculated results for the \{651 + 732\} (Figs. 2a to 3b), \{510 + 431\} (Figs. 4a to 5b) and \{330 + 411\} reflections (Figs. 6a, b) are dealt with.

In Figs. 2(a), 2(b), 4(a) and 4(b) the calculated intensities [according to (11–1) and (10)] \( \tilde{P}_{651} \), \( \tilde{P}_{732} \), \( \tilde{P}_{510} \) and \( \tilde{P}_{432} \) are plotted for both \( \varphi = 0 \) and \( \varphi = \pi/2 \) as a function of \( \sin^2 \psi \). These intensities all exhibit

![Fig. 2. (a) Single-reflection intensities \( \tilde{P}_{651} \) and \( \tilde{P}_{732} \) as a function of \( \sin^2 \psi \) plotted for \( \varphi = 0 \). The intensities cannot be measured separately. They have been calculated from the o.d.f. of a cold-rolled low-carbon steel sheet specimen (Brakman, 1985a). Definitions of \( \tilde{P}_{651} \) and \( \tilde{P}_{732} \) are given in (15) and (16). (b). As (a) but results are for \( \varphi = \pi/2 \). Note that the single-reflection intensities oscillate more strongly for \( \varphi = 0 \) than in the \( \varphi = \pi/2 \) case. The angle \( \varphi \) is determined with respect to the rolling direction in the plane of the sheet.](image-url)
stronger oscillations (with respect to \( \sin^2 \psi \)) for \( \varphi = 0 \) than obtained for the \( \varphi = \pi/2 \) case.

In Figs. 3(a), 3(b), 5(a), 5(b), 6(a) and 6(b) the calculated [13] diffraction strains are exhibited for the \( \{651 + 732\} \), \( \{510 + 431\} \) and \( \{330 + 411\} \) reflections.

The quantity \( \langle e(\psi, \varphi) \rangle \) has been divided by \( s_0 \) (single-crystal elastic anisotropy) times \( \sigma_{11} \). This allows treatment of the problem for the 'general' stress state \( \eta = \sigma_{22}/\sigma_{11} \). Here \( \eta \) was taken as +1. This comes close to the residual stress state often found after cold rolling of low-carbon steels. Both \( \sigma_{11} \) and \( \sigma_{22} \) are then compressive and approximately equal in magnitude (Dölle & Cohen, 1980).

In Figs. 3(a), 5(a), 6(a) and 6(b) the heavy lines represent the complete expression (13) (or its equivalent for the \( \{510 + 431\} \) and \( \{330 + 411\} \) cases). The thin line exhibits only the first two terms of the RHS of (13). The differences seem to be small but the full expression (13) oscillates somewhat more strongly. In Figs. 3(b) and 5(b) only the heavy line is drawn since the differences were very small.

It follows for all reflections that for \( \varphi = 0 \) (Figs. 3a, 5a and 6a) stronger oscillations of the diffraction strain \( \sin^2 \psi \) are obtained than for \( \varphi = \pi/2 \) (Figs. 3b, 5b and 6b) case.

The strong oscillations obtained for the calculated intensities (Figs. 2a and 4a) do not occur in the diffraction-strain graphs. It follows (Figs. 5a and 6a) that care must be taken in drawing straight lines through the curves. However, it seems reasonable to use only the first two members of the RHS of (13), omitting the complicated d.f. expressions \( B_j \) to \( E_j \).

The conclusion is drawn for \( \eta = +1 \) but it also holds for other stress states (not shown).* The conclusion also depends on the strength and the type of the texture. Barral (1983, Figs. 61 and 66) calculated a much stronger oscillating behaviour for the 651 and

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* \( \eta = +1 \) is a special stress state; any differences between the \( \varphi = 0 \) and \( \varphi = \pi/2 \) curves must be due to texture.

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Fig. 3. (a). Calculated diffraction strain for the \( \{651 + 732\} \) multiple reflection as a function of \( \sin^2 \psi \) plotted for \( \varphi = 0 \). A stress state of only non-zero \( \sigma_{11} \) and \( \sigma_{22} \), with \( \sigma_{11} = \sigma_{22} \), has been assumed. \( \sigma_{11} \) is taken to operate parallel to the rolling direction (RD) whereas \( \sigma_{22} \) points in the direction of the transverse direction (TD). Reuss model of elasticity. The definition of diffraction strain is given in (13). The diffraction strain is divided by \( s_0 \) (elastic anisotropy) times \( \sigma_{11} \). (b) As (a) but results are given for \( \varphi = \pi/2 \). For this stress state, any difference between the \( \varphi = 0 \) and \( \varphi = \pi/2 \) graphs must be due to texture. In both figures the heavy lines represent the complete expression (13). The thin line exhibits only the first two terms of its right-hand side. Only one line is drawn in (b) (no significant difference). Compare (a) and (b) with Figs. 17, 18 and 19 of Hauk (1984).

---

Fig. 4. (a) As Fig. 2(a), but single-reflection intensities \( P_{510} \) and \( P_{431} \) as a function of \( \sin^2 \psi \) plotted for \( \varphi = 0 \). (b) As (a) but results are given for \( \varphi = \pi/2 \). The single-reflection intensities oscillate more strongly for \( \varphi = 0 \) than for \( \varphi = \pi/2 \).
732 diffraction elastic constants. In that case the o.d. dependent expressions cannot be omitted. The texture types studied were different from the cold-rolling case.

Figs. 3(a) and 3(b) present a striking resemblance to the measured (651 + 732) diffraction strain curves obtained on cold-rolled steel reported by Hauk (1984, Fig. 17). There the slope of the graphs is negative, but allowing for negative (compressive) $\sigma_{11}$ in Figs. 3(a) and 3(b) also yields a negative slope [see also Hoffmann, Neff, Scholtes & Macherauch (1984) and Maurer, Neff, Scholtes & Macherauch (1987)].

Neglecting functions $B_f^j$, ..., $E_f^j$ and writing

$$s_i'(651,\psi,\varphi) = s_i(651)\bar{P}_{651}(\psi,\varphi)/\bar{P}_{651+732}(\psi,\varphi)$$

(19)

$$\frac{1}{2}s_2'(732,\psi,\varphi) = \frac{1}{2}s_2(732)\bar{P}_{732}(\psi,\varphi)/\bar{P}_{651+732}(\psi,\varphi)$$

(20)

etc. one obtains

$$\langle s_i(\psi,\varphi) \rangle = [\frac{1}{2}s_2'(651,\psi,\varphi) + \frac{1}{2}s_2'(732,\psi,\varphi)]$$

\[ \times (\sigma_{11} + \sigma_{22}) \]

\[ + [\frac{1}{2}s_2(651,\psi,\varphi) + \frac{1}{2}s_2(732,\psi,\varphi)] \]

\[ \times \sigma_{\varphi} \sin^2\psi \]

(21)

plus similar expressions for the 510 + 431 and 330 + 411 reflection cases. If there were no texture at all, functions $B_f^j$, ..., $E_f^j$ would equal zero, but then it would also hold that

$$\bar{P}_{651} = \bar{P}_{732} = \bar{P}_{651+732} = 1 \text{ etc.}$$

Then (21) reduces to a simple (weighted) averaging equation,

$$\langle s_i(\psi,\varphi) \rangle = s_i'(651,732)(\sigma_{11} + \sigma_{22})$$

\[ + \frac{1}{2}s_2'(651,732)\sigma_{\varphi} \sin^2\psi \]

(22)

Fig. 5. (a). Calculated diffraction strain for the {310 + 431} multiple reflection as a function of $\sin^2\psi$ plotted for $\varphi = 0$. See also Fig. 3(a). Definition of diffraction strain: the {310 + 431} equivalent of (13). The heavy line represents the full \{13\}-equivalent expression, the thin line only the first two terms of its right-hand side. (b) As (a) but results are given for $\varphi = \pi/2$. Only one line drawn (no significant difference). Note that the {310 + 431} diffraction strains oscillate more strongly for $\varphi = 0$ than for $\varphi = \pi/2$.

Fig. 6. (a). Calculated diffraction strain for the {330 + 411} multiple reflection as a function of $\sin^2\psi$ plotted for $\varphi = 0$. See also Fig. 3(a). Definition of diffraction strain: the {330 + 411} equivalent of (13). (b) As (a) but results given for $\varphi = \pi/2$. In both figures the heavy lines represent the full \{13\}-equivalent expression, the thin lines only the first two terms of its right-hand side. The {330 + 411} diffraction strains oscillate more strongly for $\varphi = 0$ than for $\varphi = \pi/2$. In all diffraction-strain graphs shown, the oscillations are weak. The difference between the full \{13\}-equivalent expression and its first two terms only is small in all cases. The texture-dependent functions $B_f^j$ to $E_f^f$ can consequently be neglected.
Table 1. Texture-free multiplicity-weighted diffraction elastic constants \( s' \) and \( \frac{1}{2}s'' \) according to equation (23) calculated for the b.c.c. \{330 + 411\}, \{510 + 431\} and \{651 + 732\} multiple reflections

<table>
<thead>
<tr>
<th>Double reflection</th>
<th>( s' ) ((10^{-6} \text{MPa}^{-1}))</th>
<th>( \frac{1}{2}s'' ) ((10^{-6} \text{MPa}^{-1}))</th>
<th>( t_1 ) ((10^{-6} \text{MPa}^{-1}))</th>
<th>( \frac{1}{2}t_2 ) ((10^{-6} \text{MPa}^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>330 + 411</td>
<td>-1.91</td>
<td>+7.62</td>
<td>-2.14</td>
<td>+8.20</td>
</tr>
<tr>
<td></td>
<td>((0.50 \leq \sin^2\psi \leq 0.95))</td>
<td></td>
<td>((0.50 \leq \sin^2\psi \leq 0.95))</td>
<td></td>
</tr>
<tr>
<td>510 + 431</td>
<td>-1.74</td>
<td>+7.11</td>
<td>-1.69</td>
<td>+6.93</td>
</tr>
<tr>
<td></td>
<td>((0.30 \leq \sin^2\psi \leq 1.00))</td>
<td></td>
<td>((0.30 \leq \sin^2\psi \leq 1.00))</td>
<td></td>
</tr>
<tr>
<td>651 + 732</td>
<td>-1.54</td>
<td>+6.50</td>
<td>-1.54</td>
<td>+6.33</td>
</tr>
<tr>
<td></td>
<td>((0 \leq \sin^2\psi \leq 1.00))</td>
<td></td>
<td>((0 \leq \sin^2\psi \leq 1.00))</td>
<td></td>
</tr>
</tbody>
</table>

\( \phi = 0 \)

\( \phi = \pi/2 \)

\( s'_{i}(h_{1},h_{2}) = [s_{i}(h_{1})m(h_{1}) + s_{i}(h_{2})m(h_{2})] \times [m(h_{1}) + m(h_{2})]^{-1} \)

(23)

and a similar expression can be written for \( \frac{1}{2}s'' \).

The question arises of whether completely texture-free behaviour could be assumed in any case [using (22) instead of (21)].

For the sections of the graphs exhibiting approximately straight-line behaviour in Figs. 3(a), 3(b), 5(a), 5(b), 6(a) and 6(b) one may formally write

\[ <(\psi,\phi)> = t_{1} (\sigma_{11} + \sigma_{22}) + \frac{1}{2} t_{2} \sigma_{\phi} \sin^{2}\psi. \]

(24)

The calculated results (taken from the graphs) for the straight-line parameters \( t_{1} \) and \( \frac{1}{2} t_{2} \) are presented in Table 1. From this table it follows that assuming texture-free behaviour [and consequently using \( s'_{i} \) and \( \frac{1}{2}s'' \) according to (22)] is quite feasible in most cases. This is a surprising feature of these reflections but it remains to be seen whether this holds generally.

Only the sections of the graphs exhibiting stronger departures from linearity \((0 \leq \sin^{2}\psi \leq 0.50, \text{Fig. 6a}; 0 \leq \sin^{2}\psi \leq 0.30, \text{Fig. 5a})\) would require use of (21).

5. Concluding remarks

The XEC \( s'_{1}, s'_{2}, \frac{1}{2}s'_{2}, \frac{1}{2}s'' \) and \( \frac{1}{2}s'' \) have all been written for the Reuss model of elasticity. For a realistic approximation of the stresses these XEC can be achieved with those for the Voigt-model prediction (Brakman, 1987a) according to the Hill (1952) procedure. Then the effect of the deviations from linearity in the figures is halved.

For two-phase materials stresses of the second kind have to be taken into account (Appendix III). The full stress tensor must then be considered. Consequently, treatment of an example would be cumbersome. It has been omitted.

The derived equations (obtained for m3m or 432 crystals and normal scattering) can be extended to the case of the other cubic point groups in conjunction with both normal and anomalous scattering using the considerations of Brakman (1987b).

For three double reflections treated the calculated diffraction strains exhibit no or only small nonlinearities when plotted with respect to \( \sin^{2}\psi \), although the single-reflection intensities oscillate quite strongly. In all three cases the diffraction strain only depends weakly on orientation distribution function expressions. They can be neglected. Then only the single-reflection intensities remain as texture-dependent quantities. In some sections of the graphs of diffraction strain vs \( \sin^{2}\psi \) texture-free behaviour may be assumed. However, the behaviour is not general; it depends on the type and strength of the texture.

In summary, expressions have been derived connecting the \((2\theta)\) line shift of the centroid of an arbitrary number of coinciding or partially overlapping diffraction peaks to (residual) stress tensor elements of textured cubic single-phase or two-phase materials. In the final expressions the so-called 'quasi-isotropic' diffraction elastic constants (XEC) \( s'_{1} \) and \( \frac{1}{2}s'' \) become connected to texture-dependent quantities, i.e. to the (not directly measurable) intensities of the single reflection peaks. The multiple-reflection XEC are found as an average of single-reflection XEC weighted by the single-reflection intensities and the multiplicities. The multiple-reflection XEC also exhibit expressions depending on the o.d.f. of the crystallites in the specimen. Diffraction-strain results have been calculated for a textured cold-rolled low-carbon steel sheet specimen for the \{330 + 411\}, \{510 + 431\} and \{651 + 732\} b.c.c. double reflections. In the \{651 + 732\} case a strong resemblance is found to measured diffraction strain data obtained on similar steel specimens reported in the literature. For the three double reflections indicated diffraction strain depends only weakly on the texture. Only single-reflection intensities then remain as texture-dependent quantities.

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References


Appendix I: Theoretical considerations: odfs, point-groups and structure factors.

I.1. The crystallite orientation distribution function (odf)

The odf yields the fraction crystallite orientations in the orientation interval between orientations $g$ and $g + dg$. It relates the volume fraction of the crystals in the interval to the interval itself: $dV/V = f(g)dg$ (Bunge, 1982, p. 42).

The odf is defined such that it is a function of orientations obtained by rotations only. It is defined on the rotation group in $R_3$.

For crystals belonging to pure-rotation point-groups it is necessary to distinguish between right-handed and left-handed crystals. They may occur in different fractions in one and the same specimen and they exhibit different odfs: $f^L(g)$ and $f^R(g)$ (Bunge, 1982, p. 103).

For the left-handed crystals the crystal reference frame is first inverted and then $f^L(g)$ is treated as a function of rotations only, just like $f^R$. It can be shown that for crystal point-groups exhibiting an explicit centre of inversion $f^L$ and $f^R$ are identical. For point-groups exhibiting mirror planes or inversion axes but not the explicit centre of inversion, $f^L$ and $f^R$ are one-to-one correlated. In the latter two cases only the right-handed odf $f^R$ needs to be taken into account.
I.2. The polycrystalline diffraction experiment

I.2.1. Crystallite orientations exhibiting the same hkl interplanar lattice spacing ($d_{hkl}$) in the direction of the scattering vector.

Upon diffraction all crystallites exhibiting an $<hkl>$ vector parallel to the scattering vector $Q$ (definition of $Q$ according to Sayer, 1984) contribute. Consider a specimen consisting of triclinic crystals, point-group $1$. The $(\bar{h}k\bar{l})$ interplanar lattice spacing equals its $(hkl)$ counterpart. Therefore, two physically different, right-handed crystallite orientation types contribute at the same time:

(i) The orientation type determined by [hkl] parallel to $Q$, arbitrary rotation angle about $Q$ (orientation "a" in Fig. 1).

(ii) The orientation type with [$\bar{h}\bar{k}\bar{l}]$/$Q$, arbitrary rotation angle about $Q$ (orientation "b" in Fig. 1).

Note that the second orientation is not obtained from the first one by inversion of the crystal's reference axes. For the general case i.e. $h$, $k$ and $l$ different from each other, the two orientations are physically different. They can never be made to coincide whatever the rotation angle about $Q$.

If the crystals belong to point-group $\bar{1}$ (triclinic, centrosymmetric case) both orientations have to be treated as well but two differences arise:

(i) The squared structure factors of both reflections are always equal whatever the scattering mode.
(ii) The centre of inversion is a point-group allowed symmetry-operation and it can be used to deduce that:
\[ f^L(g) = f^R(g) \] (Bunge, 1982, p. 105).

For cubic crystals (whatever the point-group) 48 crystallite orientation types exhibiting an \( \langle hkl \rangle \) vector parallel to \( Q \), contribute at the same time. They all have the same \( d_{hkl} \) in the direction of \( Q \). The number of 48 can be reduced considering physically equivalent crystallite orientations.

I.2.2. Physically equivalent crystallite orientations

Every crystallite orientation obtainable from another orientation using a point-group allowed rotational symmetry-operation (thus avoiding the problem of switching from the right-handed odf to the left-handed odf) is physically equivalent to that orientation. The odf's values in such orientations are equal.

Consider point-group \( \bar{4}3m \): it does not exhibit a 4-fold rotation axis. Consequently, the orientation type of say, \( [kh\bar{l}]//Q \), arbitrary rotation angle about \( Q \) (orientation "c"), is physically different from orientation "a". The "minus" orientation type i.e. \( [\bar{k}h\bar{l}]//Q \) (orientation "d") also needs considering. As a result there are four physically different crystallite orientation types for this point-group (Table I-1). Each represents a set of twelve physically equivalent orientations obtained using the point-group's rotational symmetry elements (three 2-fold rotations, four 3-fold rotations of \( 2\pi/3 \), four 3-fold rotations of \( 4\pi/3 \) and the identity operation).

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For point-groups 432 and m3m only two different sets of 24 physically equivalent orientations remain since orientation "c" can be obtained from "a" using a 4-fold rotational symmetry operation. For m3m the structure factors of the (hkl) and (h-k-l) reflections are equal whatever the scattering mode. In the 432 case they may be unequal for the anomalous scattering mode.

I.2.3. Structure factor considerations

Upon diffraction, all crystallite orientations exhibiting the same $d_{hkl}$ in the direction of $\mathbf{Q}$ contribute to the (hkl) reflection. However, not always the same structure factors occur then. Even for the normal scattering mode they may differ (point-groups 23 and m3, see Brakman (1987b)). For the anomalous scattering mode more differences arise (Table I-1). It can not be expected in the general case that the odf exhibits equal values in the a and b (or a, b, c and d) orientations*.

* It can also be shown that the theoretical (hkl) and (h-k-l) intensities differ (Bunge, 1982, p. 106; Brakman, 1985b). The same holds with respect to the (khl) and (k-h-l) intensities for the m3m case.
As a result the expression representing the total diffracted intensity or diffraction strain consists of the added, structure-factor weighted odf contributions** (Brakman, 1987b). These odf-contributions have to be taken into account because physically non-equivalent crystallite orientations (a, b, c and d) exhibit the same $d_{hkl}$.

** On top of this, the left-handed odf-contributions have to be added for the pure-rotation point-group case.
Appendix II: Definition of intensity and strain quantities

\[ P_{-h_j}, \langle \varepsilon \rangle_{-h_j}, \text{ etc.} \]

Denoting the odf by the symbol \( f \), the following quantity is defined:

\[ P_{-h_j}(\psi, \phi) = (2\pi)^{-1} \int_{0}^{2\pi} f(\psi, \phi, [\overline{hkl}]_j, \phi_2) d\phi_2 \]  \hspace{1cm} (II-1)

where:

\[ \phi_2 = \text{rotation angle about } Q. \]

\[ P_{-h_j} = \text{theoretical intensity of the } [\overline{hkl}]_j \text{ reflection}. \]

The integral only regards those crystallites exhibiting \([\overline{hkl}]_j \parallel Q\). The factor \((2\pi)^{-1}\) is a normalization factor.

Similar definitions apply to the \(+h_j\) reflection etc.

The relationship between the symbol \( P_{-h_j} \) and the quantity \( \int_{2\pi} I_{-h_j}(2\psi) d2\psi \) is the following:

Although the odf may be non-zero in eq. (II-1), the structure factor square \( S^2(-H_j) \) determines whether any intensity can actually be observed. Therefore:

\[ \int_{2\pi} I_{-h_j}(2\psi) d2\psi = c_j S^2(-H_j) P_{-h_j} m(-h_j) \]  \hspace{1cm} (II-2)

where \( m(-h_j) \) is the multiplicity of the \([\overline{hkl}]_j \) reflection according to the definition given in section 2.

A similar definition holds for the \(+h_j\) reflection etc. The constant \( c_j \) (assumed to be equal for the \([hkl]_j \) and the \([\overline{hkl}]_j \) reflections) depends on:
A normalization factor depending on the experiment.

The Lorentz-polarization factor, the Debye-Waller temperature factor and the absorption.

A number of constant factors.

If the case of two or more partially or completely coinciding reflections from two different metallurgical phases is treated, the $c_j$'s may be different for different $j$ values. In the general treatment following, the $c_j$'s are therefore retained.

The definition of $\langle \epsilon(\psi,\phi) \rangle_{-h_j}$ occurring in eq. (5) reads:

$$\langle \epsilon(\psi,\phi) \rangle_{-h_j} = \langle 2\pi P_{-h_j} (\psi,\phi) \rangle^{-1} \int_0^{2\pi} f(\psi,\phi,[\bar{hk}l]_j,\phi_2) \epsilon([hk\bar{l}]_j,\phi_2) d\phi_2$$  \hspace{1cm} \text{(II-3)}$$

where $\epsilon([\bar{hk}l]_j,\phi_2)$ is the single crystallite strain in the direction of $Q$ of those crystallites of which the orientations are determined by $[\bar{hk}l]_j // Q$ and the angle $\phi_2$ about $Q$. A similar definition holds for the $+h_j$ reflection etc. In eq. (6) the symbol $g(-h_j)$ is used for the numerator of eq. (II-3).
Appendix III: Double reflections obtained on two-phase materials.

In this case interplanar lattice spacings exactly equal to one another in both phases, seldom occur. Consider the case of two phases $\alpha$ and $\beta$, exhibiting different volume fractions in the specimen. Assume that the $(h_1 k_1 l_1)_\alpha$ and $(h_2 k_2 l_2)_\beta$ reflections partially overlap. The symbols $(h_1 k_1 l_1)_\alpha$, $(h_2 k_2 l_2)_\alpha$, $(h_1 k_1 l_1)_\beta$, and $(h_2 k_2 l_2)_\beta$ are shortened in what follows to: $h_\alpha$, $-h_\alpha$, $h_\beta$, and $-h_\beta$ or $H_\alpha$, $-H_\alpha$, $H_\beta$, and $-H_\beta$ respectively. Similar to eq. (II-2) it holds:

$$
\int_{2\theta}^{2\theta_0} I_{-h_\alpha} (2\theta) d2\theta = c_\alpha V_\alpha S^2(H_\alpha) m(-h_\alpha) P_{-h_\alpha} \tag{III-1}
$$

$$
\int_{2\theta}^{2\theta_0} I_{h_\beta} (2\theta) d2\theta = c_\beta V_\beta S^2(H_\beta) m(h_\beta) P_{h_\beta} \tag{III-2}
$$

Two similar expressions may be written for the $h_\alpha$ and $-h_\beta$ reflections respectively. The multiplicities are denoted using the symbols $m(-h_\alpha)$ etc. and the volume of material irradiated of both phases is given by $V_\alpha$ and $V_\beta$. The total volume irradiated is taken equal to $V$. The volume-fractions irradiated read: $w_\alpha = V_\alpha / V$ and $w_\beta = V_\beta / V$ subject to:

$$
w_\alpha + w_\beta = 1.
$$

The factors $c_\alpha$ and $c_\beta$ are subject to the same considerations as apply to eq. (II-2). However, they also comprise the squares of the $\alpha$ and $\beta$ unit cell volumes.

For the normal scattering case (or centro-symmetric crystals) the diffraction strain can be written similarly to eq. (8):
\[ \langle \epsilon(\psi, \phi) \rangle_t = N(2\pi D)^{-1} \]  

(III-3)

where:

\[
N = \omega_{\alpha} S^2(H_\alpha) m(h_\alpha) \{ g(-h_\alpha) + g(h_\alpha) \} 
+ \omega_{\beta} S^2(H_\beta) m(h_\beta) \{ g(-h_\beta) + g(h_\beta) \} \tag{III-4a}
\]

\[
D = \omega_{\alpha} S^2(H_\alpha) m(h_\alpha) \{ P_{-h_\alpha}(\psi, \phi) + P_{h_\alpha}(\psi, \phi) \} 
+ \omega_{\beta} S^2(H_\beta) m(h_\beta) \{ P_{-h_\beta}(\psi, \phi) + P_{h_\beta}(\psi, \phi) \} \tag{III-4b}
\]

Defining (cf. eq. (6a)):

\[
Z = 2\omega_{\alpha} S^2(H_\alpha) m(h_\alpha) + 2\omega_{\beta} S^2(H_\beta) m(h_\beta) \tag{III-5}
\]

and:

\[
c_1(\alpha, \beta) = 1/(1 + \frac{\omega_{\beta} S^2(H_\beta) m(h_\beta)}{\omega_{\alpha} S^2(H_\alpha) m(h_\alpha)}) \tag{III-6a}
\]

\[
c_2(\alpha, \beta) = 1 - c_1(\alpha, \beta) \tag{III-6b}
\]

and dividing numerator and denominator of eq. (III-3) by \(Z\) leads to:

\[
P_{\alpha + \beta}(\psi, \phi) = \frac{1}{2} c_1(\alpha, \beta) (P_{-h_\alpha}(\psi, \phi) + P_{h_\alpha}(\psi, \phi))
\]
\begin{align}
+ \frac{1}{2} c_2(\alpha, \beta) (p_{-\beta} (\psi, \phi) + p_{\beta} (\psi, \phi)) \tag{III-7} \\
p_{-\alpha} (\psi, \phi) = (2\pi)^{-1} \int_0^{2\pi} f_{\alpha} (\psi, \phi, [hkl]_{\alpha}, \phi_2) d\phi_2 \tag{III-8a} \\
p_{\beta} (\psi, \phi) = (2\pi)^{-1} \int_0^{2\pi} f_{\beta} (\psi, \phi, [hkl]_{\beta}, \phi_2) d\phi_2 \tag{III-8b}
\end{align}

Two similar expressions can be written for the \(h_\alpha\) and \(-h_\beta\) reflections.

The symbol \(\beta^\alpha_{\alpha+\beta}\) stands for the (normalized in terms of "times random") measured pole-figure intensity in the direction of \(\psi\) of the combined \(\alpha+\beta\) reflection.*

*footnote: It holds that: \(\int (p_{-\alpha} (\psi, \phi) + p_{\alpha} (\psi, \phi)) \sin \psi d\psi d\phi = 4\pi\)

and the same holds for the \(\beta\)-phase reflection. Since \(c_1(\alpha, \beta) + c_2(\alpha, \beta) = 1\) it follows: \(\int \beta^\alpha_{\alpha+\beta} (\psi, \phi) \sin \psi d\psi d\phi = 4\pi\)

which means that \(\beta^\alpha_{\alpha+\beta}\) has been normalized correctly. For the case of a single-phase material \(\alpha = \beta\) it holds that \(c_1(\alpha, \beta) = 1\) and \(c_2(\alpha, \beta) = 0\) and eq. (III-7) reduces to eq. (13).
For the line-shift strain of eq. (III-3) it follows:

\[
<\varepsilon(\psi, \phi)>_t = \\
(4\pi^2 \rho_\alpha \rho_\beta (\psi, \phi))^{-1} \left\{ c_1(\alpha, \beta) \left[ g(-h_\alpha) + g(h_\alpha) \right] \\
+ c_2(\alpha, \beta) \left[ g(-h_\beta) + g(h_\beta) \right] \right\} 
\]

(III-9)

Evidently, this represents the centroid's shift of the combined \(\alpha + \beta\) reflection line-profile.

Since the equations derived apply to a two-phase material, both stresses of the first and the second kind (Macherauch, Wohlfahrt & Wolfstieg, 1973) have to be taken into account. In any case it must be true that the measured line-shift strain is a consequence of the algebraic sum of the stresses of both kinds. Writing \(\sigma_{11}^{I+II, \alpha}\) and \(\sigma_{11}^{I+II, \beta}\) (\(ii = 11\) or \(22\)) for these sums (i.e. \(\sigma_{11}^{I+II} = \sigma_{11}^{I} + \sigma_{11}^{II}\)) and since it also must hold:

\[
\sigma_{11}^{I, \alpha} = \sigma_{11}^{I, \beta} = \sigma_{11}^{I}
\]

(III-10a)

\[
w_\alpha \sigma_{11}^{II, \alpha} + w_\beta \sigma_{11}^{II, \beta} = 0 \quad (ii = 11 \text{ or } 22) 
\]

(III-10b)

(Hauk, 1984; Stuitje, 1985) it follows generally that the actual stresses in \(\alpha\) and \(\beta\) phases are unequal. Only \(\sigma_{11}\) and \(\sigma_{22}\) (and in some cases \(\sigma_{12}\)) can occur as both first and second kind stresses.

Using the symbols \(\sigma_{11}^{\alpha}\) for \(\sigma_{11}^{I+II, \alpha}\) and \(\sigma_{11}^{\beta}\) for \(\sigma_{11}^{I+II, \beta}\) it follows for eq. (III-9):

\[
<\varepsilon(\psi, \phi)>_t = 
\]

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\[ c_1(\alpha, \beta)(s_{11}(h)\sigma_{11}^{\alpha} + \sigma_{22}^{\alpha}) + \frac{1}{2}s_2(h)\sigma_\phi^\alpha\sin^2\psi \beta_\alpha(\psi, \phi)/\beta_{\alpha+\beta}(\psi, \phi) \]

\[ + (2\beta_{\alpha+\beta}(\psi, \phi))^{-1} c_1(\alpha, \beta)((\sigma_{11}^{\alpha} - \sigma_{22}^{\alpha})\sin2\phi\sin\psi) j_1\mu \]

\[ E_j^H(\psi, \phi)F_3(h_\alpha, j, \mu) \]

\[ + \sigma_\phi^\alpha\sin2\psi \ j_1\mu \ D_j^H(\psi, \phi)F_3(h_\alpha, j, \mu) \]

\[-(\sigma_{11}^{\alpha} - \sigma_{22}^{\alpha})\cos2\phi - \sigma_\phi^\alpha\sin^2\psi \ j_1\mu \ B_j^H(\psi, \phi)F_1(h_\alpha, j, \mu) \]

\[-(\sigma_{11}^{\alpha} - \sigma_{22}^{\alpha})\sin2\phi\cos\psi \ j_1\mu \ C_j^H(\psi, \phi)F_1(h_\alpha, j, \mu) \]

(for the $\alpha$-phase contribution) +

\[ c_2(\alpha, \beta)(s_{11}(h)\sigma_{11}^{\beta} + \sigma_{22}^{\beta}) + \frac{1}{2}s_2(h)\sigma_\phi^\beta\sin^2\psi \beta_\beta(\psi, \phi)/\beta_{\alpha+\beta}(\psi, \phi) \]

\[ + (2\beta_{\alpha+\beta}(\psi, \phi))^{-1} c_2(\alpha, \beta)((\sigma_{11}^{\beta} - \sigma_{22}^{\beta})\sin2\phi\sin\psi) j_1\mu \]

\[ E_j^H(\psi, \phi)F_3(h_\beta, j, \mu) \]

\[ + \sigma_\phi^\beta\sin2\psi \ j_1\mu \ D_j^H(\psi, \phi)F_3(h_\beta, j, \mu) \]

\[-(\sigma_{11}^{\beta} - \sigma_{22}^{\beta})\cos2\phi - \sigma_\phi^\beta\sin^2\psi \ j_1\mu \ B_j^H(\psi, \phi)F_1(h_\beta, j, \mu) \]

\[-(\sigma_{11}^{\beta} - \sigma_{22}^{\beta})\sin2\phi\cos\psi \ j_1\mu \ C_j^H(\psi, \phi)F_1(h_\beta, j, \mu) \]

(III-11)

(for the $\beta$-phase contribution).

Note that the functions $B_j^H$, $C_j^H$, $D_j^H$ and $E_j^H$ differ for the $\alpha$ and $\beta$ phase cases. They depend on the $\alpha$ and $\beta$ phase odfs respectively.

Functions $F_1$ and $F_3$ have been defined for all cubic crystal point-groups in Brakman (1987b).
In complete analogy to eq. (13) it holds: \( \beta_\alpha = \frac{1}{2}(p_{-h_\alpha} + p_{h_\alpha}) \)

and \( \beta_\beta = \frac{1}{2}(p_{-h_\beta} + p_{h_\beta}) \). Therefore, if only one phase would be present \( (c_1(\alpha, \beta) = 1; c_2(\alpha, \beta) = 0) \) eq. (III-11) reduces to the one-phase, single-reflection case as given in Table 4 of Brakman (1985b). If no crystallographic texture were present functions \( B_{j \mu}E_{j \mu} \) reduce to zero.

However, eq. (III-11) is not complete, it should be extended with the contributions of the stresses of the second kind \( \sigma_{13} \), \( \sigma_{23} \) and \( \sigma_{33} \) of both phases. These stresses also obey the compensation rule similar to eq. (III-10b):

\[
\omega_{\alpha} \sigma_{13}^{II, \alpha} + \omega_{\beta} \sigma_{13}^{II, \beta} = 0
\]

(III-12)

\((i = 1, 2 \text{ or } 3)\). See: Hauk (1984), Stuitje (1985), Hauk, Oudelhoven & Vaessen (1981).

Eq. (III-11) can be extended for these stresses using Table 4 of Brakman (1985b)*. The expressions are similar to those given in eq. (III-11).

* footnote: In that paper three small errors have persisted in the right-hand (odf) column of Table 3:

coefficients of \( \cos \phi_2 \): the 2nd \( \sin \theta \) should read: \( \cos \theta \).

coefficients of \( \cos 2\phi_2 \): the 1st \( \sin \theta \) should read: \( \cos \theta \).

coefficients of \( \sin 2\phi_2 \): the 2nd \( \sin \theta \) should read: \( \cos \theta \).
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<td>(f(a) = f(c))</td>
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<td>\bar{6}3m</td>
<td>a, b</td>
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<td>(f(a) = f(c))</td>
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6. THE INFLUENCE OF TEXTURE ON THE STRAIN MEASURED BY DIFFRACTION.
The Influence of Texture on the Strain Measured by Diffraction

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Abstract

Strain, as determined by diffraction techniques, is calculated from its constituents. First, the fraction of the crystals that have the proper orientation for diffraction. One degree of freedom is present: the angle of rotation \( \varphi \) about the scattering vector that the diffracting crystals have in common. The proper orientations, expressed in Euler angles, lie on a line ('trace') in orientation space. The density along the trace is asserted to be known as a Fourier series in \( \varphi \). Second, the strain in the diffracting crystals. The simplest possible models are discussed: the Voigt and Reuss approximations. The symmetries of the crystal (m3 or m3m) and of the orientation distribution function (o.d.f.) are taken into account. The dilatation in spacing of the reflecting planes is found as a Fourier series in \( \varphi \) also. Only the zeroth, first and second harmonic (including phase angles: five parameters) play a part. The diffraction strain is the average over the angle \( \varphi \) of the dilatation, weighted with the product of the orientation density and the square of the structure factor. For each contributing trace, the corresponding Fourier coefficients have to be multiplied and added to obtain the diffraction strain. The symmetry of the diffraction pole figure is derived.

1. Introduction

The existence of lattice distortions in polycrystalline (metal) samples is well established by means of diffraction techniques. The interpretation of these strains is still the subject of discussion. More specifically, the question whether these strains can be explained by longer-range internal stresses and the character of the relation between the measured strain and the originating stresses is not yet clear. In this paper the influence of texture in the sample is studied. A very simple model is adopted: the material is supposed to be single phase, the orientation distribution function is known and either the stress (Reuss model) or the strain (Voigt model) is uniform over the irradiated volume.* Even in this model the treatment is elaborate because of the many parameters involved. The measured diffraction strain is a weighted average of the dilatation in spacing of the diffracting set of planes. The average is split into its constituents: the volume fraction of the differently oriented grains that diffract, where the texture plays a part, and the strain in these crystals, where the elastic anisotropy is determining. It is shown that texture leads to the observed 'non-linearities' and 'oscillations' in the plots of \( d_{HKL} \) vs \( \sin^2 \psi \). Comparison with experiments must show whether the texture is responsible for the entire effect or that the other causes mentioned in the literature (Dölle, 1979; James & Cohen, 1980; Hauk, 1984) play a part also.

2. Experimental procedures to measure diffraction strain

The spacing in the set of reflecting planes \((HKL)\) is determined by diffraction techniques. The mono-

* This implies that any effect of prior plastic deformation leading to a correlation between stress or deformation state and orientation of the grain is not considered.

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chromatic incident beam selects for reflection those grains in the specimen that have the proper orientation, i.e. the scattering vector matches the proper reciprocal-lattice vector. The orientation of the scattering vector is determined by the angle \( \varphi \) with respect to the normal to the surface and the angle \( \varphi \) with respect to a specified direction in the surface of the specimen. We return to these definitions in § 3. The diffracted beam can be analysed for three properties:

(i) The intensity, which depends on the volume fraction of the grains with the proper orientation for diffraction. This volume fraction depends on the orientation distribution function (o.d.f.) that describes the texture. For given \( \psi \) and \( \varphi \), all grains that have the direction \([HKL]\) in common contribute to the diffracted intensity. Apparently there is still one degree of freedom in the orientation over which it is integrated: the rotation angle \( \varphi_2^2 \) about the axis \([HKL]\). As pointed out in the Introduction, the o.d.f. is considered to be known. The orientation density as a function of \( \psi \) and \( \varphi \), for given \( HKL \) and integrated over \( \varphi_2^2 \), is the pole figure \( HKL \).

(ii) The direction of the diffracted beam defines an averaged Bragg angle and, with given wavelength, an averaged lattice spacing. In general this spacing is not equal to the equilibrium spacing observed in single crystals. The difference is transformed into a strain (dilatation) \( \epsilon_{out} \). Detailed measurements show that this 'diffraction strain' depends on the angles \( \psi \) and \( \varphi \). In the literature much attention is paid to the relation between this strain and \( \sin^2 \psi \). It is the aim of this paper to calculate this diffraction strain for given stress and texture for the simplest cases: the Voigt and the Reuss model.

(iii) The line width of the diffraction peak is usually much larger than for stress-free single crystals. Even a correction for the small size of the diffracting grains is not sufficient to explain the observed width. In view of the fact that all diffracting grains do not have the same orientation (degree of freedom \( \varphi_2^2 \)), one expects that elastic anisotropy may cause a variation in diffraction strain as a function of \( \varphi_2^2 \). The line width then represents a measure for this variation in diffraction strain. In this paper we do not deal with this aspect, although the treatment given here would allow for such a study.

3. Frames of reference and orientation relations

In textured materials the orientation of a particular grain in the specimen is important. The orientation relation is described by assigning frames of reference and giving the rotation that brings one frame into coincidence with the other. Symmetry implies that more than one choice of frame is possible and leads to equivalences that complicate matters. In this section we deal with these choices and ambiguities.

All frames of reference that are introduced will be right handed, so that two axes suffice to determine the third.

The lab frame is based on the diffraction set up. The scattering vector is the \( z' \) axis. The \( y' \) axis is perpendicular to the plane of incidence. The vector product of the wave vectors of the incident \( (k_i) \) and diffracted \( (k_r) \) beams \((k_i \times k_r)\) points in the positive \( y' \) direction. The \( \varphi \) is indicative of components in the lab frame of reference.

The specimen frame. It is assumed that the specimen is flat: rolled or ground. The \( z \) axis is normal to the flat surface and pointing outwards. The \( x \) axis is parallel to the rolling or grinding direction. In this paper, symmetry in the specimen refers to symmetry in the orientation distribution function (see § 5). Since the orientation is given with right-handed frames only, mirror or inversion symmetry cannot be present in the specimen. In a ground specimen one may expect that a rotation over 180° about the \( y \) axis results in an equivalent orientation. Grinding the top face in one direction is equivalent to grinding the bottom face in the opposite direction. Accordingly, the properties of the ground specimen belong to the monoclinic point group, with a twofold axis parallel to the transverse \((y)\) direction. A rolled specimen may belong to the orthorhombic point group. Both the transverse and the rolling direction are twofold axes, with the result that the surface normal is twofold also. In a ground specimen, two orientations are always equivalent and in a rolled specimen four.

In the crystal frame all components are given in capital letters. Only cubic crystals are considered. The frame of reference coincides with the cube axes. If the crystal structure does not possess an inversion centre, then distinction has to be made between left- and right-handed crystals, which must be treated as different phases, each with its own o.d.f. We avoid this complication by introducing an inversion centre. Two point groups remain: \( m3 \) and \( m3m \). The crystals in \( m3 \) can be represented by one of 12 equivalent right-handed frames of reference (point group 23). For crystals in point group \( m3m \) there are 24 equivalent frames of reference (point group 432).

Now turn to the description of the orientation relation. Consider a fixed direction in space. Its coordinates depend on the frame in which the reference is made:

\[
\text{specimen frame: } r \\
\text{lab frame: } r' \\
\text{crystal frame: } R
\]

The relations between these three can be given by a \( 3 \times 3 \) matrix:

\[
\begin{pmatrix}
-\sin \varphi & \cos \varphi & 0 \\
-\cos \varphi \cos \psi & -\sin \varphi \cos \psi & \sin \psi \\
+\cos \varphi \sin \psi & +\sin \varphi \sin \psi & \cos \psi
\end{pmatrix}
\]

(1)
Only the 'experimental' angles $\phi$ and $\psi$ are involved.

\[
R = \begin{pmatrix}
\alpha_k \cos \varphi_z - \beta_k \sin \varphi_z & \alpha_k \sin \varphi_z + \beta_k \cos \varphi_z & h \\
\alpha_l \cos \varphi_z - \beta_l \sin \varphi_z & \alpha_l \sin \varphi_z + \beta_l \cos \varphi_z & k \\
\alpha_i \cos \varphi_z - \beta_i \sin \varphi_z & \alpha_i \sin \varphi_z + \beta_i \cos \varphi_z & l
\end{pmatrix}
\]  

(2)

In this relation, indices $hkl$ occur: they represent the Miller or Laue indices of the set of reflecting planes, normalized to modulus 1. The angle $\varphi_z$ is the degree of freedom already mentioned in § 2. It distinguishes between the crystal orientations that have the direction $[HKL]$ in common. The relation may seem complicated, but it is chosen in such a way that equivalent orientations of reflecting planes, obtained by permutations and/or changes in sign of the indices $hkl$, lead to equivalent crystal orientations for equal values of $\varphi_z$. The parameters $\alpha_k, \alpha_l, \alpha_i, \beta_k, \beta_l, \beta_i$ follow from one another by cyclic interchange:

\[
\begin{align*}
\alpha_h &= h(1 - h^2 - 2I)/N, & \alpha_k &= k(1 - k^2 - 2I)/N, \\
\alpha_i &= l(1 - l^2 - 2I)/N, & \beta_k &= kl(k^2 - l^2)/N, \\
\beta_l &= lh(l^2 - h^2)/N, & \beta_i &= kk(h^2 - k^2)/N,
\end{align*}
\]

(3)

\[
I = h^2 k^2 + k^2 l^2 + l^2 h^2, \quad N = (I - 4I^2 + 3h^2 k^2 l^2)^{1/2}.
\]

The parameters $I$ and $N$ are invariant in cubic symmetry. For $[HKL]$ equal to $[001], [110]$ and $[111]$, the value of $N$ is zero. In these cases one can make use of the result for $|H| = |K|$:

\[
2h^2 + l^2 = 1, \quad t = h/k/|hk| \text{ (if } h = k = 0; t = 1),
\]

\[
\begin{align*}
\alpha_h &= 1/\sqrt{2}, \alpha_l &= t/\sqrt{2}, \alpha_i &= -h/\sqrt{2}, \\
\beta_h &= -l/\sqrt{2}, \beta_k &= +1/\sqrt{2}, \beta_l &= 0.
\end{align*}
\]

The $3 \times 3$ matrix consists of nine elements, whereas a rotation is characterized by only three independent parameters. Euler angles are more convenient in this respect and in common use to describe texture. We shall follow Bunge (1982) and others in introducing as Euler angles $\alpha, \beta$ and $\gamma$ in this order, with rotations around $Z, X$ and $Y$ respectively. Instead of $\beta$ we introduce $\lambda = \cos \beta$ and still refer to them as Euler angles that represent the crystal orientation with respect to the specimen frame. In symbolic notation:

\[
R = [\alpha \lambda \gamma]R.
\]

(4)

The relations between the Euler angles and the parameters introduced previously, $\psi, \varphi, hkl$ and $\varphi_z$, are

\[
\begin{align*}
\lambda &= l \cos \psi - q_k \sin \psi, \\
(1 - \lambda^2)^{1/2} \cos (\alpha - \varphi) &= \alpha_l \cos \varphi_z - \beta_i \sin \varphi_z, \\
(1 - \lambda^2)^{1/2} \sin (\alpha - \varphi) &= l \sin \psi + q_i \cos \psi, \\
(1 - \lambda^2)^{1/2} \cos \gamma &= k \cos \psi - q_k \sin \psi, \\
(1 - \lambda^2)^{1/2} \sin \gamma &= h \cos \psi - q_h \sin \psi,
\end{align*}
\]

(5)

Table 1. Orientations, in Euler angles, equivalent to $\alpha, \lambda, \gamma$ because of symmetry

The threefold axis in cubic crystals is not included because it does not correspond to a simple transformation.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>$2\varphi = a$</th>
<th>$-\lambda$</th>
<th>$\pi + \gamma$</th>
<th>$\psi$</th>
<th>twofold</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monoclinic</td>
<td>$\pi + \alpha$</td>
<td>$\lambda$</td>
<td>$\lambda$</td>
<td>$\psi$</td>
<td>twofold</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$2\varphi = a$</td>
<td>$-\lambda$</td>
<td>$\pi + \gamma$</td>
<td>$\psi$</td>
<td>twofold</td>
</tr>
<tr>
<td>Crystal</td>
<td>$\pi + \alpha$</td>
<td>$-\lambda$</td>
<td>$\lambda$</td>
<td>$\psi$</td>
<td>twofold</td>
</tr>
<tr>
<td>$m\bar{3}$</td>
<td>$\pi + \alpha$</td>
<td>$-\lambda$</td>
<td>$\lambda$</td>
<td>$\psi$</td>
<td>twofold</td>
</tr>
<tr>
<td>$m3m$</td>
<td>$\pi + \alpha$</td>
<td>$-\lambda$</td>
<td>$\lambda$</td>
<td>$\psi$</td>
<td>twofold</td>
</tr>
</tbody>
</table>

Table 2. Representative traces for cubic symmetry

A: \(-H, K, L, \varphi_z \rightarrow\) Euler angles $\alpha, \lambda, \gamma$

B: \(-K, H, L, \varphi_z \rightarrow\) $\alpha, \lambda, \gamma + \pi/2$

C: \(-H, -K, -L, \pi - \varphi_z \rightarrow\) $2\varphi = a, \alpha, \lambda, \gamma + \pi$

D: \(-K, -H, -L, \pi - \varphi_z \rightarrow\) $2\varphi = a, \alpha, \lambda, \gamma + \pi/2$

with

\[
\begin{align*}
q_k &= \alpha_k \sin \varphi_z + \beta_k \cos \varphi_z, \\
q_i &= \alpha_i \sin \varphi_z + \beta_i \cos \varphi_z.
\end{align*}
\]

(6)

These equations may be used to verify the transformations given in Tables 2 and 4.

4. Symmetry in crystal and specimen

Expressed in Euler angles, the crystal symmetries (except the threefold axis in cubic crystals) and the specimen symmetry are simple transformations. In Table 1 the results relevant for our study are given.

From a diffraction point of view, however, the other description with $\psi, \varphi, hkl, \varphi_z$ is more convenient, because it gives the orientation of the diffracting grains. Since $\varphi_z$ is variable this set of orientations corresponds to a line in orientation space. We refer to such a set of orientations as a 'trace', with $\varphi_z$ as parameter along the trace. In cubic crystals $H^2 + K^2 + L^2$ determines the spacing of the reflecting planes. There are 48 different combinations (permutations and changes in sign) of $HKL$ that contribute to the diffracted intensity. In point group $m\bar{3}$ they can be split into four groups of 12. Within each group all choices are equivalent. For each group a representative trace is chosen (Table 2). Note that in the transformation from $A$ to $C$ or $D$ the value of $\varphi_z$ also changes. In all comparisons between traces such a transformation in $\varphi_z$ must be taken into account (see also Table 4).

In point group $m\bar{3}$ the four traces in Table 2 have to be taken into account when discussing diffraction. But it can be seen immediately that a rotation over 90° about the $Z$ axis transforms $A$ into $B$ and $C$ into $D$. Hence in point group $m\bar{3}$ the traces $A$ and $B$ are equivalent as are $C$ and $D$. Symmetry in the indices of the reflecting planes also leads to
Influence of Texture on Strain Measurement

Table 3. Equivalent traces

<table>
<thead>
<tr>
<th>Crystal</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>m3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>m3m</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HHL</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0KL</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

where \( dV/V \) is the volume fraction of the grains that have an orientation within the interval \( d\alpha \, d\lambda \, d\gamma \) around \( \alpha, \lambda, \gamma \). The factor \( 1/(8\pi^2) \) is a normalizing factor to make the integral of the o.d.f. over all orientations equal to unity. The symmetry of the crystal and specimen must be visible in the o.d.f. The conditions are given in Table 1. Equivalent traces (Tables 2-5) must give the same values as a function of \( \phi_2 \).

6. Stress and strain

To obtain the strain tensor an assumption has to be made concerning the strain in each diffracting crystal. In general, strain and stress in a particular grain are not uniform and do not depend solely on the orientation of the grain. Factors such as grain shape and the orientation with respect to neighbours are important. Since this problem has not been solved and only an o.d.f. is available, we assert that the strain in each grain is uniform and consider two extreme cases for the magnitude of the strain: the Voigt and the Reuss approximation.

In the Voigt model, the strain is equal in all grains. With the strain as a second-rank tensor \( \varepsilon_{ij} \) on specimen axes, straightforward tensor transformation yields the dilatation in the direction \( \phi, \psi \) we are interested in. One finds

\[
\varepsilon_{12} = \cos^2 \phi \sin^2 \psi e_{11} + \sin^2 \phi \sin^2 \psi e_{22} + \cos^2 \phi \cos^2 \psi e_{33} + \sin \phi \sin \psi \sin 2\phi e_{13} + \cos \psi \sin 2\psi e_{13} + \sin 2\psi \sin^2 \phi e_{12}. \tag{8}
\]

The strain measured by the deformation technique yields in this model a result that is the same for every set of reflecting planes and is independent of texture. If the strain has to be translated into a stress field, then the texture will play a part in elastically anisotropic crystals. We do not consider such a transformation.

Another approximation is the Reuss model: all crystals are subject to the same stress. The stress is defined as a second-rank tensor \( \sigma_{ij} \) on specimen axes. To determine the dilatation in the direction \( [HKL] \) of a particular grain, the stresses and the elastic constants of the single crystal \( (s_{11}, s_{12}, s_{44}) \) have to be transformed to the lab frame. Both calculations involve straightforward tensor transformations. Since we consider \( \phi_2 \) and the stress components as independent variables we present the result as follows:

\[
\varepsilon'_{12} = \sum_{k=1}^{6} \{ E_{k0} + s_{0}N(E_{k1} \cos \phi_2 + E_{k2} \sin \phi_2) + s_{0}A[E_{k3} \cos(2\phi_2 - \chi) + E_{k4} \sin(2\phi_2 - \chi)] \}
\]

The contribution of each stress component is given
Table 6. The coefficients $E_{ik}$ in the Fourier series for $\epsilon_{zz}$

<table>
<thead>
<tr>
<th>$i$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>$-2 \sin \phi \cos \theta$</td>
<td>$-2 \sin \phi \cos \theta$</td>
<td>$-\sin \phi \cos \theta$</td>
<td>$-\sin \phi \cos \theta$</td>
</tr>
<tr>
<td>1</td>
<td>$-2 \sin \phi \cos \theta$</td>
<td>$-2 \sin \phi \cos \theta$</td>
<td>$-\sin \phi \cos \theta$</td>
<td>$-\sin \phi \cos \theta$</td>
</tr>
<tr>
<td>2</td>
<td>$0$</td>
<td>$-\sin \phi \cos \theta$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>3</td>
<td>$2 \sin \phi \cos \theta$</td>
<td>$2 \sin \phi \cos \theta$</td>
<td>$2 \sin \phi \cos \theta$</td>
<td>$2 \sin \phi \cos \theta$</td>
</tr>
<tr>
<td>4</td>
<td>$2 \sin \phi \cos \theta$</td>
<td>$2 \sin \phi \cos \theta$</td>
<td>$2 \sin \phi \cos \theta$</td>
<td>$2 \sin \phi \cos \theta$</td>
</tr>
</tbody>
</table>

as a Fourier series in the angle $\varphi_{zz}$. The parameters $N$, $A$, and $\chi$ depend only on $hkl$.

$$s_0 = s_{11} = s_{12} = 2s_{11}$$

$$A \cos \chi = \Gamma^2 - 2h^2k^2l^2(1-3\Gamma^2)/N^2$$

$$A \sin \chi = hkl(h^2-k^2+l^2)+h^2(\Gamma^2-k^2)/N^2$$

(10)

The values of the coefficients $E_{ik}$ are given in Table 6.

The coefficients $E_{00}$ are not shown in Table 6 because they can be found more elegantly in another way. The transformation of $E_{00}$ back to the specimen frame yields a result that is independent of $\psi$ and $\varphi$, an analogous situation to the Voigt model where one strain tensor suffices to describe the diffraction strain.

Furthermore, since the strain tensor is proportional to the stress, this $\varphi_{zz}$-independent part of the strain gives rise to the definition of 'effective' elastic constants, which give the $\varphi_{zz}$-independent part of the strain as a function of stress

$$s_{11} = s_{11} - 2s_0 \Gamma; \quad s_{12} = s_{12} + s_0 \Gamma;$$

$$s_{44} = 2(s_{11} - 3s_{12} - 3s_0 \Gamma).$$

In the literature (Hauk, 1955; Macherauch & Müller, 1961; Dölle & Hauk, 1977; Dölle, 1979; James & Cohen, 1980; Hauk, 1984), $s_{11}$ and $s_{44}$ are referred to as $s_1$ and $\frac{1}{2}s_2$, respectively, the so-called quasi-isotropic diffraction elastic constants.

The symmetry in elasticity is the same for crystals in the classes $m\bar{3}$ and $m\bar{3}m$. Hence, the strain along traces $A$ and $B$ is equal for the same value of $\varphi_{zz}$, and also along the traces $C$ and $D$. But along the traces $A$ and $C$ the strain is different.

7. Diffraction strain pole figure

In the diffraction experiment a weighted average of the single-crystal strains is measured. In general, the weighting has to be done over more than one trace, dependent on the symmetry of the crystal, specimen and strain. The highest number is 4 according to Table 3 but the lowest number depends on the stress present. In general, the strains along the traces $A$ and $C$ are unequal and these two traces have to be taken into account in spite of any symmetry in the crystal or the reflecting plane.

The weighting factor is in essence proportional to the intensity of the beam diffracted by crystals with orientation $\varphi_{zz}^0$. It consists, accordingly, of two parts: a structure-factor part and an o.d.f. part. The diffracted intensity is proportional to the square of the modulus of the structure factor. In general, the structure factor, for given $HKL$, is independent of $\varphi_{zz}$ and may be considered as constant along the trace. For non-equivalent traces the structure factor may be different, with one notable exception: $HKL$ and $-H+K-L$. In crystals with an inversion centre, which we consider here, the structure factors for the traces along $A$ and $C$ (and also along the pair $B, D$) are equal. The o.d.f. part of the weighting factor is proportional to the o.d.f. value. The weighting factor must be normalized by means of a constant factor to make its average along all relevant traces together equal to unity.

The strain along the trace was found as a Fourier series. The integration over the variable $\varphi_{zz}$ can be replaced by a summation, if the o.d.f. values along the trace are also known as a Fourier series. We need to know only the constant (average) and the first and second harmonic, since these occur only in the strain. This means that we have to know of the entire o.d.f. only five Fourier coefficients for each relevant trace.

The o.d.f. is obtained from intensity pole figures for different $HKL$ by a method introduced by Bunge (1982) and expressed as Fourier series in $\alpha$ and $\gamma$ and Jacobi polynomials in $\lambda$. What in fact has to be done is to transform the o.d.f. as found on the specimen frame to the lab frame. The Fourier coefficients that are needed then appear immediately.

To summarize, the procedure to calculate the diffraction strain in a stressed textured material is as follows:

(i) For given crystal and o.d.f. symmetry, determine the number of non-equivalent traces, $t$, for given orientation of the diffraction vector $(\psi, \varphi)$ and given set of reflecting planes $(HKL)$.

(ii) Calculate for the grain with orientation $h, k, l, \psi, \varphi, \varphi_{zz}^0 = \alpha, \lambda, \gamma$:

(a) the dilatation in spacing $e'_{zz}$ (equation 9);
(b) the volume fraction $D$ (§ 5);
(c) the modulus of the structure factor $F$ (§ 7 above).

(iii) Calculate the diffraction strain:

$$e_{zz} = T e'_{zz} DF^2 d\varphi_{zz}^0$$

$$DF^2 d\varphi_{zz}^0$$

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The integrals extend from 0 to 2$\pi$ along the $t$ traces. Since $e'_{zz}$ and $D$ are known as a Fourier series in $\varphi_{zz}$, the integrals can be replaced by a summation:

$$e_{zz} = \sum_{t=1}^{4} \sum_{r=0}^{4} \frac{1}{2}(1+\delta_{r,0})(e'_{zz})_r D_{\upsilon,r} F_r^2 \sum_{s=1}^{4} D_{s,0} F_s^2.$$

(12)

8. Symmetry diffraction strain pole figure

To determine whether the diffraction strain possesses simple symmetries, one has to substitute the
Table 7. Equivalent traces in a stressed specimen

In m3 crystals there exist also sets where A and C are replaced by B and D respectively.

\[ \sigma_1 \sigma_2 \equiv \{ A \text{ Aa} Cb \text{Cc} \} \quad \{ Cb \text{ Ca} Ab \text{ Ac} \} \]

\[ \sigma_3 \equiv \{ A \text{ Aa} Cb \text{Cc} \} \quad \{ Ca \text{ Cb} Ab \text{ Ac} \} \]

\[ \sigma_4 \equiv \{ Aa \text{ Aa} Cb \text{Cc} \} \quad \{ Ab \text{ Ac} Ca \text{ Cb} \} \]

\[ \sigma_5 \equiv \{ Aa \text{ Aa} Cb \text{Cc} \} \quad \{ Ac \text{ Ab} Ca \text{ Cb} \} \]

Table 8. Symmetry in the diffraction strain pole figure

For monoclinic point groups the symmetry axis is given in parentheses.

<table>
<thead>
<tr>
<th>Specimen symmetry</th>
<th>Stresses present</th>
<th>Point group of strain pole figure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monoclinic 2 (y)</td>
<td>( \sigma_1 \sigma_2 \sigma_3 \sigma_4 )</td>
<td>Monoclinic 2/m(y)</td>
</tr>
<tr>
<td>Orthorhombic 222</td>
<td>( \sigma_1 \sigma_2 \sigma_3 \sigma_4 )</td>
<td>Monoclinic 2/m(x)</td>
</tr>
<tr>
<td></td>
<td>( \sigma_1 \sigma_2 \sigma_3 \sigma_4 )</td>
<td>Monoclinic 2/m(y)</td>
</tr>
<tr>
<td></td>
<td>( \sigma_1 \sigma_2 \sigma_3 \sigma_4 )</td>
<td>Orthorhombic mmm</td>
</tr>
</tbody>
</table>

orientation relations given in Table 4 into the equation for the diffraction strain. If the change in orientation of the scattering vector does not lead to a change in the coefficients of \( \sigma_s \), then the orientations are equivalent. The result of such an analysis is given in Table 7.

The trace \( Ai \), also given in Table 4, is for all stress components equivalent to trace C. So, if one considers an experiment where the opposite scattering vector is active, the traces \( Ai \) and \( Ci \) contribute (as well as \( Bi \) and \( Di \) in m3 crystals). But the o.d.f., strain and structure factor along these traces are equal to the values along the traces \( C \) and \( A \) (as well as \( D \) and \( B \) in m3 crystals) for \( \varphi_2 \) values that are \( \pi \) larger. Integration along the relevant traces hence will result in the same diffraction strain for any scattering vector as compared with its opposite. The diffraction strain pole figure shows inversion symmetry. In fact, the only symmetry needed to reach this conclusion is that the structure factors for \( HKL \) and \( -H - K - L \) are equal, so that this conclusion holds for any situation where Friedel's law is valid.

From Table 7 the symmetry in the diffraction strain pole figure can be deduced. Results are given in Table 8.

Absence of '\( \psi \) splitting' indicates that the \( z \) axis possesses twofold symmetry. According to Table 8 this is only the case in orthorhombic specimen symmetry if \( \sigma_x = \sigma_y = 0 \). The presence of \( \psi \) splitting hence indicates either the presence of \( \sigma_z \) and/or \( \sigma_s \) in an orthorhombic specimen or the absence of orthorhombic symmetry in the o.d.f. of the specimen.

A linearity in \( \sin^2 \psi \) vs diffraction strain for given \( \varphi \) is present in the Voigt model and in the \( \phi_2 \)-independent (isotropic) part of the strain in the Reuss model. In textured materials, however, there are, for every trace involved, four other terms that contribute to the diffraction strain, each comprising a stress factor and an o.d.f. factor. The dependence of the stress factor on \( \psi \) is given in Table 6. How the o.d.f. factor depends on \( \psi \) is determined by the texture. No off-hand expectations can be given.

The conclusion must be that in textured materials a linear relation between the diffraction strain and \( \sin^2 \psi \) is not to be expected. According to our analysis (equation 9), all deviations from linearity are proportional to the elastic anisotropy \( s_0 \).

9. Example and concluding remarks

The magnitude of the effect of texture will be illustrated with two examples: cold-rolled steel and cold-rolled copper. The texture of these materials is very different. The main components are (111)[211] and (100)[001], respectively. The o.d.f. data needed in the calculations were derived from experimentally determined o.d.f.s (steel: Brakman, 1985a; copper: Brakman, 1985b). The elastic constants used are \( s_{11} = 7.57 \) (14.93), \( s_{12} = -2.82 \) (6.26) and \( s_{0} = 6.03 \) (14.56) in

Fig. 1. The 112 diffraction strain in cold-rolled steel as a function of \( \sin^2 \psi \). For details see text.

Fig. 2. The 224 diffraction strain in cold-rolled copper as a function of \( \sin^2 \psi \). For details see text.
\(10^{-12} \text{ m}^2 \text{ N}^{-1}\); the data for copper are given in parentheses. The stress was assumed to be uniaxial and parallel to the rolling direction. Angle \(\varphi = 0\). The diffraction strain was calculated for the 112 reflection in steel and the 224 reflection in copper. The results for steel are given in Fig. 1 and for copper in Fig. 2. The straight line gives the results for the texture-free materials; the curves are the results for the actual materials.

Our conclusion is that in practical cases the presence of texture may lead to an amplitude of the oscillations in \(d_{\text{HKL}} \text{ vs } \sin^2 \psi\) that is of the same order of magnitude as the diffraction strain itself.

References


Note added: in eq. (10) of this paper a quantity \(A\) occurs. In fact it stands for an hkl-permutation invariant expression:

\[
A = \left( \Gamma^2 - 3 \ h^2 k^2 l^2 \right)^{\frac{1}{2}}
\]

It is interesting to note that a similar and equivalent expression also occurs as:

\[
F_{33} = \left( F_0 - 3 \omega_1^2 \omega_2^2 \omega_3^2 \right)^{\frac{1}{2}}
\]

7. NON-LINEAR DIFFRACTION STRAIN VS SIN $^2 \Psi$ PHENOMENA IN SPECIMENS EXHIBITING ROLLING-TYPE TEXTURE.
Non-linear Diffraction Strain vs $\sin^2 \psi$ Phenomena in Specimens Exhibiting Rolling-Type Texture

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Abstract
Non-linearities in measured diffraction strains are frequently observed in textured materials. For the case of textured cold-rolled low-carbon steel sheet specimens the diffraction strain is analysed in its constituents: single-crystallite strain and the orientation distribution function of the crystallites. With only macro-stresses $\sigma_1$ and $\sigma_2$ taken into account, a satisfactory explanation of practical measurements on these steel specimens is obtained.

1. Introduction
The ‘$\sin^2 \psi$ method’ (Hauk, 1955; Macherauch & Müller, 1961; Dölle & Hauk, 1977; Dölle, 1979; James & Cohen, 1980; Hauk, 1984; Hauk & Macherauch, 1984) is used to determine (residual) stresses from diffraction data. The measured diffraction line-shift strain often exhibits straight-line behaviour when plotted vs $\sin^2 \psi$. From intercepts and slopes the stresses may be calculated. The symbol $\psi$ stands for the angle between the scattering vector and the specimen's normal direction (ND). The symbol $\phi$ is used for the angle between the projection of the scattering vector on the plane of the specimen and rolling direction (RD).

In textured specimens, significant deviations from linearity frequently occur (Faninger & Hauk, 1976; Hauk, Herlach & Sesemann, 1975; Hauk & Sesemann, 1976; Hauk & Kockelmann, 1977, 1978; Marion & Cohen, 1977; Hauk, Krug & Vaessen, 1981; Dölle & Cohen, 1980; Hauk & Vaessen, 1985; Hauk, Vaessen & Weber, 1985; Maurer, Neff, Scholtes & Macherauch, 1987). These reports concern cold-rolled steel sheets and $\phi = 0$. Small or negligible non-linearities are reported for measurements in the plane $\phi = \pi/2$. Examples are given in Figs. 1 and 2. In all cases the 211 reflection was used.

It is the purpose of this paper to clarify the physical nature of this non-linear diffraction strain behaviour for textured cold-rolled low-carbon steel specimens using the 211 reflection. The specimens are considered to be single phase. The orientation distribution function (o.d.f.) of the crystallites (Bunge, 1982) offers a quantitative description of crystallographic texture. Diffraction strain is an o.d.f.-weighted average of all single crystallite strains of the grains engaged in the diffraction. The o.d.f. depends in an irregular way on $\psi$ and $\phi$. Accordingly, linear diffraction strain behaviour with respect to $\sin^2 \psi$ cannot be expected. It is shown that the behaviour of the o.d.f.'s of cold-rolled steel leads to diffraction strain phenomena measured in practice.

An assumption has to be made concerning the stress state of the specimen. Only principal stresses $\sigma_1$ and $\sigma_2$ are considered. They operate parallel to the rolling
NON-LINEAR DIFFRACTION STRAIN

direction (RD) and transverse direction (TD), respectively. These stresses are taken to be macro-stresses. No use is made of the so-called stresses of the second kind (Macherauch, Wohlfahrt & Wolfstieg, 1973) for the explanation of non-linearity (Hauk, Væssen & Weber, 1985; Maurer et al., 1987). It is shown that crystallographic texture in conjunction with macro-stresses $\sigma_1$ and $\sigma_2$ offers an explanation of cold-rolled steel non-linear diffraction strain phenomena.

2. Theoretical

It has been shown in the previous paper (paper 1) (Penning & Brakman, 1988) that, for the case of $m3m$ crystals in conjunction with the 211 reflection, only one trace in orientation space needs to be considered [i = 1 in equation (12), paper 1]. In what follows only the measurement planes $\varphi = 0$ and $\varphi = \pi/2$ are taken into account.

In paper 1, both single-crystallite strain and the orientation distribution function (o.d.f.) of the crystallites are written as Fourier series with respect to the rotation angle about the scattering vector, $\varphi_z$.

2.1. Single-crystallite strain

The Fourier series of the dilatation in spacing $d_{hkl}$ of a crystallite with [hkl] parallel to the scattering vector only exhibits five terms: equation (9), paper I. The values of $\chi$, $\Gamma$, $A$, $N$ and $E_{1i}$ to $E_{4i}$ can be determined from equations (3) and (10) and Table 6 of paper I, and the $E_{k0}$ are defined (only $\sigma_1$ and $\sigma_2 \neq 0$) by

$$\sum_{k=1}^{2} E_{k0} \sigma_k = s_{12}^{\text{eff}}(hkl)/(\sigma_1 + \sigma_2)$$

$$+ \frac{1}{2} s_{44}^{\text{eff}}(hkl)(\sigma_1 \cos^2\varphi + \sigma_2 \sin^2\varphi) \sin^2\psi,$$

where $s_{12}^{\text{eff}}$ and $s_{44}^{\text{eff}}$ have been defined in paper I.

It can be shown that, for $\varphi = 0$ and $\varphi = \pi/2$, $E_{1i} = E_{3i} = E_{14} = E_{24} = 0$. For the 211 reflection, $\chi = 0$. Consequently, the coefficients of $\cos \varphi_2$ and $\sin 2\varphi_2$ in equation (9), paper I, equal zero. Of the five Fourier coefficients only three remain: $(e_{12}^1, e_{22}^1)$ and $(e_{12}^2, e_{22}^2)$ of equation (12), paper I. They are connected to $\cos 0\varphi_2$, $\sin \varphi_2$ and $\cos 2\varphi_2$, respectively.

In Figs. 3(a), (b) and 4, these Fourier coefficients are given as a function of $\sin^2\psi$ for the case of Fe crystals. Two stress states are considered: $\sigma_1 = -\sigma_2$ and $\sigma_1 = \sigma_2$.

2.2. The orientation distribution function (o.d.f.) of the crystallites

In Table 2 of Brakman (1985b), the Fourier coefficients of the o.d.f. with respect to the angle $\varphi_2$ are given. The relationship between $\varphi_2$ and $\varphi_2'$ of the present paper is given by $\varphi_2' = \varphi_2 + \arg z_i(hkl)$. In the Fourier coefficients the texture-dependent functions

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Fig. 1. Measured 211 relative intensities (upper figures) and 211 diffraction strains (lower figures) as $\sin^2\varphi$ for $\varphi = 0$ (left-hand figures) and $\varphi = \pi/2$ (right-hand figures). Specimen: low-carbon steel reduced 75% by cold rolling. After Döle & Cohen (1989). RD = rolling direction; TD = transverse direction.

Fig. 2. Measured relative intensities (lower figures) and interplanar lattice spacing for angles $\varphi = 0$ (left-hand figures) and $\varphi = \pi/2$ (right-hand figures). 211 reflection used but interplanar lattice spacing converted to (100) spacing. Specimen: low-carbon structural steel reduced 75% by cold rolling. Solid circles: positive $\psi$ angles; open circles: negative $\psi$ angles. Absence of $\psi$ splitting. After Hauk, Væssen & Weber (1985). Diffraction strain 'oscillation' for $\varphi = 0$; approximate straight-line behaviour for $\varphi = \pi/2$ in both Figs. 1 and 2.
$C'_{\psi}(\psi, \varphi)$ and $E'_{\psi}(\psi, \varphi)$ also occur. They are equal to zero for both $\varphi = 0$ and $\varphi = \pi/2$. Their definition and that of arg $z$ is given in equations (11-13), (11-15) and (19-10), respectively, of Brakman (1985b). Rearrangement of the Fourier coefficients with respect to $\varphi_x$ leads to the result that, for the $\varphi$ angles mentioned, the o.d.f.'s Fourier coefficients* connected to $\cos \varphi_x^2$ and $\sin 2\varphi_x^2$ equal zero for the 211 reflection.

Consequently, in equation (12), paper I, only the Fourier coefficients $D_0$, $D_2$, and $D_3$ need to be considered. In Figs. 5(a) and (b), $D_0$, $D_2$, and $D_3$ of the cold-rolled steel texture are depicted vs $\sin^2 \psi$ for $\varphi = 0$ and $\varphi = \pi/2$. It follows that the $\varphi = 0$ o.d.f. Fourier coefficients oscillate more strongly with respect to $\sin^2 \psi$ than the $\varphi = \pi/2$ coefficients do. Note that $D_0$ is equal to the (normalized in terms of 'times random') measured intensity.

* For specimen symmetries lower than orthorhombic this only holds for $\varphi = 0$.

Fig. 3. Fourier coefficients vs $\sin^2 \psi$ of Fe single-crystallite strain for $\varphi = 0$ (a) and $\varphi = \pi/2$ (b), [112] parallel to scattering vector, i.e. the $\psi, \varphi$ direction. Single-crystallite strain Fourier series according to equation (9) of paper I. Stress state assumed: $\sigma_1 = \sigma_2 = 0$, other stresses equal to zero. $\sigma_1$ parallel to rolling direction; $\sigma_2$ parallel to transverse direction of rolled sheet. $\bullet$: zero-order Fourier coefficient; $\times$: coefficient of $\sin \varphi_x^2$; $\Delta$: coefficient of $\cos 2\varphi_x^2$. Fourier coefficients divided by $s_5$ times $\sigma_1$.

Fig. 4. Single-crystallite strain Fourier coefficients vs $\sin^2 \psi$. As Fig. 3 but stress state $\sigma_1 = \pm \sigma_2$. Figure applies to all $\varphi$ angles. The single-crystallite strains and consequently their Fourier coefficients, for two $\varphi$ angles $\pi/2$ rad different from each other, are related by $c_{\psi}(\psi, \varphi, hkl, \varphi_x^2, \eta) = s_{\psi}(\psi, \varphi, hkl, \varphi_x^2, 1/\eta)$, where $\eta = \sigma_2/\sigma_1$.

Fig. 5. Fourier coefficients $D_0$, $D_2$ and $D_3$ vs $\sin^2 \psi$ of the cold-rolled steel o.d.f. for $\varphi = 0$ (a) and $\varphi = \pi/2$ (b), [112] parallel to scattering vector, i.e. the $\psi, \varphi$ direction. O.d.f. coefficients according to equation (12), paper I. $\bullet$: zero-order coefficient $D_0$. $\times$: coefficient $D_2$ of $\sin \varphi_x^2$; $\Delta$: coefficient $D_3$ of $\cos 2\varphi_x^2, \varphi = 0$ coefficients oscillate more strongly vs $\sin^2 \psi$ than the $\varphi = \pi/2$ coefficients. Specimen: low-carbon steel sheet reduced 64% by cold rolling. Details of o.d.f.: Brakman (1985a). $D_0$ equals the pole-figure intensity in the $\psi, \varphi$ direction. Compare $D_0$ with the intensity graphs of Figs. 1 and 2.
3. Results and discussion

A synthesis according to equation (12), paper 1, of single-crystallite strain and o.d.f. Fourier coefficients is given in Figs. 6 and 7. The o.d.f. of the cold-rolled steel specimen used has been given elsewhere (Brakman, 1985a). The two macro-stress states \( \sigma_1 = -\sigma_2 \) and \( \sigma_1 = \sigma_2 \) are dealt with in Fig. 6 and Fig. 7 respectively. All other stress-tensor elements have been taken equal to zero.

The heavy curved lines in the graphs represent the mean diffraction strain according to equation (12), paper 1. The single-crystallite strain distribution with respect to the rotation angle \( \phi \), exhibits a minimum and a maximum. For every orientation of the scattering vector, the extremal crystallite strains are represented by the thin upper and lower curved lines. The diffraction strain is the o.d.f.-weighted average of the single-crystallite strains. Therefore, the diffraction strain curve is always between the extremal strain curves. The straight line represents the texture-free (Reuss model) diffraction strain, i.e. \( \varepsilon_{\text{eq}} \). The single-crystallite strain data were calculated using the Fe compliances: \( s_{11} = 7.57 \), \( s_{12} = -2.82 \) and \( s_{44} = 8.64 \left( 10^{-12} \text{ m}^2 \text{ N}^{-1} \right) \). Both diffraction and single-crystalline strain in Figs. 6 and 7 have been divided by the elastic anisotropy \( S_0 \) times \( \sigma_1 \).

In both Figs. 6 and 7 the \( \varphi = \pi/2 \) diffraction strain graphs exhibit small oscillations with respect to the texture-free straight line as compared with the \( \varphi = 0 \) case. This also holds for other stress states (not shown). Evidently, this is a consequence of the behaviour of the o.d.f. Fourier coefficients as depicted in Fig. 5. The single-crystallite strain Fourier coefficients only have a small influence since they behave smoothly with respect to \( \sin^2 \psi \).

Deformation textures of steel develop almost irrespective of chemical composition and processing.

Fig. 6. Calculated 211 diffraction strain as \( \sin^2 \psi \) for \( \varphi = 0 \) (a) and \( \varphi = \pi/2 \) (b) for stress state \( \sigma_1 = -\sigma_2 \). Heavy curved lines: synthesis of Figs. 3 and 5 according to equation (12), paper I. Straight lines: texture-free diffraction strain. Reuss model of elasticity. All strains divided by \( S_0 \) times \( \sigma_1 \). Thin curved lines: minimal and maximal values of single-crystallite strain distributions with respect to rotation angle about the scattering vector. Diffraction strain as an o.d.f.-weighted average of single-crystallite strains is contained within these extremal strain curves. The vertical distance between the extremal strain curves represents theoretical line breadth. Note that the \( \sigma_1 = -\sigma_2 \) case yields a larger line breadth than found for \( \sigma_1 = +\sigma_2 \).

Fig. 7. As Fig. 6, but 211 diffraction strain as \( \sin^2 \psi \) for \( \varphi = 0 \) (a) and \( \varphi = \pi/2 \) (b) for stress state \( \sigma_1 = +\sigma_2 \). Strains divided by \( S_0 \) times \( \sigma_1 \). The literature (Hauk, Veesen & Weber, 1985; Dölle & Cohen, 1980; Maurer et al., 1987) reports a biaxial compressive stress state after cold rolling of low-carbon steels. On multiplication of (a) and (b) by \( S_0 \) times negative \( \sigma_1 \), a close approximation of Figs. 1 and 2 is obtained. The oscillations are predicted very well. However, the amplitudes are too large. They can be reduced by adopting the Hill (1952) approximation and averaging the Reuss- and Voigt-model results. A fit to practical measurements can be obtained allowing departures from the \( |\sigma_1| = |\sigma_2| \) condition and using the magnitudes of \( \sigma_1 \) and \( \sigma_2 \) as fitting parameters.

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conditions. Therefore, a comparison of Figs. 6 and 7 with the measured diffraction strain data of Figs. 1 and 2 (obtained on similar but not identical steels) is possible.

For cold-rolled steels a compressive biaxial stress state results (Dölle & Cohen, 1980; Hauk, Vaessen & Weber, 1985; Maurer et al., 1987) exhibiting approximately equal $\sigma_1$ and $\sigma_2$ values. Multiplying Fig. 7 by $-1$, it follows that the $\eta = +1$ graphs indeed strongly resemble the measured curves of Figs. 1 and 2. Differences may be due to deviations from $\eta = +1$, different actual magnitudes of $\sigma_1$ and/or $\sigma_2$ and small texture differences.

The essence, however, is that macro-stresses $\sigma_1$ and $\sigma_2$ in conjunction with crystallographic texture qualitatively explain the non-linearities observed. No use has to be made of other stress-tensor elements or the so-called stresses of the second kind (Macherauch et al., 1973).

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8. DIFFRACTION ELASTIC CONSTANTS FOR THE DETERMINATION OF STRESSES IN TEXTURED CUBIC MATERIALS. AN EXPERIMENTAL TEST.
DIFFRACTION ELASTIC CONSTANTS FOR THE DETERMINATION OF STRESSES IN TEXTURED CUBIC MATERIALS. AN EXPERIMENTAL TEST

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Abstract

Previously derived relations between diffraction strains and (residual) stresses in textured materials are tested experimentally. The relations are based on the Volgt and Reuss models for elastic polycrystal coupling; crystallographic texture is incorporated by using the orientation distribution function (ODF). The tests are performed by applying known stresses to cold-rolled specimens mounted in a tensile device on an X-ray diffractometer. The 'Hill average' of the ODF-modified Reuss and Voigt expressions gives an accurate quantitative description of measured diffraction strains. As a consequence, the effect of crystallographic texture can be accounted for in diffraction stress determinations.
1. Introduction

X-ray and neutron diffraction are frequently used for the determination of
stresses. Then, as a function of angles $\psi$ and $\phi$ (see Fig. 1), the strain $\varepsilon(\psi, \phi)$ is
determined from the difference between the lattice spacing $d(\psi, \phi)$
measured in the $\psi, \phi$ direction and the reference spacing $d_0$ determined
from a stress-free specimen. Almost exclusively the so-called $\sin^2\psi$ method
is employed, which is based on the following equation [Klug and Alexander,
1974]:

$$\varepsilon(\psi, \phi) = \frac{d(\psi, \phi) - d_0}{d_0} = s_1(\sigma_{11} + \sigma_{22}) + \frac{1}{2}s_2(\sigma_{11}\cos^2\phi + \sigma_{22}\sin^2\phi)\sin^2\psi$$  \hspace{1cm} (1)

where $\sigma_{11}$ and $\sigma_{22}$ are principal stresses parallel to the specimen surface
and $s_1$ and $\frac{1}{2}s_2$ are the X-ray Elastic Constants (XEC). Many presuppositions
underlie eq. (1), e.g. it is implicitly assumed that in the volume sampled by
the radiation employed the state of stress and strain is independent of
position, which implies $\sigma_{13} = 0$ ($i = 1, 2, 3$) [van Baal, 1983].

In many practical cases a straight line according to eq. (1) fits the
experimental data. A number of cases however is known, where eq. (1) is not
applicable [Dölle, 1979; James and Cohen, 1980; Hauk, 1984]. Certain cases
are well understood and procedures were developed to obtain detailed
information about the stresses in the specimen.

In the case of specimens with preferred orientation of elastically
anisotropic crystallites (crystallographic texture) it is understood why in a
plot of $\varepsilon(\psi, \phi)$ versus $\sin^2\psi$ the data points do not lie on a straight line [Dölle
and Hauk, 1978]. However, in such a case no reliable procedure is available
to obtain the stresses in the specimen.

For specimens without texture, where eq. (1) is valid, the XEC can be
obtained from diffraction strain measurements of specimens with known stresses. Alternatively, the XEC can be obtained to a high degree of accuracy from the single crystal elastic constants by (i) application of Kröner's model for elastic polycrystal coupling [Kröner, 1958, 1967] or (ii) following Hill [1952], by taking the average of the XEC calculated by application of the Reuss [1929] and the Voigt [1928] models for elastic polycrystal coupling.

For specimens with texture the XEC depend on $\psi$ and $\phi$. For cubic materials analytic expressions are available that relate measured strains to stresses, angles $\psi$ and $\phi$ and texture [Brakman, 1983; 1985a; 1987]. The relations are based on the Reuss and Voigt models and the information about the texture is incorporated via the crystallite orientation distribution function (ODF) [Bunge, 1982]. In the next section the theory is summarized.

It is the purpose of this paper to test experimentally the merits of these relations for the determination of stresses in specimens with crystallographic texture. The tests were performed by applying known stresses to steel specimens mounted in a tensile device in situ on an X-ray diffractometer. Precautions were taken to exclude from the experiment any effect in equipment and specimens, except crystallographic texture, that might cause a non-linear $\sin^2\psi$ plot. Non-linear diffraction strain behaviour with respect to $\sin^2\psi$ can also occur as a consequence of the so-called 'plastic anisotropy' [Maurer, Neff, Scholtes and Macherauch, 1987; Hauk, 1984; Marion and Cohen, 1977]. During plastic deformation of a specimen some crystallites may have more difficulty in accommodating the imposed plastic strain than others. After the deformation, such crystallites may exhibit strain-states quite different from those of other crystallites. Non-linear $\sin^2\psi$ plots can be observed then. This phenomenon is excluded from the present experiments; this paper is restricted to the combined influence of crystallographic texture and single crystal elastic anisotropy.

It emerged from the present experiments that for textured cubic
materials a 'Hill average' of ODF-modified Reuss and Voigt expressions (i) describes quantitatively the non-linear $\sin^2\psi$ plots and (ii) allows reliable stress determinations.

2. Summary of theory

When a "macroscopic" stress is imposed on a polycrystalline specimen, differently oriented crystallites will experience different stresses and strains* because of elastic anisotropy. To relate macroscopic stresses and strains to the stresses and strains in the crystallites three models are currently employed: (i) the Reuss [1929] model in which it is assumed that all crystals have the same state of stress, (ii) the Voigt [1928] model in which it is assumed that all crystals have the same state of strain, and (iii) the Kröner [1958, 1967] model in which the concept of "elastic polarization" is introduced to describe elastic polycrystal coupling. Kröner's model yields the most realistic results.

The strain $e(\psi,\phi)$ derived from a diffraction experiment is in fact an average of the strains in the $(\psi,\phi)$ direction present in the diffracting crystals. All diffracting crystals have the normal to the diffracting hkl planes parallel to the $(\psi,\phi)$ direction but they may be rotated with respect to each other over an angle ($\alpha$) around the normal to the diffracting planes. In texture-free specimens the volume fraction of crystallites that contributes to the diffraction at each $\alpha$ is constant, in specimens with texture however it is not. Therefore, in the calculation of average strains and stresses in specimens with texture, the volume fraction of crystallites within a specified

* Stresses in polycrystalline specimens not only lead to diffraction line shifts but also to diffraction line broadening [Sayers, 1984].

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orientation interval has to be introduced as a weighing factor. This can be achieved by incorporation of the so-called series-expansion method for the ODF [Bunge, 1982] in the Reuss and Voigt models [Brakman, 1983, 1985a, 1987]. The Kröner model cannot be employed in explicit form.

The present experiments are carried out in such a way that \( \sigma_{11} \) and \( \sigma_{22} \) are parallel to the specimen surface, that their directions are known (see section 3) and that \( \sigma_{33} = 0 \) in the volume sampled by the X-rays. Then it can be written [Dölle, 1979]:

\[
e(\psi, \phi) = \langle e'_{zz}(\psi, \phi) \rangle = F_{11}(\psi, \phi)\sigma_{11} + F_{22}(\psi, \phi)\sigma_{22} \tag{2}
\]

where \( \langle e'_{zz}(\psi, \phi) \rangle \) is the average strain in the direction \((\psi, \phi)\), i.e. in the direction of the normal to the diffracting hkl planes considered.

For the Reuss model (superscripts "R") it can be derived [Brakman, 1986]:

\[
F_{11}^R(\psi, \phi) = s_1^R + \frac{1}{2} s_2^R \cos^2 \phi \sin^2 \psi +
- \frac{s_0}{2P(\psi, \phi)} \sum_{j \neq \mu} F_j(\psi, \phi) \left[ (\cos 2\phi - \cos^2 \phi \sin^2 \psi) B_j^\parallel(\psi, \phi) + \sin 2\phi \cos \psi C_j^\parallel(\psi, \phi) \right] +
+ \frac{s_0}{2P(\psi, \phi)} \sum_{j \neq \mu} F_3(\psi, \phi) \left[ \cos^2 \phi \sin 2\psi D_j^\parallel(\psi, \phi) + \sin 2\phi \sin \psi E_j^\parallel(\psi, \phi) \right] \tag{3}
\]

where \( s_i^R \) and \( \frac{1}{4} s_2^R \) are the XEC calculated on the basis of the Reuss model for a texture-free specimen [Dölle, 1979] and \( s_0 \) stands for the single crystal elastic anisotropy in terms of compliances: \( s_0 = s_{1111} - s_{1122} - 2s_{1212} \). \( P(\psi, \phi) \) is the ratio of the intensities measured in the \((\psi, \phi)\) direction of the specimen under investigation and of a texture-free specimen (all other conditions being the same). \( F_1 \) and \( F_3 \) depend on h, k, l and B, C, D, E
contain the information about the texture. (Texture-free: B = C = D = E = 0). 

$F_{22}^V$ is obtained from eq. (3) when $s_0$ is replaced by $-s_0$ and in the second term $\cos^2\phi$ is replaced by $\sin^2\phi$ and between the brackets $\cos^2\phi$ is replaced by $-\sin^2\phi$.

For the Voigt model (superscripts "V") it can be derived [Brakman, 1987]:

$$
F_{11}^V(\psi, \phi) = s_1^V + \frac{1}{2} s_2^V \cos^2\phi \sin^2\psi + 
+ c_0 [T_0 + T_1 \sin^2\psi + T_2 \cos^2\phi \sin^2\psi] 
$$ (4)

where $s_1^V$ and $\frac{1}{2} s_2^V$ are the XEC calculated on the basis of the Voigt model for a texture-free specimen [Dölle, 1979], $c_0$ stands for the single crystal elastic anisotropy in terms of stiffnesses: $c_0 = c_{1111} - c_{1122} - 2c_{1212}$.

$T_0$, $T_1$ and $T_2$ contain single-crystal elastic constants and the information about the texture (see appendix I). $F_{22}^V$ is obtained from eq. (4) when $\cos^2\phi$ is replaced by $\sin^2\phi$ and $T_0$, $T_1$ and $T_2$ by $U_0$, $U_1$ and $U_2$, respectively.

$U_0$, $U_1$ and $U_2$ contain single-crystal elastic constants and the information about the texture (see appendix I) (texture-free: $T_0=T_1=T_2=U_0=U_1=U_2=0$).

In the absence of texture, only the terms with $s_1$ and $\frac{1}{2} s_2$ remain in eqs. (3) and (4) and plots of $\varepsilon^R(\psi, \phi)$ and of $\varepsilon^V(\psi, \phi)$ versus $\sin^2\psi$ yield a straight line. With texture however, a plot of $\varepsilon^R(\psi, \phi)$ versus $\sin^2\psi$ does not yield a straight line owing to the factors $P(\psi, \phi)$, $\sin \psi$, $\sin 2\psi$ and $\cos \psi$ in eq. (3), but a plot of $\varepsilon^V(\psi, \phi)$ versus $\sin^2\psi$ still yields a straight line which is shifted (term $c_0 T_0$ in eq. (4)) and has a different slope as compared to the straight line obtained in the absence of texture.

Evidently, for elastically isotropic crystals, i.e. $s_0 = c_0 = 0$, all texture-dependent terms vanish from eqs. (3) and (4).
3. Experimental
3.1. Diffraction strain measurements

Specimens and specimen preparation

In this investigation 1.0 mm thick cold-rolled deep drawing ferritic steel was used (if recrystallized, equivalent to quality FeP04, Euronorm 32). The steel contained: 0.05 wt% C, 0.23 wt% Mn, 0.005 wt% S, 0.010 wt% P and 0.06 wt% Al. The ultimate tensile strength was 628 MPa parallel to the rolling direction and 616 MPa perpendicular to the rolling direction. The hardness was 209 HV10. Optical microscopy showed a single phase structure with a grain size of ASTM 6 in the rolling direction and of ASTM 9 in the transverse direction.

Two tensile specimens, coded R and T, were manufactured; their dimension and orientation with respect to the rolling direction and their annealing treatment are given in Table 1 and Fig. 2. The annealing was carried out in order to annihilate initial macrostresses, macrostress gradients and effects of prior plastic deformation. After the annealing treatments the material was still of single phase structure, the original texture and grain size were retained and only small compressive stresses remained (see Fig. 5). In order to obtain high stresses at the loads feasible, the R specimen was uniformly thinned by alternately grinding both faces of the specimen.

Preparation of the investigated face of the specimens was performed as follows. The specimens were bonded onto a glass plate and hand-ground using waterproof grinding paper of grades 240, 320, 400 and 600. Subsequently they were hand-polished using diamond polishing compound of grades 6, 3, 1 and 1/4 μm. Between two successive polishing stages an intermediate etching with 1% nital was applied. After the final polishing
treatment an etching with 0.5% nital was performed. It was verified experimentally that the surface preparations of the specimens did not introduce plastic deformation or changes in texture.

*Equipment and procedures*

In situ strain measurements were performed using a diffractometer equipped with a tensile device. This device was constructed for a maximum load of 4.9 kN (cf. Fig. 2). The load was applied to the specimen via needle bearings to avoid bending strains.

Calibration of the built-in load cell (Entran Devices, ELF-c1000-100) was achieved as follows:

A tensile specimen with a Wheatstone bridge (strain gauges HBM6/120 LY-11) cemented onto the surface, was mounted in series connection with a force calibrating device (Mohr & Federhaff AG, nr. 866, 20kN) in a standard tensile machine. Hinge-joints were used to prevent bending couples. The output of the Wheatstone bridge was recorded as a function of the applied load. By putting the same specimen in the tensile device for the diffractometer, the load cell was calibrated via the Wheatstone bridge output (accuracy of stresses better than 3%).

The alignment of the tensile device on the diffractometer was achieved as follows. First the diffractometer with the standard specimen holder was well aligned. Then, the tensile device was mounted on the diffractometer; its correct $\omega=0^\circ$ setting was performed in an optical way (accuracy $\pm 0.1^\circ$). In order to determine the specimen displacement (i.e. the distance between specimen surface and diffractometer axis) a 5$\mu$m layer of silicon powder (NBS SRM 640-a) was pasted onto the surface of the tensile specimen. From the deviation of the correct $2\theta$-position of the Si 220-reflection (as determined with the standard specimen holder), the specimen
displacement was calculated (Wilson, 1963) and subsequently cancelled with
the aid of a micrometer on the tensile device (Fig. 2). The correction for
specimen displacement was performed after each change in loading
conditions [accuracy $\pm 5\mu m$].

The strain measurements were performed on a Siemens type F
diffactometer; the axis for the $\psi$-tilt was perpendicular to the
diffactometer plane ($\omega$-axis). The diffactometer was equipped with a
diffracted beam graphite monochromator and CrK$\alpha$-radiation was used. The
ferrite 211 reflection ($2\theta \approx 156^\circ$) was measured with a stepsize of 0.05$^\circ$$\theta$.
The divergence of the incident beam was chosen small ($0.8^\circ$) to minimize
defocusing. The irradiated area on the specimen surface was about 18x3
mm$^2$. The effective penetration depth was 4$\mu$m. To achieve good counting
statistics, at least 3000 net counts at the top of the reflection were
measured. For background determination, large portions of the tails of the
reflection were recorded. The ambient temperature was continuously
recorded; changes did not exceed 1$^\circ$C. Reproducibility, including
remounting the specimen and reapplying the load, was checked: the
differences in peak positions did not exceed 0.005$^\circ$$\theta$ (see below).

Data evaluation

The measured line profiles were corrected for background (linear),
LP-factor (Delhez, Mittemeijer, Keijser and Rozendaal, 1977), absorption
and K$\alpha_2$-component (Delhez and Mittemeijer, 1975). The peak position of
the profile was determined by a parabola fit to the datapoints with intensities
above 75% of the peak intensity. The lattice spacings $d(\psi,\phi)$ were calculated
for a reference temperature of 25$^\circ$C. The error in peak position was about
0.005$^\circ$$\theta$, which corresponds to an error in the 211 lattice spacing of
$1 \times 10^{-6}$ nm. Apart from the peak-position of the line profile, also the integral line-breadth and the integral intensity (corrected for absorption and $\psi$-dependency) were determined.

As the applied loads were in the elastic region of the stress-strain curve of the material, the linear superposition principle of stresses and of strains can be applied: subtracting the measured strains and applied stresses for two loads from each other leads to a $\sin^2\psi$ plot that corresponds to a homogeneous purely uniaxial stress. This method has the advantage of eliminating effects due to instrumental aberrations (defocusing and alignment errors) and originally present stress/strain gradients. Above all, a very accurate strain-free lattice spacing value $d_0$ needs not to be known, as follows directly from eq. (1):

$$
\epsilon_\Delta(\psi, \phi) = \epsilon_p(\psi, \phi) - \epsilon_q(\psi, \phi) = \frac{d_p(\psi, \phi) - d_q(\psi, \phi)}{d_0}
$$

where the subscripts $p$ and $q$ apply to the data obtained from the experiments with loads $p$ and $q$. Since $d_0$ now occurs only in the denominator, an uncertainty in its absolute value leads to a negligible error in $\epsilon_\Delta(\psi, \phi)$. For the strain-free material of the present investigation $d_0$ was measured to be $0.117028$ nm at $25^\circ C$.

Since the specimens originated from coiled material, they showed a slight curvature. The thin specimen (R) was stretched completely at the minimum applied load, but this was not the case with the thick specimen (T). Although the curvature was found to be small a correction to the stress was carried out (see appendix II). Changes in the specimen position caused by the stretching were eliminated by use of the Si 220 reflection (see above).
3.2. Texture measurements

Specimens

A composite sample technique [Meieran, 1962; Leber, 1965; Elias and Heckler, 1967] has been employed. The composite specimen surface normal exhibited three equal angles of \( \text{arccos} \left( \frac{1}{\sqrt{3}} \right) \) with respect to RD, TD and ND respectively. The specimen consisted of a number of stacked sheet samples enclosed in a resin-bonded steel frame, which was machined such that it fitted directly in the specimen holder of the texture goniometer. The examined surface was given the same preparation treatment as described in section 3.1.

Equipment and procedure

Measurements were performed on a Siemens Lücke-type texture goniometer in the Schulz reflection geometry [Schulz, 1949]. The use of an energy dispersive Si(Li)-detector assured pole figures measured with almost purely monochromatic radiation (MoK\textsubscript{\alpha}).

The 110, 200, 211 and 222 pole figures were determined. The inclination of the specimen normal with respect to the plane of diffraction ranged from 5/6° to 54 \( \frac{5}{2} \)° with intervals of 5/3°. The increment of rotation about the specimen normal was 2 degrees, with a counting time per increment of 4 seconds. Hence, the complete spherical triangle defined by RD, TD and ND (Fig. 1) was covered.

For the centre of the pole figures measured, backgrounds were measured on both sides of the reflection at a distance of 1.5 \( \theta \) from the top position. The mean value was used for background correction. Defocusing correction was performed by using a texture-free sputtered Au-layer of effectively
infinite thickness. From the corrected, integrated intensities of the pole figures the even order ODF series expansion coefficients were calculated using a truncation of the series at \( l_{\text{max}} = 22 \) [Bunge, 1982]. The detailed ODF of the material investigated is given elsewhere [Brakman, 1985b].

For the 211 reflection used in the present strain measurements, the pole figure as calculated from the ODF is shown in Fig. 3; sections for \( \phi = 0 \) and \( \phi = \pi/2 \) are shown in Figs. 4a and 4b. The solid lines in Figs. 4a and 4b, obtained from the ODF, correspond to intensities averaged over the cross section of the steel sheet (because of the composite sample technique used). The dashed lines in Figs. 4a and 4b represent intensities measured directly from the steel sheet and stem therefore from the surface region of the sheet. Because the solid- and dashed lines agree very well, it is concluded that there is no texture gradient in the sheet.

4. Results and discussion

The R and T specimens were subjected to stresses as given in Table 1. In Fig. 5 measured 211 lattice spacings of the R specimen are plotted versus \( \sin^2 \psi \). Three facts are clearly displayed:

(i) the +12 MPa curve shows a weak oscillation; on the average the slope is slightly negative (experiments with a strain-free specimen show that this negative slope is not due to instrumental aberrations). This indicates that in the unloaded specimen a small compressive residual stress is present despite the annealing (see Table 1). Evidently, an external stress of +12 MPa was not enough to cancel the small residual compressive stress completely.

(ii) the +448 MPa curve clearly depicts an oscillation, on the average the slope of the curve is positive. The oscillation is quite similar to the one reported by Faninger and Hauk [1976] for a cold-rolled structural steel
under an external tensile load. The same type of oscillation, but with reversed curvature, is frequently reported in the literature for cold-rolled low-carbon steels with compressive residual stresses [Dölle and Cohen, 1980; Marion and Cohen, 1977; Hauk, Krug and Vaessen, 1981; Hauk, Vaessen and Weber, 1985 and Maurer et al., 1987]. This is understandable since the texture of these cold-rolled steels is comparable to the texture of the specimens of the present investigation.

(iii) the +12 MPa and +448 MPa curves exhibit an opposite behavior, i.e. the oscillation is observed to reverse when the stress changes from compressive to tensile. This was also observed by Marion and Cohen [1977, Fig. 4]. This opposite behavior follows directly from eq. (2).

As already argued in section 3, the study of differences of measured strains in relation to differences of the corresponding applied stresses should be preferred over a direct study of measured strains in relation to the applied stress:

\[ \frac{\varepsilon_\Delta}{\sigma_\Delta} = \frac{\varepsilon_p - \varepsilon_q}{\sigma_p - \sigma_q} \]  

(6)

where \( p \) and \( q \) apply to the data obtained from the experiments with loads \( p \) and \( q \). \( \varepsilon_\Delta \) and \( \sigma_\Delta \) correspond to purely uniaxial loading. The orientation of the specimen (either \( R \) or \( T \), see Table 1) determines whether the applied stress difference \( \sigma_\Delta \) is either of \( \sigma_{11} \) or \( \sigma_{22} \) type (For both \( R \) and \( T \) specimens measurements were performed for \( \phi = 0 \) and \( \phi = \pi/2 \), see Table 2). The quotient \( \varepsilon_\Delta/\sigma_\Delta \) has the dimension of a compliance and corresponds, in the present experiments, to the diffraction elastic constant \( F_{11} \) or \( F_{22} \) [see eq. (2)].
The experimental $\varepsilon_\Delta/\sigma_\Delta$ obtained for three $\sigma_\Delta$ are shown in Figs. 6 and 7, together with the texture-dependent $F_{11}^R$, $F_{22}^R$ and $F_{11}^V$, $F_{22}^V$ calculated according to eqs. (3) and (4), respectively. At each $(\psi, \phi)$ the data obtained for the three different $\sigma_\Delta$ coincide within the experimental error, which is in accordance with the linear superposition principle of strains and stresses. The Reuss- and Voigt-model based $F_{11}$ and $F_{22}$ do not fit to the experimental data. However, the Reuss-model based $F_{11}$ and $F_{22}$ show oscillations which compare fairly well to the experimental $\varepsilon_\Delta/\sigma_\Delta$. Figs. 6 and 7 strongly indicate that also in the case of specimens with texture the suggestion by Hill [1952] can be followed [i.e. $F^H = (F^R + F^V)/2$]. This is substantiated in Figs. 8 and 9: only small deviations between theory and experiment occur. Undoubtedly, errors in the ODF determination contribute to these deviations.

The present experimental data may also serve to estimate the accuracy with which stresses in textured specimens can be obtained on the basis indicated above. The results of least-squares fits of the right-hand side of eq. (2), with $F=F^H$, to the experimental $\varepsilon_\Delta$ at each $\phi$ are gathered in Table 3. Systematic errors in $\sigma_{11}$ and $\sigma_{22}$ occur. But still the deviations are of the same order of magnitude as normally encountered in stress measurements on texture-free materials.

It is concluded that the effect of crystallographic texture on diffraction elastic constants can be obtained by taking the average of the Reuss- and Voigt-based $F_{11}$ and $F_{22}$ according to eqs. (3) and (4), respectively.

Textures of cold-rolled low-carbon steels are almost independent of composition and processing variables. Therefore, the present results could apply to the case of other cold-rolled steel specimens. Then, either the present Hill-approximated or the measured diffraction elastic constants (Figs. 8 and 9) could be employed.
5. Conclusion

The effect of crystallographic texture can be accounted for in diffraction stress determination. It has been experimentally verified for a cold-rolled steel that texture modified Reuss- and Voigt-model expressions, averaged according to the Hill approximation, yield a quantitative description of diffraction elastic constants.

Acknowledgements

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Appendix I

Coefficients $T_0$, $T_1$ and $T_2$ used in eq. (4)

For the rolling-type texture of the specimens investigated the coefficients $T_0$, $T_1$ and $T_2$ are obtained from appendix B and eq. (19) of Brakman [1987]:

$$T_0 = \frac{1}{15D\sqrt{21(c_{1212} + \frac{4}{3}c_0)}} \left\{ \left( c_{1212} + \frac{4}{3}c_0 \right) (2C_4^{11} - C_4^{12}/5) + \right.$$  

$$+ \frac{c_0}{30\sqrt{21}} \left( 2|C_4^{11}|^2 - 5|C_4^{12}|^2 + 2C_4^{11}C_4^{13}/35 \right) \right\}$$  

$$T_1 = \frac{1}{30D\sqrt{21}} \left\{ -5C_4^{11} + 2C_4^{12}/5 + C_4^{13}/35 \right\}$$  

$$T_2 = -\frac{1}{15D\sqrt{21}(c_{1212} + \frac{4}{3}c_0)} \left\{ \left( c_{1212} + \frac{4}{3}c_0 \right) (C_4^{11} - C_4^{12}/5 + C_4^{13}/35) + \right.$$  

$$+ \frac{c_0}{10\sqrt{21}} \left( 2|C_4^{11}|^2 - 5|C_4^{12}|^2 + 2C_4^{11}C_4^{13}/35 \right) \right\}$$

where
\[ D = 4\left(c_{1212} + \frac{1}{3} c_0\right)^2 + \frac{2c_0}{15\sqrt{3}}\left(c_{1212} + \frac{1}{3}c_0\right)(C_4^{11}\sqrt{7} + C_4^{13}\sqrt{5}) + \]
\[ + \frac{c_0^2}{1575} \left(2[C_4^{11}]^2 - 5[C_4^{12}]^2 + 2C_4^{11}C_4^{13}\sqrt{35}\right) \]

The \( C_4 \) are the 4th order series-expansion coefficients of the ODF.

\( U_0, U_1 \) and \( U_2 \) are obtained from \( T_0, T_1 \) and \( T_2 \) respectively, by replacing \( C_4^{12} \) by \(-C_4^{12}\).
Appendix II

Stresses induced by stretching a curved specimen

When a curved specimen is stretched, the tensile stress is not uniform over the cross-section. The stress distribution is determined in this appendix.

The specimen has a width w, thickness t and length 2L. The area of the cross-section is equal to $S = wt$. The specimen is assumed to be curved as a cylinder with a large radius $R_0$ ( $> > L$ ). The cylinder-axis is perpendicular to the X- and Z-axes, see Fig. 10. The centre of the cross-section is indicated by the coordinates $x, z$. In the force-free situation:

$$x = \frac{(L^2 - z^2)}{2R_0} \quad \text{(II.1)}$$

When a force $F$ is applied at the ends $z = \pm L$, an average stress $F/S$ is introduced. But there is also a bending moment of magnitude $Fx$ working in each cross-section. This results in stresses of the same character as the average stress $(\sigma_{zz})$, however they vary linearly from compressive in the top-layer to tensile in the bottom-layer. The maximum absolute value of these stresses is easily shown to be $6Fx/wt^2$. Hence the maximum tensile stress is not equal to $F/S$, but

$$\sigma_{zz} = (1 \pm 6x/t) \frac{F}{S} \quad \text{(II.2)}$$

where the "-" sign holds for the top-layer and the "+" sign for the bottom-layer, see Fig. 10.

Next the dependence of $x$ on $F$ has to be determined. The bending moment $Fx$ leads to an additional curvature of the specimen, equal to $-Fx/EI$, where $E$
is Young’s modulus and $I=\frac{wt^3}{12}$. Since we are dealing here with a
correction, it is not relevant which $E$ is chosen, the anisotropic one or an
average one. This leads to the differential equation for the shape of the
specimen:

$$\text{total curvature } = -\frac{d^2x}{dz^2} = \frac{1}{R_0} - \frac{Fx}{EI} \quad (\text{II.3})$$

The boundary condition reads $x=0$ for $z = \pm L$. It is convenient to introduce a
dimensionless quantity $u$, as a measure for the applied force:

$$u = \frac{L\sqrt{F/EI}}{} \quad (\text{II.4})$$

The solution now reads:

$$x = L^2 \left[ 1 - \frac{\cosh(uz/L)}{\cosh(u)} \right] / u^2 R_0 \quad (\text{II.5})$$

For a given $F$ the value of $x$ at the location of measurement ($z=0$) can be
calculated by use of eqs. (II.4) and (II.5). The total stress follows then from
eq. (II.2).
Table 1. Tensile specimens and applied loads.

The annealing was carried out in 94 vol.% N₂ + 6 vol.% H₂. The longitudinal axis and applied loads of specimens R and T are parallel and perpendicular to the rolling direction, respectively, i.e. parallel to RD and TD as indicated in Fig. 1. The stress values have been corrected for specimen curvature; see below eq. (5) and appendix II.

<table>
<thead>
<tr>
<th>specimen code</th>
<th>annealing treatment</th>
<th>specimen thickness (mm)</th>
<th>applied stresses (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>100 h 673 K</td>
<td>0.35</td>
<td>//RD : 12 ; 224 ; 448</td>
</tr>
<tr>
<td>T</td>
<td>10 h 723 K</td>
<td>0.84</td>
<td>⊥ RD : 4 ; 102 ; 231</td>
</tr>
</tbody>
</table>
Table 2. $\sigma_\Delta$ and $\varepsilon_\Delta/\sigma_\Delta$ in the present experiments.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Type of $\sigma_\Delta$</th>
<th>Type of $\varepsilon_\Delta/\sigma_\Delta$</th>
<th>Fig.</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>$\sigma_{11}$</td>
<td>$F_{11}(\psi,0)$</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$F_{11}(\psi,\pi/2)$</td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>$\sigma_{22}$</td>
<td>$F_{22}(\psi,\pi/2)$</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$F_{22}(\psi,0)$</td>
<td></td>
</tr>
</tbody>
</table>
Table 3. Stresses $\sigma_{11}$ and $\sigma_{22}$ obtained from a least-squares fit of the right-hand side of eq. (2) to the experimental $\varepsilon_\Delta$ at each $\phi$. In eq. (2) the $F$'s were taken as $F = F^H = (F^R + F^V)/2$ and $F^R$ and $F^V$ were calculated according to eqs. (3) and (4) respectively.

<table>
<thead>
<tr>
<th>Specimen R</th>
<th>Specimen T</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_\Delta$ (MPa)</td>
<td>$\sigma_\Delta$ (MPa)</td>
</tr>
<tr>
<td>$\sigma_{11}$</td>
<td>436</td>
</tr>
<tr>
<td>$\sigma_{22}$</td>
<td>--</td>
</tr>
<tr>
<td>$\sigma_{11}$</td>
<td>224</td>
</tr>
<tr>
<td>$\sigma_{22}$</td>
<td>--</td>
</tr>
<tr>
<td>$\sigma_{11}$</td>
<td>212</td>
</tr>
<tr>
<td>$\sigma_{22}$</td>
<td>--</td>
</tr>
</tbody>
</table>
Figure captions

Fig. 1. Definition of axes and angles used in this investigation
   RD = rolling direction
   TD = transverse direction
   ND = normal direction.

Fig. 2. Tensile device and tensile specimen for in situ measurements on the
diffractometer.

Fig. 3. 211 pole-figure of the material investigated as calculated from the
ODF. P is the ratio of the intensities determined from a textured and
a texture-free specimen, see below eq. (3).

Fig. 4. Normalized 211 intensities P vs. sin²ψ for $\phi = 0$ (Fig. 4a) and $\phi = \pi/2$
(Fig. 4b).
   Solid lines: calculated from the ODF as obtained by use of the
   composite sample. Dashed lines: measured directly from the steel
   sheet. The calculated and measured intensities have been set equal at
   $\psi = 0$.

Fig. 5. Measured 211 lattice spacings vs. sin²ψ of the R specimen for the
measurement plane and loads as indicated.

Fig. 6. Experimental $\varepsilon_{\Delta}/\sigma_{\Delta}$ (cf. eq. (6)) and calculated $F_{11}$ vs. sin²ψ of the R
specimen for the measurement planes and $\sigma_{\Delta}$ as indicated.

Fig. 7. Experimental $\varepsilon_{\Delta}/\sigma_{\Delta}$ (cf. eq. (6)) and calculated $F_{22}$ vs. sin²ψ of the T
specimen for the measurement planes and $\sigma_{\Delta}$ as indicated.
Fig. 8. Averaged experimental $\epsilon_\Delta/\sigma_\Delta$ (cf. eq. (6)) and calculated $F_{11}$ (according to the Hill approximation) vs. $\sin^2\psi$ of the R specimen, for the measurement planes as indicated.

Fig. 9. Averaged experimental $\epsilon_\Delta/\sigma_\Delta$ (cf. eq. (6)) and calculated $F_{22}$ (according to the Hill approximation) vs. $\sin^2\psi$ of the T specimen, for the measurement planes as indicated.

Fig. 10. Schematic drawing of curved specimen of length $2L$ under tensile load $F$ applied at $z = \pm L$. For the unloaded specimen ($F=0$) the radius of curvature equals $R_0$ and $x(z=0) = a_0$. 

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Fig. 1
Fig. 2

- needle bearings
- mirror for setting Θ/2Θ (ω=0)
- housing for gear-mechanism and load cell
- synchronous motor
- θ angle setting
- precision slide
- specimen-displacement correction
- base for mounting on diffractometer

Dimensions:
- 103mm
- 25mm

tensile specimen
Fig. 3
Fig. 4
Fig. 8
Fig. 9
SUMMARY

This thesis constitutes a contribution to the field of stress-determination in textured materials using diffraction methods. The purpose of the so-called $\sin^2 \psi$-method is the determination of unknown macro-stresses from measured diffraction strain data. (Definition of angle $\psi$: Fig. 1, 'Introduction'). Macro-stresses are assumed to be constant over distances large compared to the grain size. In many cases diffraction strain when plotted vs. $\sin^2 \psi$ exhibits straight-line behaviour. In those cases intercepts and slopes yield the stresses. In this thesis a general treatment of non-linear diffraction strain vs. $\sin^2 \psi$ behaviour is given.

In the case of materials exhibiting crystallographic texture, non-linear behaviour occurs quite often. Problems are then to explain the non-linearity and the determination of the stresses. Many causes of non-linearity may occur simultaneously.

This treatment only deals with the influence of crystallographic texture in conjunction with single crystal elastic anisotropy. Only the influence of macro-stresses is taken into account. For the quantitative description of crystallographic texture, use is made of the orientation distribution function (odf) concept. The material mainly studied is cold-rolled low-carbon steel. This material exhibits a strong development of both crystallographic texture and residual stresses.

Chapter 1 gives a general introduction.

Chapters 2 and 3 give mathematical expressions for diffraction strains of textured cubic materials for the Reuss (constant stress) and Voigt (constant strain) elasticity models, respectively. Orthorhombic and monoclinic specimen symmetries are dealt with. In the equations the series-expansion coefficients of the odf arise. In the case of the Voigt model the series truncates after the 4th order coefficients. The Voigt model predicts straight-line behaviour vs. $\sin^2 \psi$ even for textured specimens.
In Chapter 4, general expressions are derived for both diffraction strain and diffraction intensity pole-figures of textured materials for all cubic point-groups. Both normal and anomalous scattering are considered. It is shown that the 'ghost-phenomena' occurring in the analysis of intensity pole-figures do not occur in the diffraction strain pole-figure case. From the general expressions, a new type of surface spherical harmonic emerges.

Chapter 5 yields a general treatment of coinciding multiple reflections applied to residual (macro-) stress determination in textured cubic materials. Special attention is given to the \( (651 + 732) \) bcc double reflection. This reflection has been claimed by other researchers to exhibit linear vs. \( \sin^2 \gamma \) diffraction strain behaviour. Their experiments concerned the same type of material exhibiting the same type of texture as studied in this thesis.

In Chapter 6 a more general treatment of diffraction strain of textured materials is given in terms of simple physical concepts not using the series-expansion coefficients of the odf. Instead, it is assumed that the odf is known in some unspecified form. The elastic strain of the single crystallites contributing to the diffraction and the odf are written as two 5-term Fourier-series with respect to the rotation angle about the scattering vector. Diffraction strain is an average of single crystal strains. The odf occurs as a weight function in the mean value which is obtained by averaging the product of the odf and the single crystal strain. General expressions are given involving the Fourier coefficients and structure-factor squares for all cubic point-groups.

Chapter 7 constitutes an illustration of the results of Chapter 6. The analysis is applied to textured sheet steel specimens. A comparison is made with experimental results of other researchers obtained on similar materials is. It is concluded that crystallographic texture in conjunction with elastic anisotropy qualitatively explains diffraction strain phenomena observed on these materials. For this conclusion only a biaxial macro-stress state is assumed. No so-called stresses of the 2nd kind (constant over distances in the order of the grain size) are necessary for the explanation.
Chapter 8 is devoted to a practical test of the methods proposed in the preceding chapters. Experiments are described using an in-situ tensile test device on the diffractometer. It is shown that calculated and measured diffraction elastic constants of a textured cold-rolled steel specimen coincide within the experimental error. In the calculation the Hill approximation is used which represents the arithmetic mean of the Reuss and Voigt model predictions. There is no physical justification for the Hill approximation. However, its application allows determination of unknown macro-stresses in these textured materials from diffraction strain data. A curve-fitting technique can be used with the stresses as fitting parameters.
SAMENVATTING

Deze dissertatie vormt een bijdrage tot het vakgebied van de spanningsbepaling via diffractietechnieken aan getextureerde materialen. Het doel van de daarbinnen toegepaste, zogenaamde $2\psi$-methode is de bepaling van onbekende macro-spanningen uit gemeten diffractierekken (definitie van hoek $\psi$ : Fig. 1 van 'introduction'). Van macro-spanningen wordt aangenomen dat ze constant zijn over afstanden die groot zijn ten opzichte van de kristal-afmetingen. In veel gevallen vertoont de gemeten diffractierek een lineair gedrag met betrekking tot $\sin^2 \psi$. In die gevallen kunnen uit de hellingen en de afgesneden stukken van de coördinaat-assen van een dergelijke rechte de spanningen bepaald worden.

In deze dissertatie wordt een algemene verhandeling gegeven over niet-lineair diffractierek-gedrag met betrekking tot $\sin^2 \psi$.

Als materialen kristallografische textuur vertonen, wordt vaak niet-lineair gedrag van de diffractierek versus $\sin^2 \psi$ waargenomen. Het probleem is dan de verschijnselen te verklaren en toch de spanningen te bepalen. Voor die niet-lineariteit kunnen verschillende oorzaken naast elkaar voorkomen.

In deze dissertatie wordt alleen de invloed behandeld van kristallografische textuur in samenhang met de elastische anisotropie van de kristallen waaruit het preparaat is opgebouwd. Er wordt aangenomen dat alleen macro-spanningen optreden in het preparaat. Voor de kwantitatieve beschrijving van de textuur wordt gebruik gemaakt van het orientatie distributie concept (ODF) concept. Als materiaal is hoofdzakelijk koud-gewalst laagkoolstof-staal voorwerp van onderzoek geweest. Dit vertoont een stevige ontwikkeling van zowel textuur als inwendige spanning.

Hoofdstuk 1 geeft een algemene inleiding.
In Hoofdstukken 2 en 3 worden wiskundige uitdrukkingen gegeven voor diffractierekken van getextureerde kubische materialen voor de Reuss (constante spanning) en Voigt (constante rek) elasticiteitsmodellen. Orthorhombische en monokline preparaatsymmetrie worden beschouwd. In de vergelijkingen komen de reeksontwikkelings-coëfficiënten van de odf voor. In het geval van het Voigt model breekt de reeks af na de 4e orde coëfficiënten. Het Voigt model voorspelt lineair gedrag versus sin $^2\psi$ zelfs voor getextureerde preparaten.

Hoofdstuk 4 geeft een algemene behandeling van zowel diffractierek-poolfiguren als intensiteits-poolfiguren van getextureerde materialen voor alle kubische puntgroepen. Zowel normale als anomalie verstrooiing worden behandeld. Aangetoond wordt dat de zgn. 'spook'-verschijnselen die optreden bij analyse van intensiteits-poolfiguren, bij diffractierek-poolfiguren niet kunnen optreden. Uit de verkregen uitdrukkingen komt een nieuw type belfunctie naar voren.

In hoofdstuk 5 wordt een algemene behandeling gegeven van meervoudige, samenvallende of overlappende diffractiepieken toegepast op (macro-) spanningsbepaling in getextureerde kubische materialen. Speciale aandacht wordt gegeven aan de (651 + 732) dubbelreflectie. Voor deze reflectie wordt door andere onderzoekers lineair diffractierek-gedrag versus sin $^2\psi$ gerapporteerd. Hun experimenten betreffen een soortgelijk materiaal met een soortgelijke textuur als bestudeerd in deze dissertatie.

Hoofdstuk 6 geeft een behandeling van diffractierek van getextureerde materialen in termen van eenvoudige fysische beelden zonder gebruik te maken van de reeksontwikkelings-coëfficiënten van de odf. In plaats daarvan wordt aangenomen dat de odf bekend is in een of andere ongespecificeerde vorm. De elastische rek van de kristallen die bijdragen tot de diffractie en de odf zelf worden geschreven als Fourier-reeksen van 5 termen met betrekking tot de rotatiehoek om de diffractievector.
Diffractieriek is een gemiddelde van eenkristalrekken. De odf treedt op als gewichtsfunctie hierin. Rekenkundig wordt de diffractieriek verkregen door het product van odf en eenkristalrek te middelen. Algemene uitdrukkingen die de Fourier-coëfficiënten bevatten en de kwadraten van de structuurfactoren, worden gegeven voor alle kubische puntgroepen.

Hoofdstuk 7 dient als illustratie van hoofdstuk 6. De analyse wordt toegepast op getextureerde staalpreparaten. Er wordt een vergelijking gemaakt met de experimentele resultaten verkregen aan soortgelijk materiaal door andere onderzoekers. Er wordt geconcludeerd dat kristallografische textuur in samenhang met eenkristal elastische anisotropie een kwalitatieve verklaring geeft van de diffractieriek-verschijnselen die aan dit soort materialen waargenomen worden. Om tot deze conclusie te komen is het alleen nodig om een 2-assige macro-spanningstoestand aan te nemen. De zgn. spanningen van de 2de soort (constant over afstanden ter grootte van de korrelgrootte) zijn niet nodig voor de verklaring.

Hoofdstuk 8 is gewijd aan een practische test van de methoden die voorgesteld worden in de voorgaande hoofdstukken. Er worden experimenten beschreven met een in-situ trekbankje op de diffractometer. Het wordt aangetoond dat berekende en gemeten diffractie elastische constanten van een koud-gewalst staalpreparaat aan elkaar gelijk zijn binnen de meetfout. In de berekening is de Hill-benadering gebruikt die het gemiddelde neemt van de Reuss en Voigt modelvoorspellingen. Er is geen fysische basis voor de Hill benadering. De toepassing ervan echter maakt het mogelijk om onbekende macro-spanningen in deze getextureerde materialen te bepalen uit diffractieriek data. Een 'aanpas' procedure kan dan worden gebruikt met de spanningen als te bepalen parameters.