By using (61), (60), (49) together with the relation

$$\exp[-a(x-x_0)^2]*\exp[-bx^2]$$
$$= \delta(x-x_0)*\{\exp[-ax^2]*\exp[-bx^2]\},$$

we obtain (26), which is also valid for $R = 1$.

References

BONART, R., HOSEMANN, R. & McCULLOUGH, R. L. (1963). Polymer, 4, 199-211.

FISCHER, L. & RULAND, W. (1980). Colloid Polym. Sci. 258, 917-922.
FRANKLIN, R. E. (1951). Proc. R. Soc. London Ser. A, 209, 196-218.
GUENTERT, O. J. & CVIKEVICH, S. (1964). Carbon, 1, 309-313.
HOUSKA, C. R. & WARREN, B. E. (1954). J. Appl. Phys. 25, 1503-1509.
RULAND, W. (1965). Acta Cryst. 18, 992-996.
RULAND, W. (1968). Chemistry and Physics of Carbon, Vol. 4. New York: Marcel Dekker.
RULAND, W. & TOMPA, H. (1968). Acta Cryst. A24, 93-99.
RULAND, W. & TOMPA, H. (1972). J. Appl. Cryst. 5, 225-230.
WARREN, B. E. (1941). Phys. Rev. 59, 693-698.

The Influence of Texture on the Strain Measured by Diffraction

BY P. PENNING AND C. M. BRAKMAN

Delft University of Technology, Laboratory of Metallurgy, Rotterdamseweg 137, 2628 AL Delft, The Netherlands

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 φ_2'' 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 φ_2''. 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 φ_2'' 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 φ_2'' 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.

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 ψ, with respect to the normal to the surface and the angle φ, 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 ψ and φ, 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 φ_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 ψ and φ, for given *HKL* and integrated over φ_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) $\langle \varepsilon'_{zz} \rangle$. Detailed measurements show that this 'diffraction strain' depends on the angles ψ and φ. 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 model 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 φ_2''), one expects that elastic anisotropy may cause a variation in diffraction strain as a function of φ_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 ($\mathbf{k}_i$) and diffracted ($\mathbf{k}_r$) beams ($\mathbf{k}_i \times \mathbf{k}_r$) points in the positive y' direction. The ' 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:

specimen frame: r
lab frame: r'
crystal frame: R.

The relations between these three can be given by a 3×3 matrix:

$$r' = \begin{pmatrix} -\sin \varphi & \cos \varphi & 0 \\ -\cos \varphi \cos \psi & -\sin \varphi \cos \psi & \sin \psi \\ +\cos \varphi \sin \psi & +\sin \varphi \sin \psi & \cos \psi \end{pmatrix} r. \quad (1)$$

Only the 'experimental' angles φ and ψ are involved.

$$R = \begin{pmatrix} \alpha_h \cos \varphi_2'' - \beta_h \sin \varphi_2'' & \alpha_h \sin \varphi_2'' + \beta_h \cos \varphi_2'' & h \\ \alpha_k \cos \varphi_2'' - \beta_k \sin \varphi_2'' & \alpha_k \sin \varphi_2'' + \beta_k \cos \varphi_2'' & k \\ \alpha_l \cos \varphi_2'' - \beta_l \sin \varphi_2'' & \alpha_l \sin \varphi_2'' + \beta_l \cos \varphi_2'' & l \end{pmatrix} r'.$$

(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 φ_2'' 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 φ_2''. The parameters $\alpha_h \alpha_k \alpha_l$ and $\beta_h \beta_k \beta_l$ follow from one another by cyclic interchange:

$$\alpha_h = h(1 - h^2 - 2\Gamma)/N, \quad \alpha_k = k(1 - k^2 - 2\Gamma)/N,$$

$$\alpha_l = l(1 - l^2 - 2\Gamma)/N, \quad \beta_h = kl(k^2 - l^2)/N,$$

$$\beta_k = lh(l^2 - h^2)/N, \quad \beta_l = hk(h^2 - k^2)/N,$$

(3)

$$\Gamma = h^2 k^2 + k^2 l^2 + l^2 h^2, \quad N = (\Gamma - 4\Gamma^2 + 3h^2 k^2 l^2)^{1/2}.$$

The parameters Γ 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 $|H| = |K|$:

$$2h^2 + l^2 = 1, \ t = hk/|hk| \ (\text{if } h = k \equiv 0: t = 1),$$

$$\alpha_h = l/\sqrt{2}, \ \alpha_k = tl/\sqrt{2}, \ \alpha_l = -h\sqrt{2},$$

$$\beta_h = -t/\sqrt{2}, \ \beta_k = +1/\sqrt{2}, \ \beta_l = 0.$$

The 3×3 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 α, β and γ in this order, with rotations around Z, X and Z respectively. Instead of β 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, ψ, φ, hkl and φ_2'', are

$$\lambda = l \cos \psi - q_l \sin \psi,$$

$$(1 - \lambda^2)^{1/2} \cos(\alpha - \varphi) = \alpha_l \cos \varphi_2'' - \beta_l \sin \varphi_2'',$$

$$(1 - \lambda^2)^{1/2} \sin(\alpha - \varphi) = l \sin \psi + q_l \cos \psi,$$

(5)

$$(1 - \lambda^2)^{1/2} \cos \gamma = k \cos \psi - q_k \sin \psi,$$

$$(1 - \lambda^2)^{1/2} \sin \gamma = h \cos \psi - q_h \sin \psi,$$

Table 1. *Orientations, in Euler angles, equivalent to α, λ, γ because of symmetry*

The threefold axis in cubic crystals is not included because it does not correspond to a simple transformation.

Specimen				
Monoclinic	$2\pi - \alpha$	$-\lambda$	$\pi + \gamma$	y: twofold
Orthorhombic	$2\pi - \alpha$	$-\lambda$	$\pi + \gamma$	y: twofold
	$\pi + \alpha$	λ	γ	z: twofold
Crystal				
$m3$	α	λ	$\pi + \gamma$	Z: twofold
	$\pi + \alpha$	$-\lambda$	$\pi - \gamma$	X: twofold
$m3m$	α	λ	$\pi/2 + \gamma$	Z: fourfold
	$\pi + \alpha$	$-\lambda$	$\pi - \gamma$	X: twofold

Table 2. *Representative traces for cubic symmetry*

	H	K	L	φ_2''	$\rightarrow$ Euler angles	α	λ	γ
A:	H	K	L	φ_2''	$\rightarrow$	α	λ	γ
B:	$-K$	H	L	φ_2''	$\rightarrow$	α	λ	$\gamma + \pi/2$
C:	$-H$	$-K$	$-L$	$\pi - \varphi_2''$	$\rightarrow$	$2\varphi - \alpha$	$-\lambda$	$\gamma + \pi$
D:	K	$-H$	$-L$	$\pi - \varphi_2''$	$\rightarrow$	$2\varphi - \alpha$	$-\lambda$	$\gamma + 3\pi/2$

with

$$q_h = \alpha_h \sin \varphi_2'' + \beta_h \cos \varphi_2'',$$

$$q_k = \alpha_k \sin \varphi_2'' + \beta_k \cos \varphi_2'',$$

(6)

$$q_l = \alpha_l \sin \varphi_2'' + \beta_l \cos \varphi_2''.$$

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 ψ, φ, hkl, φ_2'' is more convenient, because it gives the orientation of the diffracting grains. Since φ_2'' 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 φ_2'' 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 $m3$ 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 φ_2'' also changes. In all comparisons between traces such a transformation in φ_2'' must be taken into account (see also Table 4).

In point group $m3$ 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 $m3m$ the traces A and B are equivalent as are C and D. Symmetry in the indices of the reflecting planes also leads to

Table 3. *Equivalent traces*

Of the traces given in Table 2, the equivalent ones are enclosed in { }.

Crystal $m3$	{A} {B}	{C} {D}
Crystal $m3m$	{A B}	{C D}
Reflection HHL	{A D}	{B C}
Reflection $0KL$	{A C}	{B D}

Table 4. *Traces and corresponding Euler angles for some orientations of the scattering vector*

	ψ	φ	H	K	L	φ_2''	α	λ	γ
A:	ψ	φ	H	K	L	φ_2''	α	λ	γ
Aa:	ψ	$\pi+\varphi$	H	K	L	φ_2''	$\pi+\alpha$	λ	γ
Ab:	ψ	$-\varphi$	H	K	L	φ_2''	$-2\varphi+\alpha$	λ	γ
Ac:	$\pi-\psi$	φ	H	K	L	$\pi+\varphi_2''$	$\pi+2\varphi-\alpha$	$-\lambda$	$\pi+\gamma$
C:	ψ	φ	$-H$	$-K$	$-L$	$\pi-\varphi_2''$	$2\varphi-\alpha$	$-\lambda$	$\pi+\gamma$
Ca:	ψ	$\pi+\varphi$	$-H$	$-K$	$-L$	$\pi-\varphi_2''$	$\pi+2\varphi-\alpha$	$-\lambda$	$\pi+\gamma$
Cb:	ψ	$-\varphi$	$-H$	$-K$	$-L$	$\pi-\varphi_2''$	$-\alpha$	$-\lambda$	$\pi+\gamma$
Cc:	$\pi-\psi$	φ	$-H$	$-K$	$-L$	$-\varphi_2''$	$\pi+\alpha$	λ	γ
Ai:	$\pi-\psi$	$\pi-\varphi$	H	K	L	$\pi+\varphi_2''$	$2\varphi-\alpha$	$-\lambda$	$\pi+\gamma$

Table 5. *Equivalence in traces caused by specimen symmetry*

In $m3$ crystals there exist also sets where A and C are replaced by B and D respectively.

No symmetry	{A}	(Aa Cc)	{Ab}	{Ac Ca}	{C} {Cb}
Monoclinic	{A Cb}	(Aa Cc)	{Ab C}	{Ac Ca}	
Orthorhombic	{A Aa Cb Cc}	{Ab Ac C Ca}			

The traces C and Ai are always equivalent.

equivalence in traces. The results are summarized in Table 3.

It must be mentioned that these equivalences are additive: in point group $m3m$ and reflection HHL the four traces are equivalent.

Up till now the scattering vector has been kept fixed in space and the contributing grains determined. To detect simple symmetries in the specimen with respect to diffraction, four different orientations of the scattering vector are introduced. The new values of ψ and φ result from inversion (index i), z axis twofold axis (index a), xz plane mirror (index b) and xy plane mirror (index c). A change in scattering vector leads to another set of diffracting crystals. In Table 4 the characteristics of the new trace are given for A and C. A very similar set for the traces B and D also exists. The result that the traces Aa and Cc are identical, and also the traces Ac and Ca, was to be expected: the direction $\psi, \pi+\varphi$ is opposite to $\pi-\psi, \varphi$ and also HKL and $-H-K-L$ are opposite. The trace Ai represents the opposite direction of the scattering vector for the same set of planes as in trace A. From Table 1 the equivalences given in Table 5 are found.

5. Orientation distribution function (o.d.f.)

The o.d.f. is defined as follows:

$$dV/V = f(\alpha, \lambda, \gamma) \, d\alpha \, d\lambda \, d\gamma/(8\pi^2), \qquad (7)$$

where dV/V is the volume fraction of the grains that have an orientation within the interval $d\alpha \, d\lambda \, d\gamma$ around α, λ, γ. 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 (the transformed) φ_2''.

6. Stress and strain

To obtain the diffraction strain 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 e_{ij} on specimen axes, straightforward tensor transformation yields the dilatation in the direction ψ, φ we are interested in. One finds

$$\varepsilon_{zz}' = \cos^2 \varphi \sin^2 \psi e_{11} + \sin^2 \varphi \sin^2 \psi e_{22}$$
$$+ \cos^2 \psi \, e_{33} + \sin \varphi \sin 2\psi e_{23}$$
$$+ \cos \varphi \sin 2\psi e_{13} + \sin 2\varphi \sin^2 \psi e_{12}. \qquad (8)$$

The strain measured by the diffraction 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 σ_{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 φ_2'' and the stress components as independent variables we present the result as follows:

$$\varepsilon_{zz}' = \sum_{k=1}^{6} \{E_{k0} + s_0 N(E_{k1} \cos \varphi_2'' + E_{k2} \sin \varphi_2'')$$
$$+ s_0 A[E_{k3} \cos (2\varphi_2'' - \chi)$$
$$+ E_{k4} \sin (2\varphi_2'' - \chi)]\} \sigma_k. \qquad (9)$$

The contribution of each stress component is given

Table 6. *The coefficients E_{ki} in the Fourier series for ε'_{zz}*

i	1	2	3	4
k				
1	$-\sin 2\varphi \sin \psi$	$-\cos^2\varphi \sin 2\psi$	$\sin^2\varphi - \cos^2\varphi \cos^2\psi$	$+\sin 2\varphi \cos\psi$
2	$+\sin 2\varphi \sin\psi$	$-\sin^2\varphi \sin 2\psi$	$\cos^2\varphi - \sin^2\varphi \cos^2\psi$	$-\sin 2\varphi \cos\psi$
3	0	$\sin 2\psi$	$-\sin^2\psi$	0
4	$+2\cos\varphi\cos\psi$	$-2\sin\varphi\cos 2\psi$	$\sin\varphi\sin 2\psi$	$+2\cos\varphi\sin\psi$
5	$-2\sin\varphi\cos\psi$	$-2\cos\varphi\cos 2\psi$	$\cos\varphi\sin 2\psi$	$-2\sin\varphi\sin\psi$
6	$2\cos 2\varphi\sin\psi$	$-\sin 2\varphi\sin 2\psi$	$-\sin 2\varphi(1+\cos^2\psi)$	$-2\cos 2\varphi\cos\psi$

as a Fourier series in the angle φ''_2. The parameters N, A and χ depend only on hkl.

$$s_0 = s_{11} - s_{12} - s_{44}/2$$

$$A\cos\chi = \Gamma - 2h^2k^2l^2(1-3\Gamma)/N^2$$
$$A\sin\chi = hkl\{h^4(k^2-l^2)+k^4(l^2-h^2) \tag{10}$$
$$+ l^4(h^2-k^2)\}/N^2.$$

The values of the coefficients E_{ki} are given in Table 6.

The coefficients E_{k0} are not shown in Table 6 because they can be found more elegantly in another way. The transformation of E_{k0} back to the specimen frame yields a result that is independent of ψ and φ, 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 φ''_2-independent part of the strain gives rise to the definition of 'effective' elastic constants, which give the φ''_2-independent part of the strain as a function of stress

$$s^{eff}_{11} = s_{11} - 2s_0\Gamma; \quad s^{eff}_{12} = s_{12} + s_0\Gamma;$$
$$s^{eff}_{44} = 2(s_{11} - s_{12} - 3s_0\Gamma).$$

In the literature (Hauk, 1955; Macherauch & Müller, 1961; Dölle & Hauk, 1977; Dölle, 1979; James & Cohen, 1980; Hauk, 1984), s^{eff}_{11} and $\frac{1}{2}s^{eff}_{44}$ 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 $m3$ and $m3m$. Hence, the strain along traces A and B is equal for the same value of φ''_2; 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 φ''_2. 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 φ''_2 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 A and C (and also for 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 φ''_2 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 α and γ and Jacobi polynomials in λ. 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 (ψ, φ) and given set of reflecting planes (HKL).

(ii) Calculate for the grain with orientation

$$h, k, l, \psi, \varphi, \varphi''_2 = \alpha, \lambda, \gamma:$$

(a) the dilatation in spacing ε'_{zz} (equation 9);
(b) the volume fraction D (§ 5);
(c) the modulus of the structure factor F (§ 7 above).

(iii) Calculate the diffraction strain:

$$\langle \varepsilon'_{zz}\rangle = \int \varepsilon'_{zz}DF^2 d\varphi''_2 / \int DF^2 d\varphi''_2. \tag{11}$$

The integrals extend from 0 to 2π along the t traces. Since ε'_{zz} and D are known as a Fourier series in φ''_2, the integrals can be replaced by a summation:

$$\langle \varepsilon'_{zz}\rangle = \sum_{\tau=1}^{t} \sum_{\nu=0}^{4} \tfrac{1}{2}(1+\delta_{\nu,0})(\varepsilon'_{zz})_{\tau,\nu}D_{\tau,\nu}F^2_\tau \Big/ \sum_{\tau=1}^{t} D_{\tau,0}F^2_\tau. \tag{12}$$

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.

$\sigma_1\sigma_2$	$\{A\ Aa\ Cb\ Cc\}$	$\{C\ Ca\ Ab\ Ac\}$		
σ_3	$\{A\ Aa\ Cb\ Cc$	$C\ Ca\ Ab\ Ac\}$		
σ_4	$\{A\}$	$\{C\}$	$\{Aa\ Cb\ Cc\}$	$\{Ab\ Ac\ Ca\}$
σ_5	$\{A\ Cb\}$	$\{Aa\ Cc\}$	$\{C\ Ab\}$	$\{Ac\ Ca\}$
σ_6	$\{A\ Aa\ Cc\}$	$\{Cb\}$	$\{Ab\}$	$\{C\ Ac\ Ca\}$

Table 8. *Symmetry in the diffraction strain pole figure*

For monoclinic point groups the symmetry axis is given in parentheses.

Specimen symmetry	Stresses present	Point group of strain pole figure
Monoclinic 2 (y)	$\sigma_1\sigma_2\sigma_3\sigma_5$	Monoclinic $2/m(y)$
Orthorhombic 222	$\sigma_1\sigma_2\sigma_3\sigma_4$	Monoclinic $2/m(x)$
	$\sigma_1\sigma_2\sigma_3\sigma_5$	Monoclinic $2/m(y)$
	$\sigma_1\sigma_2\sigma_3\sigma_6$	Monoclinic $2/m(z)$
	$\sigma_1\sigma_2\sigma_3$	Orthorhombic mmm

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 σ_k, 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 φ_2'' values that are π 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 'ψ splitting' indicates that the z axis possesses twofold symmetry. According to Table 8 this is only the case in orthorhombic specimen symmetry if $\sigma_4 = \sigma_5 = 0$. The presence of ψ splitting hence indicates either the presence of σ_4 and/or σ_5 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 φ is present in the Voigt model and in the φ_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 ψ is given in Table 6. How the o.d.f. factor depends on ψ 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 $(111)[2\bar{1}\bar{1}]$ 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
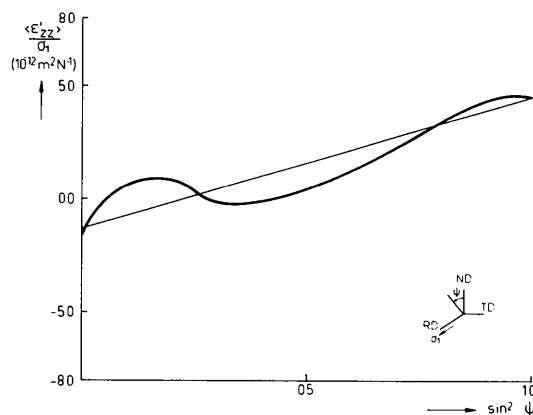

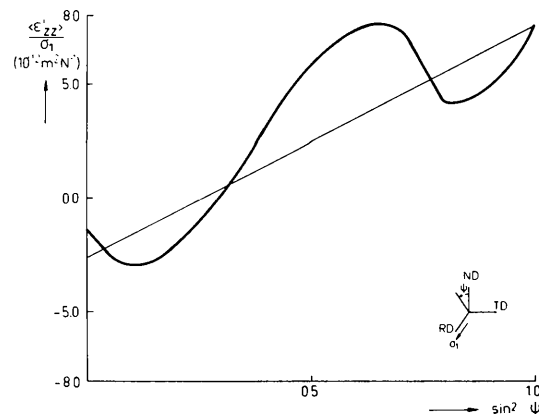Fig. 1. The 112 diffraction strain in cold-rolled steel as a function of $\sin^2 \psi$. For details see text.

Fig. 2. The 224 diffraction strain in cold-rolled copper as a function of $\sin^2 \psi$. For details see text.

10^{-12} m^2 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_{HKL} vs sin$^2 \psi$ that is of the same order of magnitude as the diffraction strain itself.

References

BRAKMAN, C. M. (1985a). *Cryst. Res. Technol.* **20**, 593–618.
BRAKMAN, C. M. (1985b). Unpublished research.
BUNGE, H. J. (1982). *Texture Analysis in Materials Science.* London: Butterworths.
DÖLLE, H. (1979). *J. Appl. Cryst.* **12**, 489–501.
DÖLLE, H. & HAUK, V. (1977). *Z. Metallkd.* **68**, 719–724.
HAUK, V. (1955). *Z. Metallkd.* **46**, 33–38.
HAUK, V. M. (1984). *Adv. X-ray Anal.* **27**, 101–120.
JAMES, M. R. & COHEN, J. B. (1980). *The Measurement of Residual Stresses by X-ray Diffraction Techniques.* In *Experimental Methods in Materials Science*, Vol. 1, edited by H. HERMAN, pp. 1–62. New York: Academic Press.
MACHERAUCH, E. & MÜLLER, P. (1961). *Z. Angew. Phys.* **13**, 305–312.

Non-linear Diffraction Strain vs sin² ψ Phenomena in Specimens Exhibiting Rolling-Type Texture

BY C. M. BRAKMAN AND P. PENNING

Delft University of Technology, Laboratory of Metallurgy, Rotterdamseweg 137, 2628 AL Delft, The Netherlands

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 σ_1 and σ_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 ψ stands for the angle between the scattering vector and the specimen's normal direction (ND). The symbol φ 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 $\varphi = 0$. Small or negligible non-linearities are reported for measurements in the plane $\varphi = \pi/2$. 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 ψ and φ. 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 σ_1 and σ_2 are considered. They operate parallel to the rolling