The Influence of Multiaxial Stress States, Stress Gradients and Elastic Anisotropy on the Evaluation of (Residual) Stresses by X-rays*

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Abstract

In recent years, nonlinear \( d \) vs \( \sin^2 \psi \) distributions have been observed in stressed materials which cannot be explained by the classical fundamentals of X-ray stress measurement. \( d \) is the interplanar spacing measured and \( \psi \) is the angle between the surface normal of the sample and the measuring direction. This paper reviews treatments for these nonlinear distributions, including stress gradients, shear stresses and anisotropic X-ray elastic constants. Methods for the evaluation of stresses are reported, and recommendations are given for the practical application of X-ray stress measurement.

1. Introduction

The X-ray method for determining residual or applied stresses in crystalline materials is based on the measurement of interplanar spacings \( d \) at various tilts, \( \varphi \) and \( \psi \), to the X-ray beam, see Fig. 1. In a polycrystalline specimen, only those grains properly oriented to diffract at each tilt contribute to the diffraction profile. This selectivity implies that the elastic constants connecting the measured strains (or change in interplanar spacings) to the stresses will vary with the particular set of planes \( (hkl) \) chosen for measurement. A recent review of this problem is contained in references, Marion & Cohen (1977); Macherauch & Wolfstieg (1977). At this point in time, theory (Bollenrath, Hauk & Müller, 1967) allows for an anisotropic grain coupled to an isotropic matrix, and the variations in X-ray elastic constants (REC) with crystallographic direction match reasonably well with measured values (Macherauch & Wolfstieg, 1977). However, their large change with plastic tensile deformation, found by Taira, Hayashi & Watase (1968), Prümmer (1969), Marion & Cohen (1977) and by Dölle, Hauk, Kloth, Over & Wichert (1977), is not yet understood.

Recently, there have been some unusual phenomena found in X-ray stress measurements suggesting that extensions of the theoretical background might permit an understanding of these new experimental results, particularly for textured materials and for materials deformed by large stresses tangent to the surface. From the theory of isotropic elasticity, with \( d_0 \) as the lattice parameter of the unstressed material (Macherauch & Müller, 1961; Barrett & Massalski, 1966),

\[
\frac{d_{\varphi \psi} - d_0}{d_0} = \frac{1}{2}s_2(hk\ell)[\sigma_1 \cos^2 \varphi + \sigma_2 \sin^2 \varphi] \sin^2 \psi + s_1(hk\ell)[\sigma_1 + \sigma_2],
\]

with the principal stresses \( \sigma_1 \) and \( \sigma_2 \) and the X-ray elastic constants (REC)

\[
\frac{1}{2}s_2(hk\ell) = [(1 + \nu)/E]^{hk\ell}; s_1(hk\ell) = (-\nu/E)^{hk\ell}.
\]
According to (1), \( d_{\text{app}} \) should be linear with \( \sin^2 \psi \), but it has recently been found that different \( d - \sin^2 \psi \) curves occur for positive and negative \( \psi \) (see Fig. 2a) after grinding (Walburger, 1973; Faninger & Walburger, 1976; Wollfsteig & Macherauch, 1976; Macherauch & Wollfsteig, 1977), or rolling friction (Christ & Krause, 1975; Krause & Jühe, 1976), or wear (Krause & Jühe, 1977), and oscillations (see Fig. 2b) may occur in textured materials (Bollenrath, Hauk & Weidemann, 1967; Shiraiwa & Sakamoto, 1970, Marion & Cohen, 1975; Hauk, Herlach & Sesemann, 1975). Since the penetration depth of X-rays depends on \( \psi \) (Wollfsteig, 1976), strong gradients can cause additional nonlinearities (Shiraiwa & Sakamoto, 1972).

It is the purpose of this paper to summarize the recent theoretical approaches taken by Shiraiwa & Sakamoto (1970, 1972) in Japan and by German groups (Evenschor & Hauk, 1975a, b; Hauk & Sesemann, 1976; Dölle & Hauk, 1976, 1977, 1978; Peiter, 1976; Peiter & Lode, 1976; Lode & Peiter, 1977) to explain the observations mentioned in the preceding paragraph. There are two major ideas involved:

(1) As the stresses calculated from lattice strains represent values averaged over the penetration depth of the X-rays, it cannot be assumed a priori that the averaged stress components normal to the surface are zero, especially when the subgrain size is small, or when steep stress gradients are present. It has been shown by Peiter (1976) and by Dölle & Hauk (1976) that shear stresses normal to the surface can explain the experimental results found after tangent plastic deformation by shear stresses.

(2) The classical equation (1) of X-ray stress analysis presumes that the X-ray elastic constants do not depend on \( \varphi \) and \( \psi \) and that \( d - \sin^2 \psi \) is linear. Occasionally large oscillations in \( d - \sin^2 \psi \) have been observed in textured materials (Fig. 2b). The current interpretations of this phenomenon are summarized in Table 1. Note that two of these utilize isotropic elastic theory and the third takes into account that in textured materials X-ray elastic constants can depend on \( \varphi \) and \( \psi \). In general, there are a number of causes of oscillations in \( d - \sin^2 \psi \) and more than one interpretation may be necessary to explain experimental observations. For example, oscillations due to microstresses or grain statistics may superimpose on the nonlinearities associated with mechanical anisotropy (texture).

The general anisotropic theory of X-ray stress measurement which will be summarized here starts from the statistical theory of elasticity (Eshelby, 1957, 1959; Kröner, 1958, 1967; Kneer, 1965; Morris, 1970; Wecker & Morris, 1978). It will be shown that the anisotropic equations reduce to the classical equations for X-ray stress analysis (Macherauch & Müller, 1961; Barrett & Massalski, 1966) when the X-ray elastic constants are isotropic.

### Table 1. Possible origins of oscillations in \( d - \sin^2 \psi \)

<table>
<thead>
<tr>
<th>Authors</th>
<th>X-ray elastic constants depending on</th>
<th>Assumed elasticity</th>
<th>Stress state</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shiraiwa &amp; Sakamoto (1970); Dölle &amp; Hauk (1978)</td>
<td>Reflection ( hkl ) and ( \varphi ) and ( \psi )†</td>
<td>Anisotropic</td>
<td>Uniform or quasi-uniform stresses as averages over the penetration depth of the X-ray beam*</td>
<td>Bollenrath, Hauk &amp; Weidemann (1967); Marion &amp; Cohen (1975)</td>
</tr>
<tr>
<td>Peiter &amp; Lode (1976)</td>
<td>Reflection ( hkl ), not ( \varphi ) and ( \psi )</td>
<td>Isotropic</td>
<td>Oscillation in stresses with ( \varphi ) and ( \psi ) due to local plastic response and texture</td>
<td>Kloner (1965)</td>
</tr>
<tr>
<td>Dölle &amp; Hauk (1976)</td>
<td>Reflection ( hkl ), not ( \varphi ) and ( \psi )</td>
<td>Isotropic</td>
<td>Superposition of strong gradients and shear residual stresses normal to the surface</td>
<td>Barrett &amp; Massalski (1966)</td>
</tr>
<tr>
<td>Shiraiwa &amp; Sakamoto (1970); Dölle &amp; Hauk (1978)</td>
<td>Reflection ( hkl ) and ( \varphi ) and ( \psi )†</td>
<td>Anisotropic</td>
<td>Uniform or quasi-uniform stresses as averages over the penetration depth of the X-ray beam*</td>
<td>Bollenrath, Hauk &amp; Weidemann (1967); Marion &amp; Cohen (1975)</td>
</tr>
</tbody>
</table>

† For \( h00 \) and \( hhh \) reflections the X-ray elastic constants of textured materials do not depend on \( \varphi \) or \( \psi \) (Dölle & Hauk, 1978).

### Table 2. Calculation of bulk elastic constants by the statistical theory of elasticity

<table>
<thead>
<tr>
<th>Authors</th>
<th>Elastic properties of matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eshelby (1957, 1959)</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Kröner (1958, 1967)</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Kneer (1965)</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Morris (1970); Wecker &amp; Morris (1978)</td>
<td>Anisotropic</td>
</tr>
<tr>
<td>Elastic properties of a grain</td>
<td></td>
</tr>
<tr>
<td>Isotropic, but different from the elastic properties of the matrix</td>
<td></td>
</tr>
<tr>
<td>Anisotropic</td>
<td></td>
</tr>
<tr>
<td>Anisotropic with hexagonal symmetry (fiber texture)</td>
<td></td>
</tr>
<tr>
<td>Anisotropic with orthotropic symmetry (rolling texture)</td>
<td></td>
</tr>
</tbody>
</table>
constants can be calculated for quasi-isotropic and textured materials, see Table 2. It is important to note that, in these treatments, the inhomogeneous surrounding grains of a crystallite are replaced by a quasi-homogeneous environment having the macroscopic isotropic or anisotropic properties of the polycrystal. Therefore, for the X-ray measurement it is necessary that the beam irradiates an area large enough so that a statistically relevant number of grains or subgrains are reflecting.

For the evaluation of stresses, it is necessary to carry out measurements of interplanar spacings \( d \) for different directions \( L_3 \), given by \( \varphi \) and \( \psi \) (see Fig. 1). Since tensor components (e.g. the lattice deformation \( \varepsilon'_{33} \)) depend on the orientation of the coordinate system* to which they are related, the calculation of stresses in the coordinate system of the sample \( P_1 \) require that two things are known: (1) the X-ray elastic constants in different laboratory systems \( L_i \) and (2) the relationship between stresses \( \sigma'_{ij} \) in the system \( P_1 \) and those in systems \( L_i \). If the material is quasi-isotropic, X-ray elastic constants do not depend on \( L_i(\varphi,\psi) \), but if it has texture, in general these constants vary with \( \varphi \) and \( \psi \), as will be shown in §3.1.

In the laboratory systems \( L_i \), the relation between interplanar spacings \( d \) or lattice strains \( \varepsilon'_{33} \) and effective stresses \( \sigma'_{ij} \) can be written as

\[
\langle d_{\varphi\psi} - d_0 \rangle / d_0 = \langle \varepsilon'_{33} \rangle = \langle (s'_{33ij} + t'_{33ij})\sigma'_{ij} \rangle,
\]

where \( d_{\varphi\psi} = \) interplanar spacing for direction \( L_3 \), \( d_0 = \) interplanar spacing of a stress-free sample, \( \varepsilon'_{33} = \) lattice strain normal to lattice planes \((hkl)\) (in direction \( L_3 \)), \( s'_{33ij} = \) single-crystal compliances in system \( L_i \), \( t'_{33ij} = \) elastic interaction of a grain and its surrounding matrix ('elastic susceptibility'), \( \sigma'_{ij} = \) stress components in system \( L_i \). The brackets in (3) indicate that an average is taken over the crystallites diffracting.

If the number of crystallites diffracting is large,

\[
\langle \varepsilon'_{33} \rangle = \langle (s'_{33ij} + t'_{33ij})\sigma'_{ij} \rangle = \langle (s'_{33ij} + t'_{33ij})\rangle \sigma'_{ij},
\]

where \( \langle \sigma'_{ij} \rangle \) are the stresses averaged over the penetration depth and the equation

\[
r'_{ij} \equiv \langle s'_{33ij} + t'_{33ij} \rangle = \langle s'_{33ij} \rangle + \langle t'_{33ij} \rangle
\]

defines the X-ray elastic constants. The interaction term \( \langle t'_{33ij} \rangle \) representing the coupling of a grain to the surrounding matrix depends on the single-crystal constants and the texture.

For quasi-isotropic materials, the averages \( r'_{ij} \) in (5) do not depend on the orientation of the axes \( L_0 \), so that the prime can be omitted. Their relationships to the X-ray elastic constants \( s_1(hkl) \) and \( s_2(hkl) \) defined by (1) are (Möller & Martin, 1939)

\[
\begin{align*}
 r_{11} &= r_{22} = s_1(hkl), \\
 r_{33} &= s_1(hkl) + \frac{1}{2}s_2(hkl), \\
 r_{12} &= r_{13} = r_{23} = 0.
\end{align*}
\]

If the interaction is neglected \( (\langle t'_{33ij} \rangle = 0) \), the Voigt averages taken over the single-crystal stiffness coefficients (constant average strain) are obtained (Glocker, 1938; Schiebold, 1938; Möller & Martin, 1939):

\[
\begin{align*}
 s'_{1y} &= \frac{3s_0(s_{1111} + 2s_{1122}) + 10s_{1212}s_{1212}}{3s_{1111} - 3s_{1122} + 4s_{1212}}, \\
 s'_{y2} &= \frac{1}{2G_v} = \frac{10s_{1212}(s_{1111} - s_{1122})}{3s_{1111} - 3s_{1122} + 4s_{1212}},
\end{align*}
\]

with

\[
\begin{align*}
 s_0 &= s_{1111} - s_{1122} - 2s_{1212}. 
\end{align*}
\]

The Reuss averages, which are taken over the single-crystal compliances (constant average stress), are (Glocker, 1938; Schiebold, 1938; Möller & Martin, 1939)

\[
\begin{align*}
 s^R_{1y}(hkl) &= s_{1112} + s_0, \\
 \frac{1}{2}s^R_{y2}(hkl) &= s_{1111} - s_{1122} - 3s_0,
\end{align*}
\]

with

\[
\begin{align*}
 \Gamma &= \frac{h^2k^2 + h^2l^2 + k^2l^2}{(h^2 + k^2 + l^2)^2}.
\end{align*}
\]

Taking the crystal coupling into account (but not texture), Bollenrath, Hauk & Müller (1967) calculated X-ray elastic constants for quasi-isotropic polycrystals, which are in good agreement with experimental results (Macherauch & Wolfstieg, 1977).

Based on the theoretical method of Eshelby (1957, 1959) and Kröner (1958, 1967) for a single-phase cubic material, the X-ray elastic constants can be calculated from (Bollenrath, Hauk & Müller, 1967)

\[
\begin{align*}
 s^V_{1y}(hkl) &= S_{3311} + t_{3311} + t_0, \\
 \frac{1}{2}s^V_{y2}(hkl) &= S_{3333} - S_{3311} + t_{3333} - t_{3311} - 3t_0,
\end{align*}
\]

with

\[
\begin{align*}
 t_0 &= t_{3333} - t_{3311} - 2t_{3331}.
\end{align*}
\]

The bulk elastic constants \( S_{3333} \) and \( S_{3311} \), which represent averages over \( s^V_{33ij} \) can be calculated from

\[
\begin{align*}
 S_{3311} &= \frac{1}{2}(1/3K - 1/2G), \\
 S_{3333} &= S_{3311} = 1/2G.
\end{align*}
\]

According to Kröner's (1958, 1967) theory of quasi-isotropic bulk elastic constants, the compressibility \( K \) and the macroscopic shear modulus \( G \) can be calculated from single-crystal compliances:

\[
\begin{align*}
 3K &= 1/(s_{1111} + 2s_{1122}), \\
 G &= G_v[1 - \frac{1}{2}s_0^2/(1 - \frac{1}{2}s_0^2a_x^2a_y^2a_z^2)],
\end{align*}
\]

with the Voigt limit \( G_v \) from (7b), and

\[
\begin{align*}
 a &= (3K + 6G_v)/(3K + 4G_v), \\
 x &= \frac{5s_0}{3s_{1111} - 3s_{1122} + 4s_{1212}}.
\end{align*}
\]

* Note that primed tensor components refer to the laboratory system \( L_i \), while unprimed refer to the sample system \( P_1 \). Principal strains and stresses have single subscripts. Single crystal compliances \( s_{ij} \) related to the principal axes of the (cubic) crystal are indicated by a tilde.
For a single-phase quasi-isotropic material, the tensor components $t_{3333}$, $t_{3311}$ and $t_{3131}$ can be calculated from

$$t_{3333} = \frac{1 - \frac{1}{3G} \left[ 2G(\ddot{s}_{1111} - \ddot{s}_{1122}) - 1 \right]}{\left\{ [8G^2 + 9KG]/(6G + 3K)(\ddot{s}_{1111} - \ddot{s}_{1122}) + 1 \right\}^{-1}},$$

(16a)

$$t_{3311} = t_{3131} = -\frac{1}{2} t_{3333}.$$ (16b)

A recent bibliography for the calculation of quasi-isotropic X-ray elastic constants of multiphase or non-cubic materials was given by Dölle & Hauk (1977). The various isotropic X-ray elastic constants calculated for iron are shown in Fig. 3. For many practical purposes the medians (Neerfeld, 1942) from X-ray elastic constants in the Voigt (7a, b) and Reuss limits (9a, b) are sufficient. For the 211 and 310 reflections usually employed, the differences between this median and the Kröner values are less than 5%. It has been observed that X-ray elastic constants of quasi-isotropic polycrystals vary with plastic deformation. Changes as large as 20–50% have been reported (Taira, Hayashi & Watase, 1968; Prümmer, 1969; Marion & Cohen, 1977; Dölle, Hauk, Kloth, Over & Wichert, 1977) for $\frac{1}{2} \Delta E(211)$ of iron. This phenomenon which depends on the reflection $hkl$ is not yet understood and it can severely affect the accuracy of a stress measurement. To avoid these errors, experimental X-ray elastic constants can be used and this should be done whenever stresses in highly deformed specimens are evaluated. Even when experimental X-ray elastic constants are used, residual stresses evaluated for different $hkl$ reflections can be different (Prümmer, 1969; Dölle, Hauk, Kloth, Over & Wichert, 1977). A thorough discussion of the effects that can cause these phenomena can be found in Garrod & Hawkes (1963) or Prümmer (1969).

### 2.2 Lattice strains in isotropic materials

The stresses related to the laboratory system $L_i$ can be calculated from stress components $\sigma_{ij}$ by

$$\sigma_{ij}' = \omega_{ij}\sigma_{jk},$$ (17)

where $\omega_{ij}$ are the direction cosines between coordinate systems $L_i$ and $P_j$. As shown in Fig. 1, $L_2$ is in the sample surface and is parallel with the axis of $\psi$ tilt. Therefore,

$$\omega = \begin{pmatrix}
\cos \phi \cos \psi & \sin \phi \cos \psi & -\sin \psi \\
-\sin \phi & \cos \phi & 0 \\
-\sin \phi \sin \psi & \sin \phi \cos \psi & \cos \psi
\end{pmatrix},$$ (18)

and the stresses $\sigma_{ij}'$ result as

$$\begin{align*}
\sigma_{11}' &= \sigma_{11} \cos^2 \phi \cos^2 \psi + \sigma_{12} \sin^2 \phi \cos^2 \psi \\
&\quad - \sigma_{13} \cos \phi \sin \phi \sin \psi + \frac{1}{2} \sigma_{22} \sin^2 \phi \cos \psi \\
&\quad - \sigma_{23} \sin \phi \sin \psi + \frac{1}{2} \sigma_{33} \sin^2 \phi \cos \psi , \\
\sigma_{12}' &= \sigma_{21}' = -\frac{1}{4} \sigma_{11} \sin 2 \phi \cos \psi + \sigma_{12} \cos 2 \phi \cos \psi \\
&\quad + \sigma_{13} \sin \phi \sin \psi + \frac{1}{2} \sigma_{22} \sin 2 \phi \cos \psi , \\
\sigma_{13}' &= \sigma_{31}' = \frac{1}{2} \sigma_{11} \cos^2 \phi \sin 2 \psi \\
&\quad + \frac{1}{2} \sigma_{12} \sin 2 \phi \sin \psi + \sigma_{13} \cos \phi \cos 2 \psi \\
&\quad + \frac{1}{2} \sigma_{22} \sin^2 \phi \sin \psi + \sigma_{23} \sin \phi \cos 2 \psi \\
&\quad - \frac{1}{2} \sigma_{33} \sin 2 \psi , \\
\sigma_{22}' &= \sigma_{11} \sin^2 \phi - \sigma_{12} \sin 2 \phi + \sigma_{22} \cos^2 \phi , \\
\sigma_{23}' &= \sigma_{32}' = -\frac{1}{4} \sigma_{11} \sin 2 \phi \psi + \sigma_{12} \cos 2 \phi \psi - \sigma_{13} \sin \phi \cos \phi \psi \\
&\quad + \frac{1}{2} \sigma_{22} \sin 2 \phi \psi + \sigma_{23} \cos \phi \cos \phi \psi , \\
\sigma_{33}' &= \sigma_{11} \cos^2 \phi \sin^2 \psi + \sigma_{12} \sin 2 \phi \psi \\
&\quad + \sigma_{13} \cos \phi \sin \phi \sin \psi + \sigma_{22} \sin^2 \phi \psi \\
&\quad + \sigma_{23} \sin \phi \sin \phi \sin \psi + \sigma_{33} \cos^2 \phi \psi .
\end{align*}$$ (19)

According to (4), (5) and (19) the relationship between multiaxial stress states and lattice deformation $\varepsilon_{33}$ or change in interplanar spacing $d$ is (Dölle & Hauk, 1976)

$$d_{\phi \psi} - d_0 = \varepsilon_{33} = \frac{1}{2} s_{33}(hkl) \left[ \sigma_{11} \cos^2 \phi + \sigma_{12} \sin 2 \phi \\
+ \sigma_{22} \sin^2 \phi \sin^2 \psi + \frac{1}{2} s_2(hkl) \sigma_{33} \cos^2 \psi \\
+ \frac{1}{2} s_1(hkl) \sigma_{11} + \sigma_{22} + \sigma_{33} \right] + \frac{1}{2} s_2(hkl) \left[ \sigma_{13} \cos \phi + \sigma_{23} \sin \phi \right] \sin 2 \psi ,$$

(20)

where the stress components $\sigma_{ij}$ are to be interpreted as average values over the penetration depth of the X-rays.

Consider the following four stress tensors whose components are given relative to the sample system $P_i$:  

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![Image](https://via.placeholder.com/150)

Fig. 3. Isotropic X-ray elastic constants for iron as $3\Gamma$, calculated in (a) Voigt, (b) Reuss and (c) Eshelby–Kröner limits.
While the tensors (21a, b) represent (residual or applied) stresses in free surfaces, the tensors (21c, d) may represent residual stress states in the interior of a material or stress states caused by multiaxial loading. It is obvious that for the tensors a and c, the principal axes of the stress state coincide with the sample system Pi. The 'classical' $d \sin^2 \psi$ law (1) (Macherauch & Müller, 1961) results when (21a) is substituted into (20). For the tensors (21b, c) there are additional terms, but $d \sin^2 \psi$ is still linear. For the most general stress state (21d), $d$ is no longer linear vs $\sin^2 \psi$. The terms $\sigma_{13}$ and $\sigma_{23}$ in (20) have a $\sin 2 \psi$ dependence. This results in different $d \sin^2 \psi$ relationships for $\psi > 0$ and $\psi < 0$ as illustrated in Fig. 2(a). This effect has been termed 'lp splitting' (Dölle & Hauk, 1977) and has actually been detected by Walburger (1973) in ground steel. In recent years, these lattice-strain distributions were found after grinding or milling (Faninger & Walburger, 1976; Wolfstieg & Macherauch, 1976; Macherauch & Wolfstieg, 1977; Dölle & Cohen, 1979), or on the surfaces of wheels and wear (Christ & Krause, 1975; Krause & Jühe, 1976, 1977).

2.3 The evaluation of the stress tensor for isotropic materials

The lattice strain for the direction $L_3$ is (Evenschor & Hauk, 1975b)

$$
\varepsilon_{33} = \varepsilon_{11} \cos^2 \phi \sin^2 \psi + \varepsilon_{12} \sin 2 \phi \sin^2 \psi \\
+ \varepsilon_{13} \cos \phi \sin 2 \psi + \varepsilon_{23} \sin^2 \phi \sin^2 \psi \\
+ \varepsilon_{33} \sin \phi \sin 2 \psi + \varepsilon_{33} \cos^2 \psi.
$$

(22)

Introducing the average strain, $a_1$, and the deviation, $a_2$, from this average strain ('splitting'), we find

$$
a_1 = \frac{1}{2} [\varepsilon_{\phi \phi} + \varepsilon_{\phi \psi} - ] = (d_{\phi \phi} + d_{\phi \psi} - )/2d_0 - 1 \\
= \varepsilon_{33} + \left[ \varepsilon_{11} \cos^2 \phi + \varepsilon_{12} \sin 2 \phi \right] \\
+ \varepsilon_{22} \sin^2 \phi - \varepsilon_{33} ] \sin^2 \psi,
$$

(23a)

$$
a_2 = \frac{1}{2} [\varepsilon_{\phi \phi} - \varepsilon_{\phi \psi} - ] = (d_{\phi \phi} - d_{\phi \psi} - )/2d_0 \\
= \left[ \varepsilon_{13} \cos \phi + \varepsilon_{23} \sin \phi \right] \sin [2\psi].
$$

(23b)

Thus, $\varepsilon_{33}$ can be determined from the intercept of $a_1$ vs $\sin^2 \psi$, if $d_0$ is known. As a check on this result, note that this value is independent of $\phi$. The tensor components $\varepsilon_{11} \varepsilon_{12} \varepsilon_{22}$ can be obtained from $(\delta a_1 / \delta \sin^2 \psi)$. For $\phi = 0$, $(\varepsilon_{11} - \varepsilon_{33})$ is obtained, whereas for $\phi = 90^\circ$, $(\varepsilon_{22} - \varepsilon_{33})$ is evaluated. The tensor component $\varepsilon_{12}$ can then be evaluated from $(\delta a_1 / \delta \sin^2 \psi)$ at $\phi = 45^\circ$. From $(\delta a_2 / \delta \sin [2\psi])$, $\varepsilon_{13}$ results when $\phi = 0$, and $\varepsilon_{23}$ when $\phi = 90^\circ$.

Taking the crystallographic anisotropy into account, the stress components $\sigma_{ij}$ can be calculated from

$$
\sigma_{ij} = \frac{1}{2} [s_{\phi \phi}^2(hkl) + \Delta s_{\phi \phi}^2(hkl) + s_{\phi \phi}^2(hkl)] \\
\times (\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}).
$$

(24)

This method, developed by Dölle & Hauk (1976), can also be used when there is no $\psi$ splitting (which implies that $\sigma_{13} = \sigma_{23} = 0$). It may be a useful procedure to determine whether or not the surface stress condition $\sigma_{33} = 0$ is fulfilled.

An experimental example of this kind of study (Dölle & Cohen, 1979) is discussed below. On ground steel, the $\varepsilon \sin^2 \psi$ curves shown in Fig. 4 were measured at the 211 reflection; the evaluation of stresses resulted in the residual stress tensor

$$
\begin{pmatrix}
390 & 14 & 63 \\
14 & 306 & -1 \\
63 & -1 & 92
\end{pmatrix}
$$

(components in MPa).

It is remarkable how well (20) with the stress tensor (25) substituted fits the data points. The principal axes of the stress tensor evaluated by principal axes transformation were tilted about the transverse direction of the sample $P_2$ by about $11^\circ$.

3. Stress measurement on textured materials

3.1 X-ray elastic constants of textured materials

For textured materials, the X-ray elastic constants defined by (5), even for the same $hkl$ reflection, depend on the direction $\phi \psi$ of the measurement (Dölle & Hauk, 1978). Neglecting the interaction of crystallites $(\tilde{t}^{\psi}_{33 ij} = 0)$, we will calculate the anisotropic X-ray elastic constants for a sharp texture in cold-rolled $\alpha$-iron, as an example of the procedures. Since the averages will be taken over single-crystal compliances $s'_{33 ij}$, the X-ray elastic constants will result in the Reuss limit. It will be assumed that the orientation distribution of the crystallites can be idealized by some combination of

$$
\begin{align}
\varepsilon_{33} &= \varepsilon_{11} \cos^2 \phi \sin^2 \psi + \varepsilon_{12} \sin 2 \phi \sin^2 \psi \\
+ \varepsilon_{13} \cos \phi \sin 2 \psi + \varepsilon_{23} \sin^2 \phi \sin^2 \psi \\
+ \varepsilon_{33} \sin \phi \sin 2 \psi + \varepsilon_{33} \cos^2 \psi.
\end{align}
$$

(22)

Thus, $\varepsilon_{33}$ can be determined from the intercept of $a_1$ vs $\sin^2 \psi$, if $d_0$ is known. As a check on this result, note that this value is independent of $\phi$. The tensor components $\varepsilon_{11} \varepsilon_{12} \varepsilon_{22}$ can be obtained from $(\delta a_1 / \delta \sin^2 \psi)$. For $\phi = 0$, $(\varepsilon_{11} - \varepsilon_{33})$ is obtained, whereas for $\phi = 90^\circ$, $(\varepsilon_{22} - \varepsilon_{33})$ is evaluated. The tensor component $\varepsilon_{12}$ can then be evaluated from $(\delta a_1 / \delta \sin^2 \psi)$ at $\phi = 45^\circ$. From $(\delta a_2 / \delta \sin [2\psi])$, $\varepsilon_{13}$ results when $\phi = 0$, and $\varepsilon_{23}$ when $\phi = 90^\circ$.

Taking the crystallographic anisotropy into account, the stress components $\sigma_{ij}$ can be calculated from

$$
\sigma_{ij} = \frac{1}{2} [s_{\phi \phi}^2(hkl) + \Delta s_{\phi \phi}^2(hkl) + s_{\phi \phi}^2(hkl)] \\
\times (\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}).
$$

(24)

This method, developed by Dölle & Hauk (1976), can also be used when there is no $\psi$ splitting (which implies that $\sigma_{13} = \sigma_{23} = 0$). It may be a useful procedure to determine whether or not the surface stress condition $\sigma_{33} = 0$ is fulfilled.

An experimental example of this kind of study (Dölle & Cohen, 1979) is discussed below. On ground steel, the $\varepsilon \sin^2 \psi$ curves shown in Fig. 4 were measured at the 211 reflection; the evaluation of stresses resulted in the residual stress tensor

$$
\begin{pmatrix}
390 & 14 & 63 \\
14 & 306 & -1 \\
63 & -1 & 92
\end{pmatrix}
$$

(components in MPa).

It is remarkable how well (20) with the stress tensor (25) substituted fits the data points. The principal axes of the stress tensor evaluated by principal axes transformation were tilted about the transverse direction of the sample $P_2$ by about $11^\circ$.
single-crystal orientations with different volume fractions $\lambda^i$, and including a volume fraction $\lambda^f$ of randomly oriented crystallites. A model similar to this has been employed by Alers & Liu (1966) for the calculation of anisotropic bulk elastic constants. Since the X-ray measurement is selective, it is necessary to modify their model in the following ways:

(1) Since preferred orientations are assumed there are only a few directions $\Phi_i\psi_i$ for which strong reflections are obtained.

(2) Because the averages have to be taken over reflecting crystallites only, the anisotropic X-ray elastic constants are obtained only for these directions $\Phi_i\psi_i$. Therefore, the orientation distribution functions, which are constant for quasi-isotropic materials, can be represented by the $\delta$ function being zero unless $\phi = \Phi_i$ and $\psi = \psi_i$.

Using the isotropic X-ray elastic constants $r_{ij}(hkl)$, (6), the anisotropic X-ray elastic constants $R_{ij}$ of such an idealized polycrystal, we can calculate by assuming (Dölle, Hauk & Zegers, 1978)

$$R_{ij}(hkl\Phi_i\psi_i) = [\lambda^i r_{ij}(hkl) + \lambda^a \langle s_{33ij} \rangle^a](\lambda^i + \lambda^a), \quad (26)$$

where anisotropic averages $\langle s_{33ij} \rangle^a$ have to be taken over the preferred orientations. If the crystallites with random orientations are neglected, $\lambda^a = 0$, and there is no superposition of the different preferred orientations for a given direction $\Phi_i\psi_i$, $R_{ij}$ does not depend on the volume fractions $\lambda^i$. In this case, $R_{ij}$ is equal to the single-crystal compliances $s_{33ij}$ referred to the laboratory system $L_i(\Phi_i\psi_i)$. If there are no preferred orientations, $\lambda^a = 0$, the isotropic X-ray elastic constants in the Reuss limit $(9a,b)$ result from (26). It is evident that by taking the weighted averages (26), the texture of the material is taken into account in a quantitative way. However, these averages and the isotropic and anisotropic limits discussed above do not consider the interaction of crystallites. Additionally, real orientation distributions of crystallites are much more complicated than the assumed ones, but it will be shown that this anisotropic theory of X-ray measurement can explain many of the observed phenomena associated with textured materials, at least qualitatively and in some cases quantitatively.

In what follows, the directions $\Phi_i\psi_i$ of strong reflections and the anisotropic averages $\langle s_{33ij} \rangle^a$ related to the laboratory systems $L_i(\Phi_i\psi_i)$ will be calculated for the following preferred orientations of $\alpha$-iron:

$$\begin{align*}
(211) [01\overline{1}] \text{ or } [0\overline{1}1], \\
(111) [21\overline{1}] \text{ or } [2\overline{1}1], \\
(100) [01\overline{1}] .
\end{align*} \quad (27)$$

A (211) $[01\overline{1}]$ orientation implies that the (211) plane of a crystallite is parallel to the rolling plane and the [01\overline{1}] direction is parallel to the rolling direction. Therefore, the unit vectors coinciding with the rolling (RD), transverse (TD) and normal (ND) directions are

$$\begin{align*}
\text{RD: } & B_1 = \frac{1}{\sqrt{2}} [01\overline{1}], \\
\text{ND: } & B_3 = \frac{1}{\sqrt{6}} [21\overline{1}], \\
\text{TD: } & B_2 = B_3 \times B_1 = \frac{1}{\sqrt{3}} [\overline{1}1\overline{1}] .
\end{align*} \quad (28)$$

where components of the unit vectors $B_i$ are related to the crystal axes $A_j$. The direction cosines $\beta_{ij}$ describing the orientation of a crystallite with respect to the coordinate system $B_i$ are

$$\beta_{ij} = (B_i \cdot A_j) = \begin{pmatrix} 0 & 1/2 & \frac{1}{\sqrt{3}} \\
1/\sqrt{3} & 1/3 & 1/3 \\
2/\sqrt{6} & 1/\sqrt{6} & 1/\sqrt{6} \end{pmatrix} . \quad (29)$$

If a sample is cut from a rolled sheet in an arbitrary way, the orientation of a crystallite with respect to the coordinate system $P_i$ of the sample is

$$\pi_{ij} = (P_i \cdot A_j) = \eta_{ik} \beta_{kj} . \quad (30)$$

The matrix elements $\eta_{ij}$ ($j = 1,3$) are the components of the unit vectors $P_i$ with respect to the crystal axes $A_j$, and $\eta_{ik}$ are the direction cosines between the coordinate systems $P_i$ and $B_k$.

$$\eta_{ik} = (P_i \cdot B_k) . \quad (31)$$

If samples are cut with the rolling planes in their surfaces ($P_3 = B_3$), $\eta$ has the form:

$$\eta = \begin{pmatrix} \cos \zeta & \sin \zeta & 0 \\
-\sin \zeta & \cos \zeta & 0 \\
0 & 0 & 1 \end{pmatrix} , \quad (32)$$

where $\zeta$ is the angle from the rolling direction $B_1$ to the longitudinal direction of the sample, $P_1$. For a sample with the rolling direction $B_1$ as $P_1 (\zeta = 0)$, $\eta$ is the unit matrix $\delta_{ij}$.

The directions $\Phi_i\psi_i$ of a strong reflection from the $\{hkl\}$ planes chosen for the measurement of interplanar spacings are called the poles of $hkl$ reflections. These angles can be calculated for each of the assumed

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{Fig. 5. Poles for the (211) (a) and (310) (b) planes, calculated for the preferred orientations of $\alpha$-iron (27). The length of the radius vector is $\sin^4 \psi$.}
\end{figure}
Table 3. Anisotropic X-ray elastic constants $R_{ij}$ and stress factors $F_{ij}$ (42) calculated for preferred orientations of $\alpha$-iron (27) with an isotropic volume fraction $\lambda_i = 0.2$

<table>
<thead>
<tr>
<th>Preferred orientation</th>
<th>$\lambda_i$</th>
<th>$\psi_i$</th>
<th>$\sin^2 \psi_i$</th>
<th>$\Phi_i$</th>
<th>$hkl$</th>
<th>$R_{ij}$ in $10^{-6}$ MPa$^{-1}$</th>
<th>$F_{ij}$ in $10^{-6}$ MPa$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>(a) For the 211 reflection</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(211)[011]</td>
<td>0.6</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>211</td>
<td>-1.66 -0.90 4.58 0.0 0.0 0.0</td>
<td>-1.66 -0.90 0.0 4.58 0.0 0.0</td>
</tr>
<tr>
<td>(211)[011]</td>
<td>0.6</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>211</td>
<td>-1.28 -1.28 4.58 0.0 0.0 0.0</td>
<td>-1.28 -1.28 0.0 4.58 0.0 0.0</td>
</tr>
<tr>
<td>(211)[011]</td>
<td>0.6</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>211</td>
<td>-0.90 -1.66 4.58 0.0 0.0 0.0</td>
<td>-0.90 -1.66 0.0 4.58 0.0 0.0</td>
</tr>
<tr>
<td>(111)[211]</td>
<td>0.2</td>
<td>19.5</td>
<td>0.111</td>
<td>0.0</td>
<td>211</td>
<td>-1.01 -1.52 4.56 0.0 0.72 0.0</td>
<td>0.06 -1.52 0.0 3.49 4.62 0.0</td>
</tr>
<tr>
<td>(111)[211]</td>
<td>0.2</td>
<td>19.5</td>
<td>0.111</td>
<td>0.0</td>
<td>211</td>
<td>-1.01 -1.52 4.56 0.0 0.72 0.0</td>
<td>-1.13 -0.34 1.37 3.49 2.31 4.00</td>
</tr>
<tr>
<td>(111)[211]</td>
<td>0.2</td>
<td>19.5</td>
<td>0.111</td>
<td>0.0</td>
<td>211</td>
<td>-1.01 -1.52 4.56 0.0 0.72 0.0</td>
<td>-1.28 -1.28 0.0 4.58 0.0 0.0</td>
</tr>
<tr>
<td>(100)[011]</td>
<td>0.2</td>
<td>35.3</td>
<td>0.333</td>
<td>0.0</td>
<td>211</td>
<td>-1.01 -1.52 4.56 0.0 -0.72 0.0</td>
<td>0.06 -1.52 0.0 3.49 4.62 0.0</td>
</tr>
<tr>
<td>(100)[011]</td>
<td>0.2</td>
<td>35.3</td>
<td>0.333</td>
<td>0.0</td>
<td>211</td>
<td>-1.01 -1.52 4.56 0.0 -0.72 0.0</td>
<td>-1.13 -0.34 1.37 3.49 2.31 4.00</td>
</tr>
<tr>
<td>(111)[221]</td>
<td>0.2</td>
<td>43.1</td>
<td>0.467</td>
<td>0.0</td>
<td>211</td>
<td>-2.07 -1.84 5.93 -0.25 0.39 -0.62</td>
<td>2.01 -1.80 1.46 1.81 7.78 2.10</td>
</tr>
<tr>
<td>(111)[221]</td>
<td>0.2</td>
<td>43.1</td>
<td>0.467</td>
<td>0.0</td>
<td>211</td>
<td>-2.07 -1.84 5.93 -0.25 0.39 -0.62</td>
<td>-0.21 0.43 4.02 1.81 5.71 5.69</td>
</tr>
<tr>
<td>(111)[221]</td>
<td>0.2</td>
<td>43.1</td>
<td>0.467</td>
<td>0.0</td>
<td>211</td>
<td>-2.07 -1.84 5.93 -0.25 0.39 -0.62</td>
<td>-1.48 1.69 2.56 1.81 2.07 7.79</td>
</tr>
<tr>
<td>(100)[011]</td>
<td>0.2</td>
<td>18.4</td>
<td>0.100</td>
<td>0.0</td>
<td>211</td>
<td>-2.07 -1.84 5.93 -0.25 0.39 -0.62</td>
<td>-0.21 0.43 4.02 1.81 5.71 5.69</td>
</tr>
<tr>
<td>(100)[011]</td>
<td>0.2</td>
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<td>0.100</td>
<td>0.0</td>
<td>211</td>
<td>-2.07 -1.84 5.93 -0.25 0.39 -0.62</td>
<td>2.01 -1.80 1.46 1.81 7.78 2.10</td>
</tr>
</tbody>
</table>

H. DOLLE
preferred orientations specified in terms of $\mathbf{P}_i$ as follows:

$$q_1 = (\mathbf{P}_1 \cdot \mathbf{E}_i), \quad q_2 = (\mathbf{P}_2 \cdot \mathbf{E}_i),$$  \hspace{1cm} (33a, b)

$$\tan \psi_i = q_2 / q_1, \quad \sin^2 \psi_i = q_1^2 + q_2^2.$$  \hspace{1cm} (34a, b)

The $\mathbf{E}_i$ are the unit vectors in the crystal's axial system belonging to the $hkl$ reflection and all planes in the form must be considered. The reflections most commonly employed in stress measurements on steels are the 211 and 310. The poles of these planes within the usual measuring range ($\sin^2 \psi \leq 0.5$) are shown in Fig. 5. The numerical values of $\phi_i$ and $\psi_i$ and the specific planes reflecting are listed in Table 3.

For the calculation of transformed single-crystal compliances $s_{3ij}$ related to the system $\mathbf{L}_i$ (see Fig. 1), it is necessary to evaluate the components of $\mathbf{L}_i$ in terms of the crystal coordinates $A_i$. The vector $\mathbf{L}_3$ is identical with the particular unit vector $\mathbf{E}_i$, whose orientation with respect to the sample system $\mathbf{P}_i$ is given by $\phi_i$ and $\psi_i$. Its components $\gamma_{3112} \gamma_{32}$ expressed in crystal coordinates are:

$$\gamma_{31} = h/(h^2 + k^2 + l^2)^{1/2}; \quad \gamma_{32} = k/(h^2 + k^2 + l^2)^{1/2};$$

$$\gamma_{33} = l/(h^2 + k^2 + l^2)^{1/2}.$$  \hspace{1cm} (35a, b, c)

The vector components $\gamma_{3112} \gamma_{222} \gamma_{23}$ of the unit vector $\mathbf{L}_2$ can be evaluated from the rotation around $P_3$, keeping in mind that $\mathbf{L}_2$ is in the sample's surface (Fig. 1):

$$\mathbf{L}_2 = \gamma_{31122} \gamma_{322} \gamma_{33} = \omega_{\phi_i} \cdot \mathbf{P}_2$$

$$= \begin{pmatrix} \cos \phi_i & \sin \phi_i & 0 \\ -\sin \phi_i & \cos \phi_i & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \gamma_{21} \\ \gamma_{22} \\ \gamma_{23} \end{pmatrix}. $$  \hspace{1cm} (36)

The unit vector $\mathbf{L}_1$ can be calculated from:

$$\mathbf{L}_1 = \begin{pmatrix} \gamma_{11} \\ \gamma_{12} \\ \gamma_{13} \end{pmatrix} = \mathbf{L}_2 \times \mathbf{L}_3.$$  \hspace{1cm} (37)

The single-crystal compliances in the laboratory system $\mathbf{L}_i$ are obtained from the usual equations for the transformation of tensor components:

$$s_{3ij} = \gamma_{3m} \gamma_{3n} \gamma_{ij} P_{mnop}.$$  \hspace{1cm} (38)

With $\delta_0$ defined in (8), the transformed tensor components $s_{3ij}$ result as:

$$s'_{311} = s_{111} + \delta_0 \gamma_{112} \gamma_{23},$$

$$s'_{322} = s_{112} + \delta_0 \gamma_{122} \gamma_{23},$$

$$s'_{333} = s_{112} + \delta_0 \gamma_{122} \gamma_{23},$$

$$s'_{312} = \delta_0 \gamma_{112} \gamma_{23},$$

$$s'_{313} = \delta_0 \gamma_{112} \gamma_{23},$$

$$s'_{323} = \delta_0 \gamma_{112} \gamma_{23}.$$  \hspace{1cm} (39a-f)

As preferred orientations have been assumed, the term $<s'_{33ij}>^d$ in (26) is given by (39). Also, as

$$(\mathbf{L}_i \cdot \mathbf{L}_j) = \gamma_{1k} \gamma_{jk} = \delta_{ij},$$  \hspace{1cm} (40)

for the $h00$ and $hhh$ reflections, quasi-isotropic X-ray elastic constants result from the anisotropic theory, which are identical with the results from (9). For these reflections, by substituting (40) in (39) it can be shown that $s'_{3112}, s'_{3313}$ and $s'_{3233}$ are zero, and therefore the same conditions as for quasi-isotropic materials (see § 2) can be expected; these reflections are not affected by texture.

Anisotropic X-ray elastic constants for the poles of the 211 and 310 reflections have been calculated for volume fractions $\lambda^2$ and $\lambda^a$ corresponding to the intensity distributions published in the literature (Shiraiwa & Sakamoto, 1970; Hauk, Herlach & Sesemann, 1975). The volume fraction assumed and the calculated anisotropic X-ray elastic constants $R_{ij}$ are listed in Table 3.

Anisotropic X-ray elastic constants recently evaluated by Dölle, Hauk & Zegers (1978) for the 211 reflection of cold-rolled steels are shown in Fig. 6. The experimental results for $\psi_i = 0$ and various angles $\zeta$ (see Fig. 5) lie between the isotropic limit calculated from (9a) and the anisotropic limit for the case of the (211)[011] or [011] orientation, which furnishes the pole for $\psi_i = 0$, see Fig. 5. As the crystallographic direction changes with the cut-out direction, the anisotropic limit depends on the angle $\zeta$. Although additional experiments are necessary, it is obvious that with increasing degree of reduction the experimental values approach the anisotropic limit. However, this limit cannot be reached with a real material because it represents the elastic behavior of a free (uncoupled) single crystal.

Fig. 6. Experimental X-ray elastic constants $R_{ij}$ (Dölle, Hauk & Zegers, 1978) for the preferred orientation (211)[011] or [011]; measured in cold-rolled steels (C: 0.10%; Si: 0.34%; Mn: 1.34%) at various directions $\phi_i = \zeta$. Reduction: $\odot$ 30%; $\square$ 50%; $\triangle$ 75%. The isotropic and anisotropic limits have been calculated from (26).
3.2 Lattice strains in textured materials

For anisotropic materials, lattice strains vs $\sin^2 \psi$ can be calculated from (Dölle & Hauk, 1978)

$$\varepsilon_{33} = \frac{(d_{\psi} - d_0)}{d_0} = R_{ij} \sigma_{ij}. \quad (41)$$

In general, $R_{12}$, $R_{13}$ and $R_{23}$ are different from zero in textured materials, see Table 3. Thus, shear stresses $\sigma_{ij}$ might also cause strains $\varepsilon_{33}$ normal to the lattice plane. Using the results from (19), the relationship between lattice strains $\varepsilon_{33}$ and stresses $\sigma_{ij}$ related to the sample system $P_i$ is (Dölle & Hauk, 1979):

$$F_{ij}(\psi) \sigma_{ij}. \quad (42)$$

As opposed to $R_{ij}$, the terms $F_{ij}$ in the above equation are not tensor components. Their numerical values for the poles of the 211 and 310 reflections are also listed in Table 3. When isotropic X-ray elastic constants (6) are substituted into (42), (20) results and if the tensor (21a) is employed, the $\sin^2 \psi$ law (1) is obtained.

Some characteristic plots of lattice strain vs $\sin^2 \psi$ will be presented for the 211 reflection. For samples cut at various angles $\zeta$ for the same stress $\sigma_{13}$ = 100 MPa, different curves of $\varepsilon$ vs $\sin^2 \psi$ result, as shown in Fig. 7. Strong oscillations which have been observed by many authors (Bollenrath, Hauk & Weidemann, 1967; Shiraiwa & Sakamoto, 1970; Marion & Cohen, 1975; Hauk, Herlach & Sesemann, 1975; Dölle, Hauk & Zegers, 1978), only occur for the rolling direction, $\zeta$ = 0. The reason for this effect is a change in the sign of $R_{13}$ for the three poles at $\psi_{1} = 0$, 19.5 and 35.3°, see Table 3. For that reason, an earlier calculation (Evenschor & Hauk, 1975a) of lattice-strain distributions under the presumption $R_{13} = 0$ could not yield the oscillations observed in experimental studies. A further examination of Fig. 6 and Table 3, especially of the X-ray constants for $\psi_{1} = 0$, shows that $R_{11}$ and $R_{22}$ (connected with $\sigma_{13}$ and $\sigma_{22}$) depend on which crystallographic direction is parallel to each $L_{ij}(\phi_{0}, \psi_{1})$. The change of the elastic constants $R_{11}$ and $R_{22}$ with the orientation $\phi_{0}$ is about three times smaller than the variation in $R_{13}$.

The amount of oscillation in $d$ vs $\sin^2 \psi$ for a coarse-grained material results from the variation of all elastic constants $R_{ij}$. Oscillations due to grain statistics are only likely in recrystallized material (aluminium) and not in cold-worked materials. It is obvious that erroneous stresses might be obtained if any two-tilt method is employed for the measurement of stresses in coarse-grained or textured materials.

From comparison of the upper diagrams of Fig. 8 (isotropic case) with the lower diagrams (calculations for the three poles in the rolling direction), it is clear that transverse stresses $\sigma_{22}$ may cause additional oscillations in $\varepsilon - \sin^2 \psi$ plots. Whereas $s_{(hkl)}$, connected with $a_{22}$ according to (20), does not depend on $\psi$, $R_{22}$ or $R_{13}$ is only likely in recrystallized material (aluminium) and not in cold-worked materials. It is obvious that erroneous stresses might be obtained if any two-tilt method is employed for the measurement of stresses in coarse-grained or textured materials.

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The amount of oscillation in $d$ vs $\sin^2 \psi$ for a coarse-grained material results from the variation of all elastic constants $R_{ij}$. Oscillations due to grain statistics are only likely in recrystallized material (aluminium) and not in cold-worked materials. It is obvious that erroneous stresses might be obtained if any two-tilt method is employed for the measurement of stresses in coarse-grained or textured materials.
elastcic constants do not depend on the direction $\phi\psi$ of the measurement, the same $\epsilon-\sin^2 \psi$ distribution as in isotropic materials appears. However, the calculations have been carried out neglecting the interaction terms $t_{33}\psi$ (5). Therefore, oscillations which might be observed with these reflections cannot be caused by elastic anisotropy but there might be additional oscillations due to grain coupling or local variations in microstresses, shear stresses and stress gradients (see Table 1 and discussion concerning it). However, recent studies (Dölle & Cohen, 1979) on a 75% cold rolled steel have shown that for the 200 reflection $d$ is linear with $\sin^2 \psi$, whereas it is not so for the 211 reflection. This result supports the interpretation that elastic anisotropy is the predominant reason for nonlinear $d$ vs $\sin^2 \psi$ distributions in textured materials. In fact, on examining Fig. 5 it is clear that the 310 reflection will exhibit fewer oscillations due to elastic anisotropy in both the rolling and transverse directions.

Measurements of interplanar spacings on aluminium, copper and nickel (Bollenrath, Evers & Hauk, 1967; Hauk & Sesemann, 1976; Hauk & Kockelmann, 1978) have shown that nonlinearities on face-centered cubic materials are smaller by a factor of two. This is partially due to the smaller anisotropy of those materials (Al) but it is also due to the fact that in f.c.c. metals only low amounts of residual stresses occur.

3.3 Evaluation of stresses in textured materials

Three methods have been described in the literature: the method of texture-independent directions by Hauk & Sesemann (1976), the Shiraiwa–Sakamoto method (1970, 1972) and the method of Marion & Cohen (1975), see Table 1. All methods presume that the directions of principal stresses are known. Recently, a method for the evaluation of multiaxial stress states (21d) in textured materials, based on the anisotropic theory of elasticity, has been developed. This new method will also be discussed here, (Dölle & Hauk, 1979).

The method of texture-independent directions has been developed to evaluate uniaxial residual or applied stresses in textured materials. For particular directions and reflections there are $\psi$ angles for which the isotropic lattice strain (20) is equal to the lattice strain in textured materials (42). These $\psi$ directions are the intersection points $\psi^*$ in Fig. 7(a). Two intersections are required and this occurs only in the rolling direction. The stresses can be calculated from the ‘quasi-isotropic’ strains by using isotropic X-ray elastic constants, see § 2.1. For uniaxial stress conditions, good agreement is obtained between stresses evaluated in this manner and the applied load (Hauk, Herlach & Sesemann, 1975). However, for multiaxial stress states this method cannot be employed because the texture-independent directions depend on the magnitude of the stress components as well as on X-ray elastic constants.

Shiraiwa & Sakamoto (1970) evaluated residual stresses in textured materials, by employing single-crystal compliances $\Delta_{ijkl}$ for strains measured at the poles in a pole figure, see Fig. 5. The equation used was

$$\varepsilon_{33} = (2\Delta_{2112} \sin^2 \psi + \Delta_{0000} \sin^2 \phi + \Delta_{1122} \sin^2 \phi + \Delta_{3322} \sin^2 \phi) + (\Delta_{3322} \sin^2 \phi + \Delta_{1122} \sin^2 \phi) \sigma_1,$$

(43)

where $\gamma_{3\Delta}$ has been explained in (35) and $\chi_{ki}$ are the direction cosines between the crystallographic axes $(k)$ and the principal axes $(i)$ of the stress tensor (21a). This model of uncoupled crystallites (Reuss, 1929; Möller & Martin, 1939) has been put in a more general form by Dölle & Hauk (1978) and has been described in §§ 3.1 and 3.2.

The method of Marion & Cohen (1975) starts from considerations of Greenough (1951) and of Bollenrath, Hauk & Weidemann (1967). While the first author considered microstresses in quasi-isotropic materials, the latter correlated the lattice strain, and especially the oscillations in $d$ vs $\sin^2 \psi$, with the deformation texture. The equation used for the evaluation of ‘macrostress’, $\sigma_1$ parallel to the rolling direction is (Weidemann, 1966; Marion & Cohen, 1975)

$$d_\phi = 0, \psi = \frac{1}{2} s_2(hk\ell) d_0 \sigma_1 \sin^2 \psi + d_B + (d_{\text{max}} - d_B) f(0, \psi),$$

(44)

where the first term describes strains due to macrostresses (linear with $\sin^2 \psi$) and the last one oscillations due to microstresses. $d_B$ is the interplanar spacing in dislocation-poor regions, $d_{\text{max}}$ the interplanar spacing for the direction of strongest reflection and $f(0, \psi)$ the intensity distribution for the rolling direction. The function $f(0, \psi)$ is normalized by setting $f(0, \psi) = 1$ for
the maximum integrated intensity. The major deficiency involved in this method is that isotropic X-ray elastic constants are used. The theory described in the previous section clearly shows that oscillations may also occur from homogeneous stresses in textured material due to elastic anisotropy but there may be more than one source of oscillations.

Starting from (42), Dölle & Hauk (1979) recently presented a method for the evaluation of multiaxial stress states (21d) in textured materials. The authors suggested carrying out measurements (intensity and peak location) for the directions $\Phi, \Psi$, of a pole figure, see Fig. 5. When the interplanar spacing $d_0$ of the stress-free state is known, stresses can be evaluated from strains by a least-squares fit to (42) using experimental values of X-ray elastic constants or those calculated according to (26) (see also Table 3). If there is evidence for a surface stress state (21a, b), the last three terms in (42) can be omitted and a least-squares fit can be computed for the variables $\sigma_{11}$, $\sigma_{12}$ and $\sigma_{22}$ only. Unfortunately, this method is not simple enough to be employed in practical situations. Therefore, as an alternative, the measurement (Dölle & Cohen, 1979) can be performed with the 310, h00 or hhh reflections. Since no (or only small) oscillations should occur according to this approach (§ 3.1), the methods of § 2.3 or the classical methods can be used to evaluate the stresses.

4. The influence of steep stress gradients

The influence of stress gradients on a stress measurement with X-rays was first discussed by Osswald (1948) and later by Macherauch (1956); Kelly, Short & Evans (1971); Shiraiwa & Sakamoto (1972); Lei & Scardina (1976). In general, corrections due to the penetration depth $\tau$ of X-rays and the removal of surface layers (Kelly, Short & Evans, 1971; Lei & Scardina, 1976) are necessary. It is well known that the average stress evaluated by X-rays deviates from the stress in the surface when gradients are bigger than 2 MPa $\mu$m$^{-1}$. However, for ground or shot-peened surfaces of steels, steep gradients sometimes occur which can be bigger than this limit by a factor of ten or more (Lessels & Brodrick, 1956; Iwanaga, Namikawa & Aoyama, 1972; Shiraiwa & Sakamoto, 1972; Schreiber, 1976).

Additionally, the influence of such stress gradients on the linearity of $d$ vs $\sin^2 \psi$ has been studied. While Shiraiwa & Sakamoto (1972) and Dölle (1978) calculated only small nonlinearities for the stress tensors (21a) with gradients in $\sigma_{11}$ and $\sigma_{22}$, Peiter & Lode (1976) argued that multiaxial stress-states (tensor 21d) and steep gradients are the reasons for oscillations in $d$ vs $\sin^2 \psi$ curves, see Table 1. However, the theory of Peiter & Lode (1976) is defective because the absorption of X-rays was taken into account in an unrealistic way and, indeed, there is no experimental evidence for this explanation, because oscillations usually persist even after the near surface layers are removed (Dölle, Hauk & Zegers, 1978; Quesnel, Mshii & Cohen, 1978).

In the following, a theoretical approach to the problem of near-surface stress gradients will be presented, which can be employed for isotropic as well as for textured materials. For the calculation it will be assumed that the interplanar spacing $d_0$ of the stress-free state and the X-ray elastic constants are not altered by a free surface (Stickforth, 1966), where $z = 0$. Actually, slow variations of both parameters will not affect the results. In the surface, only the stress tensor (21b) is possible, while in the interior of the sample the general stress state (21d) can occur. Thus, not only gradients in $\sigma_{11}$, $\sigma_{12}$ and $\sigma_{22}$ have to be taken into account, but also for the other stress components. Note that the effect of $\psi$ splitting, discussed in § 2.2, is impossible unless gradients with respect to $z$ in $\sigma_{13}$ or $\sigma_{23}$ are present, because these components must vanish at the surface. It will also be assumed that the stress components $\sigma_{ij}$ depend only on $z$, and that local strains $\epsilon_{33}^i$ ($\varphi, \psi, z$) are caused by local stresses $\sigma_{ij}$. The intensity $dI$ reflected by unit volume $dV$ at depth $z$ can be written (Macherauch, 1956; Cullity, 1956)

$$dI \approx \exp(-\mu l) dV,$$

where $l$ is the path length of the X-ray beam within the sample and $\mu$ is the linear absorption coefficient. The path length depends on $\psi$ and the Bragg angle $\theta$. For an $\Omega$ goniometer, the $\psi$ tilt occurs about the $2\theta$ axis, which is perpendicular to the diffractometer plane. Therefore,

$$l = 2z \sin \theta \cos \psi / (\sin^2 \theta - \sin^2 \psi).$$

In recent years in Europe, the $\psi$ goniometer (Macherauch & Wolfstieg, 1977) has become popular, for which the $\psi$ tilt is around an axis perpendicular to the $2\theta$ axis and parallel to the goniometer plane. For this geometry,

$$l = 2z / \sin \theta \cos \psi.$$

Defining the actual penetration depth of X-rays by

$$\exp[-\mu l] = 1/e \quad \text{for} \quad z = \tau,$$

the penetration depth becomes (Wolfstieg, 1976)

$$\tau_0 = (\sin^2 \theta - \sin^2 \psi) / 2 \mu \sin \theta \cos \psi,$$

and the intensity can be rewritten as

$$dI \approx \exp[-z/\tau] dV.$$

Therefore, the information included in a strain average $\langle \epsilon_{33}'(\varphi, \psi) \rangle$ over a depth $z$ is:

$$\langle \epsilon_{33}'(\varphi, \psi) \rangle = \int_0^D \epsilon_{33}'(\varphi, \psi, z) \exp[-z/\tau] dz / \int_0^D \exp[-z/\tau] dz,$$

where $D$ is the thickness of the sample. For isotropic materials $\epsilon_{33}'$ from (20) has to be substituted in (50). For $\varphi = 0,$
THE EVALUATION OF (RESIDUAL) STRESSES BY X-RAYS

\[
\langle \varepsilon'_{33}(\phi, \psi) \rangle = \frac{1}{2} s_2(hkl) \left[ \langle \sigma_{11} \rangle \sin^2 \psi \\
+ \langle \sigma_{13} \rangle \sin 2\psi + \langle \sigma_{33} \rangle \cos^2 \psi \right] \\
+ s_1(hkl) \left[ \langle \sigma_{11} \rangle + \langle \sigma_{22} \rangle + \langle \sigma_{33} \rangle \right],
\]

(51)

with

\[
\langle \sigma_{ij} \rangle = \int_{0}^{R} \sigma_i(z) \exp \left[ -z/\rho \right] dz/\int_{0}^{R} \exp \left[ -z/\rho \right] dz \\
\approx \sigma_i(z=0) + \int_{0}^{R} \exp \left[ -z/\rho \right] g_i(z) dz,
\]

(52)

where \( g_i(z) \) are the stress gradients with respect to the depth \( z \):

\[
g_i(z) = \frac{d}{dz} \sigma_i(z). \tag{53}
\]

Thus, the resulting \( d \) vs \( \sin^2 \psi \) will be determined by the stresses in the surface (\( z = 0 \)), the stress gradients near the surface and the penetration depth \( \tau(\psi, \theta) \). Typical \( d \) vs \( \sin^2 \psi \) plots are shown in Fig. 9. Only when steep gradients are present will the second term in (52) contribute appreciably to the average strain measured. The nonlinearities in \( d - \sin^2 \psi \) plots caused by gradients are generally small.

The theory presented is equivalent to the considerations of Shiraiwa & Sakamoto (1972) if the stress tensor \( (21a) \) is substituted into (50). Moreover, when (42) is substituted into (50), the influence of stress gradients on \( d \) vs \( \sin^2 \psi \) for textured materials can be studied.

5. Conclusions

Recommendations for the practical application of X-ray stress measurement have been developed by American, Japanese and German groups. Unfortunately, these recommendations do not include the problem of nonlinear \( d \) vs \( \sin^2 \psi \) distributions detected in recent years. Thus, the information presented here should be considered when a stress evaluation is performed on heavily cold-worked materials (Dölle & Hauk, 1977; James & Cohen, 1979).

In general, the influence of gradients, shear stresses and texture may be present at the same time but usually only one influence is dominant. If any two-tilt method is employed, nonlinear \( d \) vs \( \sin^2 \psi \) can lead to erroneous results. Therefore, this approach should be employed only when the deformation history is known and a linear \( d - \sin^2 \psi \) dependence can be expected or has been verified in the laboratory.

In order to recognize \( \psi \) splitting caused by machining, measurements are necessary for positive and negative \( \psi \) directions or with \( \psi \) positive and at \( \varphi \) and \( \varphi + 180^\circ \). Since misalignments of the goniometer can cause an apparent \( \psi \) splitting, this source of errors must be carefully eliminated in alignment, and checked by examining \( d \) vs \( \sin^2 \psi \) for \( \pm \psi \).

If the material has a strong texture, \( d - \sin^2 \psi \) distributions for the same direction in the specimen depend strongly on the \( hkl \) planes. It may be possible to circumvent these oscillations in \( d \) vs \( \sin^2 \psi \) by employing \( h00 \) or \( hhh \) reflections for any texture and/or material. Alternatively, quasi-isotropic directions or anisotropic X-ray elastic constants can be employed. With steels there is less effect with the 311 reflection than the 211. Stress gradients cause additional small nonlinearities. As the effects of shear stresses and texture superimpose on the small effects due to gradients, the stress distribution should be evaluated by etching.

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