A model for calculating diffraction elastic constants

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A model for calculating diffraction elastic constants

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A model, dubbed the inverse Kröner model, is proposed to calculate the diffraction elastic constants from the elastic constants of a single crystal. It is related to the classic Kröner model, and both are identified as bounds on the diffraction elastic constants. Through the grain shape as controlling parameter, the classic Kröner model is bound by the hkl-independent mechanical limit given by the bulk elastic constants of the matrix, while the inverse Kröner model approaches the Reuss limit.

1. Introduction

Diffraction elastic constants (DECs) provide a relationship between elastic lattice strains and macroscopic stress. As such, they form the basis of diffraction stress determination. The models used for the calculation of DECs have undergone a very long development from the Reuss model (Möller & Martin, 1939), the Reuss–Voigt average, as suggested by Hill (Hill, 1952), the Kröner model (Bollenrath et al., 1967; Behnken & Hauk, 1986), and, more recently, the use of perturbation theory by de Wit (1997). First and foremost, DECs depend on the Miller indices (hkl) of the reflection used for measuring the lattice spacings. Secondly, from Eshelby’s theory (Eshelby, 1961) it is known that the strain/stress response of a single grain depends on the elastic properties of its surroundings as well as its shape. Prominent examples where these interactions come into play are composites of hard particles that reinforce an elastically soft matrix. DECs are orientation-selective averages over a subset of all grains, and therefore these dependencies remain valid to a degree. Thirdly, it is known from various experimental results (Barral et al., 1977, 1978; Doelle et al., 1977, 1978; Baczynski et al., 1993; Dölle, 1979; Hauk, 1997) that preferred orientation of grains can have a profound effect on the magnitude and orientation dependence of DECs. Consequently, one should expect that DECs themselves depend on these factors. The Kröner theory is the only model that can account for all of these effects, yet the literature shows that, because of the relative simplicity of the calculations and despite their shortcomings, the Reuss model and the Reuss–Voigt average are used predominantly. For isotropic aggregates and multiphase polycrystals in which the elastic properties of the constituents are not too dissimilar, the Reuss–Voigt average and the Kröner model yield results in acceptable to good agreement with measured DECs. Other models such as the modified Voigt model (Murray & Noyan, 1999), de Wit’s model and the geometric average (Baczynski et al., 1993; Moraviec, 1989; Matthews & Humbert, 1993) have not yet been compared with experimental results on a wider scale.

There are relatively few comparative data for materials with preferred orientation, partly because the techniques used to compare experimental results vary widely. For example, recalculated stresses are sometimes compared with a known applied stress, thus reducing the quality measure of the DEC model used to a single number comparison. A comparison of angular distributions of measured and recalculated lattice strains has considerably more detail to offer but it also has to reproduce the magnitude of the applied stress. A more appropriate comparison can be gleaned from measured DECs themselves. However, measuring DECs requires a large number of measurements because lattice strains have to be measured for different tilt angles ψ and azimuth angles φ, as well as for several applied stresses. This type of relationship is conveniently expressed as stress factors \( F_{ij} \). An alternative expression for \( F_{ij} \) is developed in the following.

2. Theoretical considerations

The stress factors (Doelle et al., 1977, 1978; Dölle, 1979; Barral et al., 1987; Hauk, 1997; Koch et al., 2004; Ortner, 2006) are defined as

\[
\varepsilon(\varphi, \psi, hkl) = \frac{d(\varphi, \psi, hkl) - d_{ij}(\varphi, \psi, hkl)}{d_{ij}(\varphi, \psi, hkl)}
\]

\[
\frac{\partial \varepsilon(\varphi, \psi, hkl)}{\partial \sigma_{ij}} = F_{ij}(\varphi, \psi, hkl)\sigma_{ij},
\]

(1)

where \( \varepsilon(\varphi, \psi, hkl) \) is the average lattice strain of all grains oriented such that their lattice planes \( (hkl) \) contribute to the diffracted intensity in the direction given by the azimuth \( \varphi \) and tilt angle \( \psi \). Note that the reference \( d \) spacing \( d_{ij}(\varphi, \psi, hkl) \) may depend on the orientation as well, as is the case for samples with residual stresses from plastic deformation. The \( \sigma_{ij} \) parameters are the stresses that pertain to the macroscopic aggregate. For isotropic materials without preferred orientation, \( F_{ij} \) is related to the traditionally used DECs \( s_1 \) and \( \frac{1}{2} s_2 \) through (Hauk, 1997)


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The coordinate system used in the following is shown in Fig. 1. In the following, Kroener’s notation is adopted, in which fourth-rank tensors are denoted by upper case letters if they depend on the orientation and shape of the crystallite depend on the orientation and shape of the crystal. Thus, this discussion extends to composites of noncrystalline and disfiguring crystalline materials (grains) with known elastic properties. The grains in the composite are described by an ellipsoidal shape with an orientation $\omega$ of the ellipsoidal axes. Furthermore, they are characterized by their stiffness $c_{ijkl}(g)$ and compliance $s_{ijkl}(g)$, which depend on the orientation g of the crystal lattice with respect to the specimen frame. A fourth-rank tensor dependent on the orientation $g$ is expressed as

$$a_{ijkl}(g) = \frac{1}{s_{ijkl}(g)} = \frac{1}{g_{ijkl}} a_{ijkl},$$

in which $a_{ijkl}$ is the property tensor in the crystal reference frame, $a_{ijkl}(g)$ is the tensor in the specimen system and $g_{ijkl}$ is the transformation matrix [using Bunge angles $(\phi_1, \phi_2, \phi_3)$] for the transformation from the specimen reference frame to the crystal reference frame (Bunge, 1982).

$$g(\phi_1, \phi_2, \phi_3) = \begin{pmatrix}
\cos \phi_1 \cos \phi_2 & \sin \phi_1 \cos \phi_2 & \sin \phi_2 \\
-\sin \phi_1 \sin \phi_2 \cos \phi & +\cos \phi_1 \sin \phi_2 & \cos \phi \\
-\cos \phi_1 \sin \phi_2 & -\sin \phi_1 \sin \phi_2 & \cos \phi_2 \sin \phi \\
\sin \phi_1 \sin \phi & -\cos \phi_1 \sin \phi & \cos \phi
\end{pmatrix}.$$

Note that equation (3) uses the inverse of $g$ because the transformation is from the crystal frame to the specimen frame. The overall elastic constants of the composite, $C_{ijkl}$ and $S_{ijkl}$, are considered as known. The strain and stress in a single crystallite depend on the orientation and shape of the crystallite. The relationship between the strain $\varepsilon_{ijkl}(g)$ and stress $\sigma_{ijkl}(g)$ of a single grain and the macroscopic stress $\bar{\sigma}_{ijkl}$ and strain $\bar{\varepsilon}_{ijkl}$ according to Kroener (1958) and Kneer (1965) is expressed through the transfer tensors $p$ and $q$:

$$\sigma_{ijkl}(g) = p_{ijkl}(g, \omega) \bar{\varepsilon}_{ijkl},$$

$$\varepsilon_{ijkl}(g) = q_{ijkl}(g, \omega) \bar{\sigma}_{ijkl}.$$ \hspace{1cm} (5)

Appropriate averaging of equation (6) yields the Kroener model. Because of the difficulties associated with the determination of the distribution of the grain ellipsoid-axis orientations $\omega$ (not to be confused with the crystallite orientation distribution), it is assumed in the following that the ellipsoid axes $(a_1, a_2, a_3)$ align with $(RD, TD, ND)$ (defined in Fig. 1), and average values for the ellipsoid axis aspect ratios will be used, where appropriate. Through Hooke’s law one has the relationship

$$p_{ijkl}(g) = c_{ijkl}^g \bar{\sigma}_{ijkl}(g) C_{ijkl}.$$ \hspace{1cm} (7)

However, it will be shown in the following that it is advantageous to consider the inverse tensor $p_{ijkl}(g)$ instead, where the superscript indicates the inverse fourth-rank tensor. It is obvious that, in general, $p_{ijkl}(g) \neq q_{ijkl}(g)$, which, when averaged over all orientations, was shown by Kroener (1958) to represent bounds on the overall elastic constants of the polycrystal in the form

$$\bar{\sigma}_{ijkl} < S_{ijkl} < \bar{\sigma}_{ijkl}^{-1} \quad \text{or} \quad \bar{\varepsilon}_{ijkl} > S_{ijkl} > \bar{\varepsilon}_{ijkl}^{-1}.$$ \hspace{1cm} (8)

where the inequalities indicate that $\bar{\sigma}_{ijkl}$ and $\bar{\varepsilon}_{ijkl}$ can be either an upper or a lower bound, depending on the single-crystal constants, grain shape and orientation distribution. Furthermore, it was shown by Kroener (1958) and Kneer (1965) that spherical grains or ellipsoids with randomly oriented axes averaged over all crystal orientations yield $\bar{\sigma}_{ijkl} = \bar{\varepsilon}_{ijkl}^{-1}$. It must be pointed out that, because the orientation average for DECs is not complete and involves only a small subset of grain orientations, the DECs are generally subject to a relationship of the type given by equation (8). The often-used Kroener model is therefore only one of two possible formulae, and one can express a relationship between lattice strain and macroscopic stress entirely equivalent to equation (6) as

$$\varepsilon_{ijkl}(g) = \frac{1}{p_{ijkl}(g)} \bar{\sigma}_{ijkl},$$ \hspace{1cm} (9)

which in the following is referred to as the inverse Kroener model because the inverse of tensor $p(g)$ is used. Kroener (1958) derived expressions that define $p_{ijkl}(g)$ and $q_{ijkl}(g)$:

![](image-url)
where $c_{ijkl}(g)$ is the stiffness tensor of the crystallite, $C_{ijkl}$ and $S_{ijkl}$ are, respectively, the stiffness and compliance tensors of the overall composite, and $w_{ijkl}$ is the inverse Eshelby tensor (Kinoshita & Mura, 1971; Mura, 1987; Gavazzi & Lagoudas, 1990). From equation (10), Kröner established the conditions for calculating the overall elastic constants

$$\bar{r}(g) = 0 \quad \text{and} \quad \bar{r}(g) = 0,$$

where the overbars indicate the average over all crystal orientations. Note that $r(g)$ and $\bar{r}(g)$ represent different physical quantities, where $r(g)$ is determined in units of GPa and $\bar{r}(g)$ in units of GPa$^{-1}$. Equations (15) yield two solutions, $C^{(e)}$ and $C^{(o)}$, that are not necessarily equal. As indicated before, both yield the same solution only if the grains are all spherical or ellipsoids with randomly oriented axes. Similar to the Reuss and Voigt bounds but not as straightforward, the existence of two solutions, $C^{(e)}$ and $C^{(o)}$, is to be interpreted as bounds on the overall elastic moduli. The existence of bounds is rooted in the condition of continuity of displacement (fulfilled for Voigt) and equilibrium of traction (fulfilled for Reuss) at the grain–matrix interface for all grains. If the polycrystal under consideration were to consist of needle-shaped grains aligned in the same direction, then the elastic moduli may be closer to the Voigt bound in the direction of the longitudinal axis, while Reuss bounds may be closer for flat platelet grains with their short axis aligned in the same direction.

In the case of DECs, one must calculate partial orientation averages in the sense that only those orientations contribute to the average for which a given crystal direction $h$ is parallel to a given sample direction $m$. In this case, one has both $r(g) = 0$ and $\bar{r}(g) = 0$, with the consequence that

$$S + \bar{r}(g) = C + r(g) = C^{(e)}.$$  

In fact, the whole basis of the Kröner model for DEC calculation is $H(g) = 0$. From equation (16), together with equations (11) and (12), it can be concluded that the only general exception to the inequality (16) is when both $c(g) = C$ for all orientations $g$. In other words, the grains have to be elastically isotropic (tungsten comes to mind). For all other cases, DECs calculated using the Kröner model or the inverse Kröner model [first and second parts of equation (10)] will be different from each other, except for singular combinations of grain shape and grain orientation (see discussion in §3.1 below).

Using a compact notation without indices, equation (9), which is also the right-hand side of equation (16), can now be written as

$$\varepsilon(g) = p^{-1}(g) \bar{\sigma} = \left[ \left( c(g) + c(g) - C + C_{w} \right)^{-1} \right] \bar{\sigma}.$$  

As shown previously (Barral et al., 1987; Brakman & Penning, 1988; Dölle et al., 1977, 1978; Baczynski et al., 1993; Dölle, 1979; Hauk, 1997; Pina et al., 1997; Van Houtte & De Buysier, 1993), the quantity that is measurable by diffraction is that which is in the direction of the $z$ axis of an intermediate reference frame. The $z$ axis of this intermediate coordinate system is parallel to both the direction given by the tilt and azimuth angles ($\psi, \phi$) in the specimen coordinate system and the direction $h$ [normal to the diffracting lattice planes $(hkl)$] in the fixed crystal coordinate system.

$$\varepsilon_{33}^{L} = \varepsilon(\psi, \phi, hkl) = p^{-1}_{zkl}(g^{L}, \omega) \bar{\pi}_{kl},$$  

where the overbar signifies that the orientation average is taken over rotations about $h$ for grains with the direction $h$ parallel to $(\psi, \phi)$. The transformation matrix $g^{L}$ is given by (Bunge, 1982)

$$g^{L} = g_{2} \left[ \lambda, \Phi_{B}, \alpha, \beta \right] g_{1} \left[ \omega, \phi, \psi, 0 \right];$$  

as the product of the transformation $g_{1}$ from the specimen coordinate system to the intermediate system and $g_{2}$ as the transformation from the intermediate system to the fixed crystal coordinate system. The inverse of $g^{L}$ is used in equation (3) to calculate all orientation-dependent tensors in equation (17). The position of the variables in the curly brackets determines which of the angles $\{\omega, \phi, \psi\}$ they replace. The angles $\Phi_{B}$ and $\beta_{B}$ are tilt and azimuth angles of the direction $h$ in the Cartesian crystal coordinate system that is normal to the lattice planes $(hkl)$. The elastic property tensors are referenced in a Cartesian coordinate system which means that, in the case of non-Cartesian unit cells, the real space direction normal to the lattice planes $(hkl)$, i.e. the strain ‘direction’ or scattering vector direction, has to be calculated. With the lattice parameters $a, b, c, \alpha, \beta, \gamma$, and using the transformation given by Sands (1995), one obtains for $\Phi_{B}$ and $\beta_{B}$

$$\Phi_{B} = \arccos \left[ \frac{h_{x}}{\left( h_{x}^{2} + h_{y}^{2} + h_{z}^{2} \right)^{1/2}} \right], \quad \beta_{B} = \arccos \left[ \frac{h_{y}}{\left( h_{x}^{2} + h_{y}^{2} \right)^{1/2}} \right].$$

As shown previously (Barral et al., 1987; Brakman & Penning, 1988; Dölle et al., 1977, 1978; Baczynski et al., 1993; Dölle, 1979; Hauk, 1997; Pina et al., 1997; Van Houtte & De Buysier, 1993), the quantity that is measurable by diffraction is that which is in the direction of the $z$ axis of an intermediate reference frame. The $z$ axis of this intermediate coordinate system is parallel to both the direction given by the tilt and azimuth angles ($\psi, \phi$) in the specimen coordinate system and the direction $h$ [normal to the diffracting lattice planes $(hkl)$] in the fixed crystal coordinate system.
where \( V = abc(1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma)^{1/2} \). Equation (21) assumes that \( \mathbf{x} = a \mathbf{a} + b \mathbf{b} + c \mathbf{c} \) and \( \mathbf{z} = (a \times b) \times \mathbf{x} \) and \( \mathbf{z} = (a \times b) \times \mathbf{x} \), where \( (x, y, z) \) are the Cartesian base vectors of the transformed crystal lattice. The base vector orientation must agree with that used in the measurement of the elastic property tensors, which requires confirmation especially in the case of monoclinic and triclinic symmetry. The angle \( \lambda \) is the rotation angle about \( \mathbf{h} \), and it runs from 0 to \( 2\pi \). Generally, one has to assume that some degree of preferred grain orientation is present, which requires the use of averages weighed by the orientation distribution function (ODF) \( f(g^2) \). In practical terms, both Kröner-type models, the Reuss model and the Voigt models can be written as follows (Hauk, 1997; modified Voigt: Murray & Noyan, 1999):

Kröner:

\[
F_{kl} = \frac{q_{3kl}(g^2)}{2\pi} \int_{0}^{2\pi} \left[ \delta + t(g^2) \right]_{ijkl} m_{i} m_{j} f(g^2) \, d\lambda \; \; \; (22a)
\]

Inverse Kröner:

\[
F_{kl} = \frac{p^{-1}_{3kl}(g^2)}{2\pi} \int_{0}^{2\pi} \left[ C + r(g^2) \right]_{ijkl} m_{i} m_{j} f(g^2) \, d\lambda \; \; \; (22b)
\]

Voigt:

\[
F_{kl} = m_{i} m_{j} f(g^2) \; (ijkl) \; \; \; (22c)
\]

Modified Voigt:

\[
F_{kl} = m_{i} m_{j} \left[ \frac{2\pi}{0} \int f(g^2) \, d\lambda \right]_{ijkl} \; \; \; (22d)
\]

Reuss:

\[
F_{kl} = \frac{2\pi}{0} \int s_{ijkl}(g^2) m_{i} m_{j} f(g^2) \, d\lambda \; \; \; (22e)
\]

Here, \( m_{i} \) are components of the measurement direction

\[
m = (\cos \varphi \sin \psi \; \sin \varphi \sin \psi \; \cos \psi)\; \; \; (23)
\]

Alternatively, in equation (22c), the single-crystal constants \( c(g^2) \) can be replaced by matrix constants \( C_{ijkl} \) calculated using the Kröner model, which would yield a better approximation of the mechanical average. The integrations in equations (22a), (22b), (22d) and (22e) are performed numerically such that for each \( \lambda \) the matrix product (9) is calculated, and the Euler angles \( \{\varphi_{1}, \varphi_{2}, \varphi_{3}\} \) are determined from the matrix components in equation (4).

It should be emphasized that, regardless of the model used in equations (22a)–(22e), the stress factors contain no implicit statement about the stress or strain state of the grains themselves, but rather how the lattice strains change in response to changes in the macroscopic stresses. Thus, any pre-existing strains in the grains, be it from plastic anisotropy, elastic misfit or thermal expansion, are immaterial to this calculation.

3. Examples

For a discussion of examples we will focus entirely on ferritic low-alloy steel (α-iron). Because of its industrial importance, this material has the most detailed body of theoretical analysis and published experimental data. This material will allow the study of the effects of preferred orientation and grain shape with good sensitivity, owing to the appreciable elastic anisotropy visible in measured lattice strain distributions, combined with high strength (large magnitude of elastic strains).

3.1. Isotropic case (no preferred orientation)

Concentrating for now on spherical grains without preferred orientation, we find that, in terms of the familiar quantities \( s_{1} \) and \( s_{2} \), the inverse Kröner model falls between the Kröner and Reuss models (Fig. 2).

However, unlike the intersecting DECs for the Reuss and Voigt models, \( s_{2} \) and \( s_{1} \) do not intersect for either the inverse Kröner model or the Kröner model, and one is always greater than the other. One should note that, in the case of grains in the form of aligned nonspherical ellipsoids, \( s_{1} \) and \( s_{2} \) become dependent on \( (\varphi, \psi) \), and the relationship between lattice strain and macroscopic stress must be expressed by the stress factors \( F_{ij} \) in equation (1). Both models yield substantially different results if the grains are oriented such that the difference between the tensors \( [C + r(g^2)] \) in equation (17) is large, and this is amplified by extreme grain shapes as in the case of the 100 reflection. This is shown in Fig. 3.

One must be careful not to assume that the DECs display similar symmetries to the overall or matrix elastic constants. In particular, the DECs for spherical grains \( (a_{1} = 1, a_{2} = 1, a_{3} = 1) \) are not equal in both models, as predicted above in the discussion of the inequality in equation (16). This could be interpreted as placing upper and lower bounds on the DEC. However, as stated originally by Kröner [equation (8)], the tensors \( p \) and \( q \) may have interchangeable roles. In fact, the intersecting curves in Fig. 3 show that this is the case for the Kröner and inverse Kröner models, with the grain shape as the controlling factor. The asymptotic behavior of both models is particularly revealing: for grains in the form of very thin plates, the Kröner model yields stress factors that for all \( hkl \) converge to the value of the mechanical limit \( F_{11}(0,0) = -\varepsilon E \).

Note that this value is closely related to the Voigt value but numerically different, because the matrix elastic constants were calculated using the Kröner model and not the Voigt model. The opposite behavior is found for the inverse Kröner
model: the \( hkl \) dependence becomes even more apparent and the model reaches the limit of values calculated by the Reuss model for each \( hkl \). The stress factors in the mechanical limit for all \( hkl \) are calculated using equation (2) with \( s_1 = \nu/E \) and \( \frac{1}{2}s_2 = (1 + \nu)/E \). Poisson’s ratio \( \nu \) and Young’s modulus \( E \) are calculated from the matrix elastic constants (Table 1). Isotropic constants are usually sufficient in accuracy (SC isotropic in Table 1), and the following formulae can be used (Hauk, 1997):

\[
E = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{C_{11} + C_{12}} \quad \text{and} \quad \nu = \frac{C_{12}}{C_{11} + C_{12}}.
\]  

The argument presented for the asymptotic behavior of the Kröner-type models is a numerical one, i.e. it was inferred from the convergence of \( hkl \) at the extremes of elastic crystal anisotropy (100 and 111 in the cubic case) that this is the case for all \( hkl \). This procedure was applied to other materials including corundum, niobium, titanium and uranium, all of which cover a wide range of crystal symmetries and elastic anisotropies. All showed the same behavior of asymptotically reaching the respective limits of the mechanical average (Kröner) and Reuss (inverse Kröner).

### Table 1
Overall (matrix) elastic constants calculated using different models (GPa).

<table>
<thead>
<tr>
<th>Model</th>
<th>( C_{11} )</th>
<th>( C_{22} )</th>
<th>( C_{33} )</th>
<th>( C_{12} )</th>
<th>( C_{13} )</th>
<th>( C_{23} )</th>
<th>( C_{44} )</th>
<th>( C_{55} )</th>
<th>( C_{66} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Voigt</td>
<td>294.9</td>
<td>293.1</td>
<td>297.1</td>
<td>114.0</td>
<td>110.1</td>
<td>111.8</td>
<td>86.8</td>
<td>85.1</td>
<td>90.0</td>
</tr>
<tr>
<td>Reuss</td>
<td>275.3</td>
<td>273.5</td>
<td>277.6</td>
<td>123.9</td>
<td>119.8</td>
<td>121.6</td>
<td>72.1</td>
<td>70.6</td>
<td>74.4</td>
</tr>
<tr>
<td>SC [50,50,1]</td>
<td>285.5</td>
<td>282.4</td>
<td>287.3</td>
<td>119.2</td>
<td>114.3</td>
<td>117.4</td>
<td>81.6</td>
<td>79.2</td>
<td>81.5</td>
</tr>
<tr>
<td>SC [3.2,2.8,1]</td>
<td>286.0</td>
<td>283.5</td>
<td>287.2</td>
<td>118.6</td>
<td>114.1</td>
<td>116.3</td>
<td>80.1</td>
<td>78.1</td>
<td>82.4</td>
</tr>
<tr>
<td>SC, isotropic</td>
<td>282.4</td>
<td>282.4</td>
<td>282.4</td>
<td>118.3</td>
<td>118.3</td>
<td>118.3</td>
<td>82.05</td>
<td>82.05</td>
<td>82.05</td>
</tr>
</tbody>
</table>

### 3.2. Preferred orientation

A study of the literature also shows that the Fe(211) reflection is very sensitive to the elastic effects of preferred orientation in terms of the variability of the slope \( d/(\sin 2\psi) \). This reflection is also one of those most frequently used in residual stress measurements on ferritic steel. In the extreme, a large tensile stress can produce \( d \) spacings that decrease with \( \sin 2\psi = 0.2–0.4 \). This reflection is therefore well suited to studying the quality of DEC model predictions.
The samples used here are HSLA50 sheet metal extracted as uniaxial tensile samples (60 mm long ||RD, 5 mm wide ||TD, 0.7–1.0 mm thickness ||ND) from larger sheets of as-received material and from a sample strained to 20% in equibiaxial mode. HSLA50 is a high-strength low-alloy ferritic steel used for automotive applications. It has the composition given in Table 2.

The single-crystal elastic constants used throughout are for pure iron: $c_{111} = 237$, 141 and 116 GPa (Alexandrov & Ryzhova, 1961). A second sample with the same strain history was used to extract five small plates (5 x 5 mm) to form a sample of roughly cuboidal shape for neutron diffraction pole-figure measurements of the 110, 200 and 211 reflections. This mode of operation was made necessary by the relatively small area of uniform strain on the biaxially expanded sheet sample. Also, the neutron diffraction experiments, performed at NIST (Brand et al., 1997), allowed the measurement of full pole figures. The equibiaxially expanded sample was used in subsequent X-ray measurements (211 reflection, Cr Kα radiation) under five different levels of applied stress. The as-received sheet was used to extract five tensile samples, which were stacked together in a common fixture for stress testing in radiation) under five different levels of applied stress. The as-received sheet was used to extract five tensile samples, which were stacked together in a common fixture for stress testing in

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Si</th>
<th>Nb</th>
</tr>
</thead>
<tbody>
<tr>
<td>as received</td>
<td>0.05</td>
<td>0.44</td>
<td>0.009</td>
<td>0.01</td>
<td>0.03</td>
<td>0.023</td>
</tr>
<tr>
<td>20% equibiaxial</td>
<td>0.05</td>
<td>0.44</td>
<td>0.009</td>
<td>0.01</td>
<td>0.03</td>
<td>0.023</td>
</tr>
</tbody>
</table>

![Figure 4](image)

Inverse pole figures for ND, with levels in steps of 1 x multiples of random density (m.r.d.), for the HSLA as-received sample and after 20% equibiaxial deformation.

**Table 2**

Chemical composition of HSLA 50 in wt%; Fe provides the remainder.

Interpolation between neighboring values on the $5 \times 5 \times 5$ grid. The cumulative effect of the numerical uncertainty from this interpolation was determined in two ways. Firstly, using the thus-read ODF, pole figures were calculated for all 24 permutations ($hkl$, $klh$, ...) of the 211 reflection, and secondly, stress factors were calculated for the same permutations. Because each $hkl$ permutation results in a different but symmetry-equivalent fibre orientation $m|hl$ through Euler space, a comparison between fibres allows the quantification of the numerical accuracy of the method. The relative deviations among different permutations $hkl$ for both pole figures and stress factors were of the order of 2% without bias, which was regarded as sufficiently small.

Equation (17) requires the rotation of the single-crystal stiffness tensor $c(g)$, for which the orientation matrix $g$ has to be calculated in each sample direction $m = (\varphi, \psi)$ using equation (19). More specifically, the numerical integration in equations (22) over discrete rotation angles $\lambda$ requires the calculation of $g^\lambda$ from equation (19) for each $\lambda$, and then use of inverse trigonometric functions on the matrix elements in equation (4) to obtain the Bunge angles $(\varphi_1, \Phi, \varphi_2)$, together with the ODF value for $f(g^\lambda)$ in equations (22).

**3.2.2. Matrix elastic constants.** Through equation (17) the integrations in equations (22) also require the overall or matrix elastic constants of the polycrystal. These were determined through both equations (15) using a Newton–Raphson root-finding iteration. For comparison, the upper [Voigt, equation (25a) below] and lower bounds [Reuss, equation (25b) below] on the matrix elastic constants were also calculated, with the results shown in Table 1:

$$C_{ijkl}^V = \frac{\int \int c_{ijkl}(g^\lambda) f(g^\lambda) \sin \varphi \, d\varphi_1 \, d\varphi_2}{\int \int f(g^\lambda) \sin \varphi \, d\varphi_1 \, d\varphi_2}, \quad (25a)$$

$$C_{ijkl}^R = \left[ \frac{\int \int s_{ijkl}(g^\lambda) f(g^\lambda) \sin \varphi \, d\varphi_1 \, d\varphi_2}{\int \int f(g^\lambda) \sin \varphi \, d\varphi_1 \, d\varphi_2} \right]^{-1}. \quad (25b)$$

Inspection of the values in Table 1 shows that, compared with the Reuss/Voigt bounds in self-consistent (SC) estimates, the effect of both grain shape and preferred orientation on the overall elastic constants is small. Also, the SC estimates fall approximately in the middle between the Voigt and Reuss estimates. Therefore, the use of the Voigt/Reuss bounds as matrix constants should show the full extent of the matrix effect on the DECs (Fig. 5). It should be emphasized that the calculation of the matrix constants is not per se a necessity because one could use matrix elastic constants that were measured in some way. An example where this may be the more appropriate solution is a multiphase material where only the preferred orientation of one phase is known or measurable.

**Figure 4**

Inverse pole figures for ND, with levels in steps of 1 x multiples of random density (m.r.d.), for the HSLA as-received sample and after 20% equibiaxial deformation.
practical purposes they are set to the width of the SC graphs in Fig. 5. DECs, which deviate from one another by less than the line matrix elastic constants yield similarly small differences in the given in the table. As shown in Fig. 5, the effect of the matrix constants calculated using the Reuss model, UB stands for the Voigt model and SC is the self-consistent estimate for the average grain shape [3.2,2.8,1]. The values are listed in Table 1.

The average grain shape of [3.2,2.8,1] was estimated using an optical intersect method for the as-received sample (average grain shape [1.85,1.6,1]) with subsequent 20% biaxial elongation in-plane and contraction in the normal direction due to volume conservation. Electron-backscatter diffraction measurements on the strained sample were not feasible because of the high dislocation density.

In the two solutions to equation (15), the differences between components \( C_{ij}^{(r)} - C_{ij}^{(t)} \) are less than 0.1, and for practical purposes they are set to \( C^{(0)} = C^{(t)} \), with the result given in the table. As shown in Fig. 5, the effect of the matrix elastic constants is weak, and it has a visible effect on the diffraction stress factors only if the Voigt or Reuss bounds are used. The small differences between the SC estimates of the matrix elastic constants yield similarly small differences in the DECs, which deviate from one another by less than the line width of the SC graphs in Fig. 5.

\[ \begin{align*}
C_{11} & = 252,358 \text{ and } 475 \text{ MPa} \end{align*} \]

3.2.3. Stress factors. In order to facilitate the comparison of calculated stress factors with experimental data from a plastically deformed sample, it is important to separate completely the effects of intergranular strains from the stress factor measurement. Intergranular strains, also known as residual strains of the second kind (type II), are the result of plastic deformation, and they are caused by plastic anisotropy between grains of different orientations. Intergranular strains are primarily visible in the absence of other stresses, i.e., under zero applied or residual stress (see Fig. 6). Thus, any effect of intergranular strains on a stress factor measurement can be completely removed by choosing the lattice strains or \( d \) spacings at zero applied load as the reference state from which, through successive application of applied stresses, the linear elastic changes are measured for each sample direction \( \mathbf{m} = (\varphi, \psi) \). The actual stress factor determination is simply an application of Hooke’s law, here done through the slope of the linear regression of lattice strain over applied stresses (0, 141, 249, 358 and 475 MPa) (Fig. 6, right). Note that the actual sequence should start at the highest load, with the zero load measurement as the last. This way, in the absence of creep, the stress factor measurements are guaranteed to reflect only linear elastic effects, as shown in Fig. 6, right.

Using the matrix elastic constants for SC [3.2,2.8,1] from Table 1, the F11 stress factors are calculated and compared with measurements in the ND–RD plane (\( \varphi = 0^\circ \)) and in the ND–TD plane (\( \varphi = 90^\circ \)) (Fig. 7).

For the ND–RD plane, the results reflect reports in the literature (e.g., Barral et al., 1987; Baczmanski et al., 1993) that good agreement is observed using the Reuss model, while the Kröner model generally captures less well the ‘snake line’ distribution of the stress factors. Of all the models, the inverse Kröner model as introduced here shows the best agreement for platelet-shaped grains with aspect ratios [50,50,1]. Using the experimentally determined estimate of the average grain shape \([a_1 = 3.2, a_2 = 2.8, a_3 = 1]\), the agreement is still better than for the Kröner model. The modified Voigt model (Murray & Noyan, 1999) yields results very similar to the Reuss model. The sensitivity of the Kröner model to the grain shape is counterintuitive – needle grains aligned parallel to ND (not shown) would yield a better agreement than platelets.
[50,50,1]. Plate-like grains with their small dimension along ND would be expected after biaxial stretching along RD and TD. The Kröner model with [50,50,1] grains approaches the mechanical limit (close to the Voigt case). In contrast, the inverse Kröner model behaves correctly, i.e., showing better agreement as the grain shape varies from low aspect ratios [3.2,2.8,1] to thin plates [50,50,1] where, in turn, the inverse Kröner model approaches the Reuss limit of homogeneous stress. In the ND–TD plane at $\varphi = 90^\circ$, one finds a reversal of the roles of the two models. The best agreement is now found for the Kröner model using the measurement-based estimate of the grain shape [3.2,2.8,1]. For flat grains ([50,50,1]), the Kröner model approaches the mechanical limit, just as in the ND–RD plane. Remarkably, the modified Voigt model shows similarly good agreement with the measured stress factors. The inverse Kröner model, which performed best at $\varphi = 0^\circ$ with [50,50,1] as grain-shape parameters, again approaches the Reuss limit, and both show the worst agreement. Therefore, one can surmise that this type of model agreement reflects the role of $q_{ijkl}$ and $p_{ijkl}^{-1}$ as bounds, as expressed in equation (8), with the grain-shape parameters controlling the proximity to the respective Reuss or mechanical limit. Even for spherical grains, the two Kröner-type models do not start out the same, but rather in close proximity to the Reuss/Voigt average (not shown), from which, on increasing the grain aspect ratio, the Kröner model approaches the mechanical limit and the inverse Kröner model approaches the Reuss limit. This is the result of the asymptotic behavior of the Eshelby tensor for $a_1$, $a_2 >> a_3$. Here, one has nearly homogeneous strain (grain and surrounding matrix) in the directions of $a_1$ (RD) and $a_2$ (TD), while the stresses in the $a_3$ direction (ND) are zero (Mura, 1987, p. 82).

It should be pointed out that grain elongation from slip due to plastic deformation depends on the orientation of the crystal lattice of the grain. For any given orientation $(\varphi, \psi)||h$, the grains contributing to diffraction and to the integral in equation (20) will not have the same shape parameters $[a_1,a_2,a_3]$, thus making the Eshelby tensor a variable as well. This has been disregarded in this work because of the lack of appropriate data, but it provides a possible explanation of the fact that extreme ellipsoid-axes aspect ratios show the best agreement between measured and calculated stress factors in Fig. 7.

It is tempting to interpret the very good agreement of the modified Voigt model in both tilt planes (ND–RD and ND–TD) as an overall confirmation for the validity of its under-

![Figure 7](image-url)

**Figure 7**
Comparison of measured and calculated stress factors $F_{11}$ at $\varphi = 0^\circ$ (top) and $\varphi = 90^\circ$ (bottom) for the Kröner model (left), the inverse Kröner model (right), the mechanical average (calculated from SC [3.2,2.8,1] in Table 1), the Reuss model and the modified Voigt model. The sample was previously stretched to 20% equibiaxial strain. The direction of the applied stress was $\varphi = 0^\circ$, $\psi = 90^\circ$. The uncertainties (1σ) for the measured $F_{11}$, if not visible, are smaller than the size of the symbols. Orthorhombic sample symmetry (implied by the biaxial straining) was assumed and the $\psi$ and $\varphi$ branches were averaged. The matrix constants (SC [3.2,2.8,1] in Table 1) needed in the Kröner-type models were calculated from the iron single-crystal elastic constants and the ODF using equation (25a).
Table 3
Stress factors $F_{11}$ for an as-received sample of HSLA steel measured by neutron diffraction (TPa$^{-1}$).

| $hkl$ | $3\Gamma$ | $(\varphi, \psi)$ | $F_{11}$ | $1\sigma$ | Mecha-
|-------|-----------|-----------------|---------|---------|nical
|       |           |                 |         |         | modified
|       |           |                 |         |         | Voigt
|       |           |                 |         |         | Reuss
|       |           |                 |         |         | Kro-
|       |           |                 |         |         | ßner
|       |           |                 |         |         | Inverse
|       |           |                 |         |         | Kro-
  |       |           |                 |         |         | ßner
| 200 0 | (0, 0)    | -1.78 0.10      | -1.38  | -2.83  | -1.67  | -2.38  | -1.89
| 310 0 | (0, 0)    | -1.63 0.10      | -1.38  | -1.95  | -1.59  | -2.04  | -1.66
| 220 0 | (0, 0)    | -1.36 0.07      | -1.38  | -1.15  | -1.40  | -1.39  | -1.26
| 211 0 | (0, 0)    | -1.32 0.04      | -1.38  | -1.16  | -1.49  | -1.40  | -1.26
| 222 1 | (0, 0)    | -1.07 0.06      | -1.38  | -0.79  | -0.79  | -1.14  | -0.98  | -1.05

$\chi^2$ defined as $\sum([F_{11\text{meas}} - F_{11\text{calc}}^2]/F_{11\text{meas}}^2)$. Kroßer (isotropic) refers to the Kroßer model with equiaxial grains and no preferred orientation. The modified Voigt-Reuss-Kröner and inverse Kroßer models use the ODF, with these last two models using an average grain shape of $[1.85,1.6,1]$.

Table 3

4. Conclusions
A model for the calculation of diffraction stress factors, here dubbed the inverse Kroßer model, has been developed and compared with measured stress factors from a sample with strong preferred orientation. In X-ray measurements of the 211 reflection, the inverse Kroßer model yields the best

Figure 8
Measured (X-ray diffraction) and calculated stress factors $F_{11}$ (left, measured with $\sigma_{\text{appical}}|\text{RD}$) and $F_{22}$ (right, measured with $\sigma_{\text{appical}}|\text{TD}$) for the 211 reflection of the as-received sample. The Kroßer and inverse Kroßer model use the average grain shape $[1.8,1.6,1]$ and the matrix elastic constants calculated from the ODF of the as-received state. The X-ray test regimen was the same as for the equibiaxially expanded sample.
agreement with measured stress factors in the tilt plane that contains the stress direction, while the Krüner model is the best choice in the tilt plane perpendicular to the stress direction. The use of elongated flat ellipsoidal grain shapes – congruent with experimental findings – is necessary to achieve this level of agreement. For extreme grain shapes, the Krüner model reaches the $hkl$-independent limit of the bulk elastic constants, while the inverse Krüner model approaches the Reuss limit. It is concluded that both models represent bounds the Kroener principal sample directions showed a general preference for measurements of stress factors involving other closer to the respective bound.

For a sample with weak texture, neutron diffraction measurements of stress factors involving other $hkl$ along the principal sample directions showed a general preference for the Krüner model with a negligible effect from the weak texture. However, for intermediate tilt angles typical for X-ray diffraction, even weak preferred orientation has a visible effect and it should be included in stress factor calculations.

The experimental data presented here or available in the literature are not sufficient to develop a general guideline for which model to use under a given set of circumstances (grain shape, texture). However, the large differences that are expected for $h00$-type reflections for platelet grains indicate the type of experiment necessary to gain this insight. Both models should also give different results if a realistic grain shape–crystal orientation correlation (which is a result of slip) is used.

References