PROPERTIES AND GENERAL USE OF THE X-RAY ELASTIC FACTORS

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ABSTRACT

The equation \( \varepsilon(\phi, \psi, hkl) = F_{ij}(\phi, \psi, hkl)\sigma_{ij} \) can be directly deduced from Hook’s law. It is shown that the matrix \( F_{ij}(\phi, \psi, hkl) \) which is usually called X-ray elastic factors, behaves as a second rank tensor. Since this behaviour is the only criterion for the question of whether or not it is a tensor, the \( F \)-matrix must be regarded as a second rank tensor. This allows us to make some statements about the structure of the \( F \)-matrix on the basis of Neumann’s principle, to find relationships among \( F \)-matrices in different measurement directions, and to apply the methods and strategies for the measurement of a second rank tensor. All this is shown in a few examples. It is further shown that a consistent use of the \( F \)-matrix can replace all methods for data evaluation which makes use of linear regressions and in addition avoids all difficulties and disadvantages of these methods. One of these disadvantages is that the \( \sin^2\psi \)-method, as well as its derivatives, is generally not correct least square fits of the measured data. This is also shown in an example. The more complicated cases with stress or constitution gradients in the range of the probed volume or stress measurement after plastic deformation are not discussed.

INTRODUCTION

Stress measurement using X-ray and neutron diffraction seems to be strongly dominated by the \( \sin^2\psi \)-method and some methods which are similar to it or can be regarded as derivatives of the \( \sin^2\psi \)-method. They all have their merits and advantages, but also some disadvantages: (1) the necessity of having—in the theory—a linear relationship between \( \varepsilon \) and \( \sin^2\psi \), (2) the necessity of finding enough measurement points at constant azimuth \( \phi \) and in a sufficiently wide \( \sin^2\psi \) range, (3) the difficulties to apply different weights for differently accurate measurement points, and (4) because the \( \sin^2\psi \)-method is only in special cases a correct least square fit.

All these problems could be overcome if we consistently made use of the concept of the X-ray elastic factors and the standard mathematical methods for the solution of linear equations. Yet in order to do so it is also necessary to have a better understanding of the X-ray elastic factors. Only the correct understanding of the X-ray elastic factors’ properties enables us to use the full potential lying in this concept.

THE \( F_{ij}(\phi, \psi, hkl) \) MATRIX

The defining equation of the X-ray elastic factors is (see e.g. Dölle [1], Hauk [2], Lu [3], and Noyan and Cohen [4]):

\[ \varepsilon(\phi, \psi, hkl) = F_{ij}(\phi, \psi, hkl)\sigma_{ij} \]
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For $\sigma_{ij}$ one can use any stress unit, e.g. MPa or TPa, etc., therefore $F_{ij}$ must have the reciprocal unit. A notation different to Eq. (1) uses the vector $\mathbf{r}$, the measurement direction which is defined by the two angles $\varphi$, $\psi$:

$$\varepsilon(\mathbf{r}, hkl) = F_{ij}(\mathbf{r}, hkl)\sigma_{ij}$$ \hspace{1cm} (2)

The validity of Eq. (1) can simply be deduced from Hook’s law. Hook’s law not only can be applied for the relationship between an average stress and an average strain tensor, but in the same way it gives the relationship between an average stress tensor and the strain in any direction ($\mathbf{r}$), averaged over any set of grains in a polycrystalline material. If this set of different grains consists of those grains which are in the $(hkl)$ reflecting position in the direction $\mathbf{r}$ we have exactly Eq. (1) and (2).

It has been nearly 30 years since this important equation was discovered, but at the same time a statement was put forward which we regard as a mistake. This is the assertion that the matrix $F_{ij}$ must not be regarded as a tensor. We say this is not correct; $F$ is a second rank tensor. Why? Different proofs are possible, the most simple and direct is this (see also Ortner [5]): We have on the left side of Eq. (2) a value which is measured, this means it cannot change if we change the coordinate system, in other words, it is a scalar. Therefore the expression on the right side is also a scalar, one of its factors is the stress tensor, and tensor analysis tells us that the second factor, here $F_{ij}(\mathbf{r}, hkl)$, must also behave like a tensor in order that the whole expression is a scalar product. And the definition for tensor says that a matrix which behaves like a tensor is a tensor!

The question of whether $F$ is a tensor or not is more than academic hair splitting, since from the tensor character of $F$ we can draw some quite helpful conclusions.

**Symmetry of $F$**

For instance, we can deduce the symmetry of the $F$-tensor from the symmetry of the measurement direction, be it in a single crystal or in a textured polycrystalline material. This is a consequence of Neumann’s principle. An example: Let us regard a material with fibre texture, and the fibre axis is parallel to the $z$-axis [Figure 1(a)]. Then the $z$-axis has the highest possible symmetry and therefore the $F$-matrix must have this shape:

$$\begin{pmatrix} F_{11} & 0 & 0 \\ 0 & F_{11} & 0 \\ 0 & 0 & F_{33} \end{pmatrix}$$ \hspace{1cm} (3)
Figure 1. (a) Fiber texture with fiber axis parallel to $z$-axis; (b) texture with threefold symmetry axis parallel to $z$-axis.

The same would be true if the $z$-axis had a threefold symmetry as in Figure 1(b). Another example: A texture with a mirror plane (Figure 2). For any direction $\mathbf{r}$ in this plane the $F$-tensor must reflect this mirror symmetry, so its shape is

$$
\begin{pmatrix}
F_{11} & 0 & F_{13} \\
0 & F_{22} & 0 \\
F_{13} & 0 & F_{33}
\end{pmatrix}
$$

These are only a few examples regarding the symmetry of $F$, a more detailed discussion can be found elsewhere [5].

Figure 2. Texture with mirror parallel to the $x$-$z$-plane.
Relationships among $F$-tensors at different $\varphi$, $\psi$

In Figure 3(a) we see that directions A and C are crystallographically equivalent. For these two directions Eq. (5) holds, with $R$, the rotation matrix. Then the corresponding tensors are related to each other by Eq. (6), with $R^T$, the transposed rotation matrix:

$$r_C = R r_A$$  \hspace{1cm} (5)

$$F(r_C) = RF(r_A)R^T$$ \hspace{1cm} (6)

In a similar way we can also calculate $F(r_B)$ from $F(r_A)$ by applying the mirror operation with the $x$-$z$-plane as a mirror plane:

$$F(r_C) = MF(r_A)M^T$$ \hspace{1cm} (7)

Another example: fibre texture with fibre axis parallel to $z$ [Figure 3(b)]. Then all directions with the same $\psi$ are crystallographically equivalent, so for any $F(r_B)$ we have

$$F(r_B) = A(\varphi) F(r_A)A^T(\varphi):$$

$$\begin{array}{c}
\left\{ a_{ij} \right\} = \begin{pmatrix} 
\cos(\varphi) & -\sin(\varphi) & 0 \\
\sin(\varphi) & \cos(\varphi) & 0 \\
0 & 0 & 1 
\end{pmatrix} 
\end{array}$$ \hspace{1cm} (8)

A rather trivial example is the case of a quasisotropic polycrystal: All directions are equivalent and all have the highest possible symmetry. So for $F(z)$ we must have Eq. (9):
And as is well known $F_{11} = F_{22} = s_1; F_{33} = 1/2 s_2 + s_1$. From $F(z)$ we can calculate $F(r)$ for any $r$ by a simple rotation transformation. The result is Eq. (10):

$$
\begin{bmatrix}
F_{11} & 0 & 0 \\
0 & F_{11} & 0 \\
0 & 0 & F_{33}
\end{bmatrix}
$$

A closer look at $F_{11}, F_{22}, F_{12}$ shows the $\sin^2 \psi$ dependence of these in-plane components—this is the basis of the $\sin^2 \psi$-method.

**Calculation of the $F$-tensor**

The easiest case of $F$-tensor calculation is when the material has elastic isotropy. The second easiest case is that of a single crystal. When the crystal is oriented so that the crystal physical coordinate axes are parallel to the specimen axes then we have

$$
F_{ij}^{C}(r,hkl) = S_{ijkl}r_{k}r_{l}
$$

This sum at the right side is a so called tensor reduction—the forth rank compliancy tensor is reduced to a second rank tensor. Since in single crystals we are restricted to measurement directions which are orthogonal to a lattice plane $(hkl)$ we write

$$
F_{ij}^{C}(r,hkl) = S_{ijkl}h'_{k}h'_{l} / |h'|^2
$$

with $h', k', l'$ the Miller indices in the crystal physical coordinate system. And if the crystal is in any other orientation we simply have to calculate the rotated $F$-matrix, using the orientation matrix of the crystal:

$$
F_{ij}^{S}(r,hkl) = A F_{ij}^{C} A^{T}
$$

With this equation we can directly write down a formulation for the Reuss approximation of $F$ in a polycrystalline material, since we only have to calculate a mean value of the $F$-tensors of all crystallites in reflection position:
This equation looks different to what we are used to from the literature. The reason is that we do not use the so called laboratory system, but instead we go directly for each crystallite from the crystal system to the specimen system.

**Measurement of F**

Since $F$ is a symmetric second rank tensor we find the principle for its measurement in textbooks about crystal physics. The general recipe is measure longitudinal effects in different directions $s$ and then solve the resulting equation system. The longitudinal effect of a tensor $T$ in the direction $s$ is

$$T(s) = t_{ij} s_i s_j$$

What is the longitudinal effect of the $F$-tensor? We make a specimen from our material with the specimen axis in a given direction and impose a uniaxial stress on it [Figure 4(a)]. The stress is uniaxial in the test specimen but in the coordinate system of the material, $x||TD$, $y||RD$, the stress tensor looks as in Eq. (16):

$$\{\sigma_{ij}\} = \{\sigma_{ij}\} = \sigma \begin{pmatrix}
  s_1 s_1 & s_1 s_2 & s_1 s_3 \\
  s_2 s_1 & s_2 s_2 & s_2 s_3 \\
  s_3 s_1 & s_3 s_2 & s_3 s_3
\end{pmatrix}$$

---

**Equation (14)**

$$F^{S}_g (r, hkl) = F^{C}_{ma} (hkl) \frac{\int_{0}^{2\pi} a_m(\lambda) a^*_m(\lambda) f(g(\lambda)) d\lambda}{\int_{0}^{2\pi} f(g(\lambda)) d\lambda}$$
We insert Eq. (16) into Eq. (2) and divide the equation by $\sigma$:

$$\varepsilon(r,s,hkl)/\sigma = F_{ij}(r,hkl)s_i s_j$$  \hspace{1cm} (17)

Now we have the longitudinal effect of $F(r, hkl)$ in the direction $s$ and it is clear what we had to do to obtain an $F$-tensor, namely cut at least six tensile test specimens in properly chosen directions [6], apply a stress, and measure $\varepsilon$ always in the direction $r$. An example: Let us assume a free surface so $\sigma_{33} = \sigma_{23} = \sigma_{13}$ and therefore only $F_{11}, F_{22}, F_{12}$ are needed and can be measured. Eq. (2) is then reduced to

$$\varepsilon(r,hkl) = F_{11}(r,hkl)\sigma_{11} + F_{22}(r,hkl)\sigma_{22} + 2F_{12}(r,hkl)\sigma_{12}$$  \hspace{1cm} (18)

If we now take $s^A, s^B, s^C$ as in Figure 4(b) with

$$s^A = \{1,0,0\}$$  \hspace{1cm} (19)
$$s^B = \{\cos 60, \sin 60, 0\}$$  \hspace{1cm} (20)
$$s^C = \{\cos 120, \sin 120, 0\}$$  \hspace{1cm} (21)

then with Eqs. (17)–(21) we find the following simultaneous equation system which must be solved for $F_{ij}$:

$$\begin{pmatrix}
\varepsilon(r,s^A,hkl)/\sigma \\
\varepsilon(r,s^B,hkl)/\sigma \\
\varepsilon(r,s^C,hkl)/\sigma
\end{pmatrix} =
\begin{pmatrix}
1 & 0 & 0 \\
0.25 & 0.75 & \sqrt{3}/2 \\
0.25 & 0.75 & -\sqrt{3}/2
\end{pmatrix}
\begin{pmatrix}
F_{11} \\
F_{22} \\
F_{12}
\end{pmatrix}$$  \hspace{1cm} (22)

We should point to this: $r$, the measurement direction and $s$, direction of the strain samples are completely independent. Therefore with only these three samples we can measure the in-plane components of $F$ for any measurement direction $r$ and any reflecting plane $(hkl)$.

**HOW TO USE THE $F$-TENSOR**

When we look at the literature we see that there is really a great variety of different methods to calculate the stress from X-ray or neutron diffraction data. Most of them are, in one or the other way, based on the $\sin^2\psi$-method, which means they make use of a linear regression. Furthermore, all these methods have the same disadvantages as the $\sin^2\psi$-method itself, as was already described in the introduction. All these different methods can be replaced by only three equations, one is Eq. (1), the other two are derived from Eq. (1) by slight changes.

**Triaxial stress state**

When all six independent stress components are unknown we simply should use Eqs. (1) and (2) (see e.g. Lu [3] and Winholtz and Cohen [7]). And we have no reason to distinguish whether the material is a single crystal, a textured polycrystal, or a quasiisotropic polycrystal. Only the calculation of the $F$ tensors is different in each of these cases.
A method used very often to calculate all six unknown stress tensor components is one which is sometimes called Dölle-Hauk method [2] and sometimes $\psi$-differential method [3]. It is an ingenious method based on two different linear regressions. These are $[d(\phi,\psi) + d(\phi,-\psi)]/2$ over $\sin^2\psi$ and $[d(\phi,\psi) - d(\phi,-\psi)]$ over $\sin^2\psi$ (see e.g. Hauk [2], Noyan and Cohen [4], and Lu [3]). The method had clearly its merits, but since access to computers is common we would say that it is much easier to solve the linear equation system which we get from inserting the measured data into Eq. (1). And when using Eq. (1) we are not restricted to only one $hkl$, not restricted to any linear dependence, we need not to perform measurement series at constant azimuths, and with Eq. (1) we do a correct least square fit.

What difficulties can arise from the necessity to find measurement directions at constant azimuth and with sufficient difference in $\sin^2\psi$ can be inferred from Figure 5(a), the 211 pole figure of a material with (110)[001] texture.

In Figure 5(b) the intensity of the (211) reflexion for $\phi = 90^\circ$ is drawn over $\sin^2\psi$. We see that we could get measurement points only in a small range of $\sin^2\psi$, therefore we had poor accuracy of the slope $d - \sin^2\psi$. The same is true for any other azimuth ($\phi = 25^\circ$, $\phi = 55^\circ$) in Figure 5(a). When using Eq. (1) we are free to measure only in the $\phi$, $\psi$ positions with the highest (211)-intensities, and according to the rules of thumb given in Ortner [6] we would obtain a well conditioned linear equation system. We could also include without any problem one strong (220) reflection at the center of the pole figure to get an equation system with even better conditioning.

Because the above mentioned method is not a least square fit has different reasons; it is primarily attributable to the stepwise data treatment, for one azimuth after the other. In a correct least square fit all experimental data must be included in one single fitting procedure. This will be shown in more detail in a forthcoming paper [8]; here we refer only to the analogous case of the $\sin^2\psi$-method.

Figure 5. (110)[001] texture: (a) (211) pole figure; (b) intensity of (211) - $\sin^2\psi$ for $\phi = 90^\circ$. 
Biaxial stress state

A stress free surface means that $\sigma_{33} = \sigma_{23} = \sigma_{13} = 0$. With the $\sin^2\psi$-method we use only the slope of the $a$ or $c$ versus $\sin^2\psi$ plot, but we do not care about the cut between the regression line and the abscissa, which in fact means that $a_0$ is regarded as a free parameter. Doing so we obtain intermediate results, namely $\sigma$ values for three or more azimuths $\phi$, and from these we can calculate all unknown stress components $\sigma_{11}, \sigma_{22}, \sigma_{12}$. This method is the one most often used although better methods have been known for a long time [7,9].

Here we will once more explain an equation system which could replace the $\sin^2\psi$-method and so avoid all its disadvantages and errors. We again start with our basic equation Eq. (2), but now only for the in-plane stresses:

$$\varepsilon(r, hkl) = F_{11}(r, hkl)\sigma_{11} + F_{22}(r, hkl)\sigma_{22} + 2F_{12}(r, hkl)\sigma_{12} \quad (23)$$

$a_0$ is a free parameter as it is in the $\sin^2\psi$-method. So, with $\varepsilon(r, hkl) = [a(r, hkl)-a_0]/a_0$ we reshape that equation:

$$a(r, hkl) = a_0 + a_0F_{11}(r, hkl)\sigma_{11} + a_0F_{22}(r, hkl)\sigma_{22} + 2a_0F_{12}(r, hkl)\sigma_{12} \quad (24)$$

For $a_0$ we are again free to use any unit, e.g. Å, nm, or any other unit. With enough measurements $a(r, hkl)$ we obtain an equation system for four unknowns and can calculate the stress components from such an equation system. Once again the advantage is that we are free in choosing the $\phi, \psi$ pairs, and also free to combine measurements with different $hkl$s.

Back to the example of the (110)[001] texture, we can measure at exactly the intensity maxima [Figure 5(a)] and would get a well conditioned equation system. Or we could also include one 200 reflection at the center of the pole figure then conditioning would be even better.

The other advantage of Eq. (24) is it is always a correct least square fit, whereas the $\sin^2\psi$-method is only correct in some special cases. An example to demonstrate the incorrectness of the $\sin^2\psi$-method: we assume again $\sigma_{33} = \sigma_{23} = \sigma_{13} = 0$ and main stress axes known, therefore $\sigma_{12}$ can also be set to zero. Measurements are assumed to be done in the directions as shown in
Figure 6. We further assumed quasiisotropic steel with \( s_1 = -1.25 \ TPa^{-1} \), \( s_2 = 5.76 \ TPa^{-1} \). In the method according to Eq. (1), and using Eq. (10) the equation system to be solved is

\[
\begin{pmatrix}
a(0, 0) \\
a(0, 30) \\
a(0, 45) \\
a(90, 30) \\
a(90, 45)
\end{pmatrix} =
\begin{pmatrix}
1 & -1.25 & -1.25 \\
1 & 0.19 & -1.25 \\
1 & 1.63 & -1.25 \\
1 & -1.25 & 0.19 \\
1 & -1.25 & 1.63
\end{pmatrix}
\begin{pmatrix}
a_0 \\
a_0 \sigma_x \\
a_0 \sigma_y
\end{pmatrix}
\]

(25)

Eq. (25) is solved as usual with the aid of the normal equations, the result is again written in matrix notation, where the \( 3 \times 5 \) matrix on the right side is called the Moore-Penrose pseudoinverse [10]:

\[
\begin{pmatrix}
a_0 \\
a_0 \sigma_x \\
a_0 \sigma_y
\end{pmatrix} =
\begin{pmatrix}
-0.030 & 0.162 & 0.353 & 0.162 & 0.353 \\
-0.298 & 0.020 & 0.337 & -0.119 & 0.060 \\
-0.298 & -0.119 & 0.060 & 0.020 & 0.337
\end{pmatrix}
\begin{pmatrix}
a(0, 0) \\
a(0, 30) \\
a(0, 45) \\
a(90, 30) \\
a(90, 45)
\end{pmatrix}
\]

(26)

In the \( \sin^2 \psi \)-method we would plot \( a(\phi, \psi) \) over \( \sin^2 \psi \), determine the slope \( (m = a_0 \sigma_\phi 1/2s_2) \) of the regression line from which we could calculate the products \( a_0 \sigma_\phi \). This had to be done two times and independently for both azimuths \( \phi = 0^\circ \) and \( \phi = 90^\circ \).

If we do this in an analytic instead of a graphic way we can derive an equation system for \( a_0 \sigma_x \), \( a_0 \sigma_y \) similar to the second and third line of Eq. (26):

\[
\begin{pmatrix}
a_0 \sigma_x \\
a_0 \sigma_y
\end{pmatrix} =
\begin{pmatrix}
-0.347 & 0.000 & 0.347 & 0.000 & 0.000 \\
-0.347 & 0.000 & 0.000 & 0.000 & 0.347
\end{pmatrix}
\begin{pmatrix}
a(0, 0) \\
a(0, 30) \\
a(0, 45) \\
a(90, 30) \\
a(90, 45)
\end{pmatrix}
\]

(27)

To obtain \( \sigma_x \) and \( \sigma_y \) we usually insert an approximate value for \( a_0 \); in the method according to Eq. (24) we either use also an approximate value or the more accurate value which we obtain from the first line of Eq. (26).

The second and third lines of Eq. (26) and (27) are clearly different, and since we claim that using Eq. (24) gives a correct least square fit, in this case the \( \sin^2 \psi \)-method cannot be a correct least square fit. Further details about correctness or incorrectness of the \( \sin^2 \psi \)-method and similar methods will be given in another paper [8].
Constant in-plane stress

With Eqs. (1), (2), and (24) we can cover nearly all cases of X-ray stress data evaluation. Only the case where $\sigma_{13} = 0$ and $\sigma_{11} = \sigma_{22}$, $\sigma_{12} = 0$, that means $\sigma(\phi,\psi = 90^\circ) =$ constant, must be dealt in a different way. This is a simple change of Eq. (24) as given in Eq. (28):

$$a(r, hkl) = a_0 + a_0[F_{11}(r, hkl) + F_{22}(r, hkl)]\sigma_{11}$$  (28)

CONCLUSION

The X-ray elastic factors of a measurement direction ($\phi$, $\psi$) and a reflection $hkl$ constitute second rank tensors. This is especially helpful in the measurement of the entries of these matrices. The consistent use of the $F$-matrices for X-ray stress measurement, be it in single crystals or in polycrystalline materials with or without texture, in bulk materials or in thin films, has many advantages as compared to the use of the $\sin^2\psi$-method or similar methods. One advantage is the correctness in the sense of least square data fitting, which is usually not the case in the $\sin^2\psi$-method as well as in most of its derivatives (this is shown in detail in one example).

REFERENCES