WHY SHOULD WE GIVE UP THE $\sin^2 \psi$ METHOD

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ABSTRACT

The $\sin^2 \psi$ method can be formulated as a single system of simultaneous linear equations. Using this it is easy to show that the $\sin^2 \psi$ method is not a least-squares method. It further helps to compare the accuracies of the stress tensors obtained by the $\sin^2 \psi$ method and the method of least-squares. Quantitative comparisons have been made for different fictitious measurements. It is shown that the - unnecessary - loss in accuracy by using the $\sin^2 \psi$ method is quite significant and by no means negligible. The same course of action has been applied to compare the so-called Dölle-Hauk method with a least-squares method, the result is similar. Some other methods for x-ray stress determination, most often similar to the $\sin^2 \psi$ method, and their shortcomings are also discussed briefly, together with the corresponding, more effective and more versatile least-squares method.

INTRODUCTION

The $\sin^2 \psi$ method is now more than half a century old; it was - and still is - a good idea, it has been used all over the world with great success in thousands and thousands of stress measurements. But it has also some weak points, these are that it needs a special distribution of measurement directions, it is only applicable for isotropic and quasi isotropic materials, it is not applicable when measurements with different (hkl)s have been done and, in its general case, it is not a correct least-squares method.

"In the wake of the $\sin^2 \psi$ method" many different methods have been developed to overcome some of these difficulties, but without much success. These methods all suffer from one or another difficulty already found in the $\sin^2 \psi$ method.

Up to now the $\sin^2 \psi$ method has been the method of choice in the case of a stress free surface, since in this case the knowledge of the unstressed lattice constant is not necessary. If the measurement is not done at a free surface, in other words if all three diagonal elements of the stress tensor are unknowns, then a different method for the data evaluation is to be used. The traditional method used in that case is one which is similar to the $\sin^2 \psi$ method inasmuch as it also makes use of some straight line fitting, and it has difficulties similar to the $\sin^2 \psi$ method.

These above-mentioned methods – the $\sin^2 \psi$ method and some similar methods – will be discussed and compared to what I call correct methods. Special attention will be payed to the aspect of the calculated stress tensor’s accuracy.
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THE CORRECT METHOD

Methods, which are, in many respects, better than the $\sin^2 \psi$ as well as similar methods are based on two other good ideas. These are the least-squares method and Eq. (1).

$$\epsilon(\varphi, \psi, hkl) = \sum_{i,j=1}^{3} F_{ij}(\varphi, \psi, hkl)\sigma_{ij}$$

Eq. (1) was discovered nearly 30 years ago and, although one can say it is simply a very special expression of Hooke’s law, its discovery can also be regarded as an extraordinary, outstanding achievement comparable to the development of the $\sin^2 \psi$ method. Its discovery is to be credited to H. Dölle and to V. Hauk [1], [2], [3]. Therefore, in the following I will call it either Eq. (1) or Dölle-Hauk equation. For the sake of simplicity I will also use the following form of Eq. (1), where one index notation is used not only for the stress tensor but also for $F$ (see e.g. [4],[5]):

$$\epsilon(\varphi, \psi, hkl) = \sum_{i=1}^{6} F_i(\varphi, \psi, hkl)\sigma_i$$

$$\{\sigma_i\} = \{\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12}\}$$

$$\{F_i\} = \{F_{11}, F_{22}, F_{33}, 2F_{23}, 2F_{13}, 2F_{12}\}$$

All stress tensor components unknown

Eq. (2) can be directly used when all six components of the stress tensor are to be determined. The complete stress tensor can be calculated after at least six, well distributed, measurements of lattice plane distances have been made and if the unstressed lattice parameters are known. Besides that all six components of the tensor $F$ must be known. Then the stress tensor is the solution of the overdetermined system of simultaneous linear equations, Eq. (5).

$$\begin{pmatrix}
\epsilon(\varphi_1, \psi_1, hkl_1) \\
\epsilon(\varphi_2, \psi_2, hkl_2) \\
\vdots \\
\epsilon(\varphi_N, \psi_N, hkl_N)
\end{pmatrix} = 
\begin{pmatrix}
F_1(\varphi_1, \psi_1, hkl_1) & F_2(\ldots) & F_3(\ldots) & F_4(\ldots) & F_5(\ldots) & F_6(\ldots) \\
F_1(\varphi_2, \psi_2, hkl_2) & F_2(\ldots) & F_3(\ldots) & F_4(\ldots) & F_5(\ldots) & F_6(\ldots) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
F_1(\varphi_N, \psi_N, hkl_N) & F_2(\ldots) & F_3(\ldots) & F_4(\ldots) & F_5(\ldots) & F_6(\ldots)
\end{pmatrix} 
\begin{pmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_3 \\
\sigma_4 \\
\sigma_5 \\
\sigma_6
\end{pmatrix}$$

An example would be the stress measurement inside a massive specimen, where all six stress tensor components can be finite. See Figure 1.

Principal stress axes known

Very often one or all three principal stress axes are known, then the system of equations must be reduced. For example, in many cases, due to the way a rail is produced – hot rolling – it will be justified to assume that the residual stress field has the same symmetry as the geometry of the rail itself. Then, the principal stress axes at the red spot in Figure 1b can only be as drawn and $\sigma_4 = \sigma_5 = \sigma_6 = 0$ holds, therefore the last three columns in Eq. (5) can be omitted.
Figure 1: Stress measurement in a massive specimen using neutron diffraction. a) Measurement position with unknown principal axes. b) Measurement position with principal axes known.

**Stress free surface**

The most frequent case in x-ray stress measurement is when there is a stress free surface. \( \sigma_{33} = \sigma_{23} = \sigma_{13} = 0 \). Then, thanks to the fact that \( \sigma_{33} = 0 \), it is possible to establish a solvable system of linear equations in which not only the three non-vanishing components of the stress tensor are unknowns but also the unstressed lattice constant \( a_0 \). For this purpose Eq. (2) must be transformed by solving it for \( a(\varphi, \psi, hkl) \) and omitting all components with index 3, 4, 5:

\[
\epsilon(\varphi, \psi, hkl) = \frac{a(\varphi, \psi, hkl) - a_0}{a_0} = \sum_{i=1}^{6} F_i(\varphi, \psi, hkl) \sigma_i
\]

(6)

\[
a(\varphi, \psi, hkl) = a_0 + F_1(\varphi, \psi, hkl) a_0 \sigma_1 + F_2(\varphi, \psi, hkl) a_0 \sigma_2 + F_6(\varphi, \psi, hkl) a_0 \sigma_6
\]

(7)

Now there are four unknowns, namely \( a_0, a_0 \sigma_1, a_0 \sigma_2, a_0 \sigma_6 \), and only at least four measurements are necessary, the system of simultaneous equations then is:

\[
\begin{pmatrix}
    a(\varphi_1, \psi_1, hkl_1) \\
    a(\varphi_2, \psi_2, hkl_2) \\
    \vdots \\
    a(\varphi_N, \psi_N, hkl_N)
\end{pmatrix}
= \begin{pmatrix}
    1 & F_1(\varphi_1, \psi_1, hkl_1) & F_2(\ldots) & F_6(\ldots) \\
    1 & F_1(\varphi_2, \psi_2, hkl_2) & F_2(\ldots) & F_6(\ldots) \\
    \vdots & \vdots & \vdots & \vdots \\
    1 & F_1(\varphi_N, \psi_N, hkl_N) & F_2(\ldots) & F_6(\ldots)
\end{pmatrix}
\begin{pmatrix}
    a_0 \\
    a_0 \sigma_1 \\
    a_0 \sigma_2 \\
    a_0 \sigma_6
\end{pmatrix}
\]

(8)

Of course, with some extra knowledge about the stress state, be it that the principal stress axes are known or any other information about the stress tensor, Eq. (8) can be reduced by some unknowns and columns.

**Uniaxial stress state**

An example for the above-mentioned is if it is known that the stress state is an uniaxial one, that is \( \sigma_1 \neq 0 \), all others are zero. Then the system of simultaneous equations reduces to:

\[
\begin{pmatrix}
    a(\varphi_1, \psi_1, hkl_1) \\
    \vdots \\
    a(\varphi_N, \psi_N, hkl_N)
\end{pmatrix}
= \begin{pmatrix}
    1 & 1 & \vdots & \vdots & \vdots \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    1 & 1 & \vdots & \vdots & \vdots
\end{pmatrix}
\begin{pmatrix}
    a_0 \\
    a_0 \sigma_1 \\
    a_0 \sigma_2 \\
    a_0 \sigma_6
\end{pmatrix}
\]

(9)
There is one further special case for which Eq. (7) has to be transformed to a third type. This is when
the stress is independent of the direction in the surface plane. In this case Eq. (10) is to be used:

\[
\begin{align*}
a(\varphi, \psi, hkl) &= a_0 + [F_1(\varphi, \psi, hkl) + F_2(\varphi, \psi, hkl)]a_0\sigma \\
\left( \begin{array}{c}
a(\varphi_1, \psi_1, hkl_1) \\
\vdots \\
a(\varphi_N, \psi_N, hkl_N) \\
\end{array} \right) &= \left( \begin{array}{c}
1 & F_1(\varphi_1, \psi_1, hkl_1) + F_2(\varphi_1, \psi_1, hkl_1) \\
\vdots & \vdots & \vdots \\
1 & F_1(\varphi_N, \psi_N, hkl_N) + F_2(\varphi_N, \psi_N, hkl_N) \\
\end{array} \right) \left( \begin{array}{c}
a_0 \\
a_0\sigma \\
\end{array} \right)
\end{align*}
\] (10) (11)

Applicability of the correct methods

It is important to point out that in these equations one is absolutely free in choosing the \(\varphi, \psi\)
pairs (measurement directions). For instance, in a polycrystalline material one can use a traditional
distribution of measurement directions, like that in Figure 2a or, the better one, in Figure 2b. Or if, for practical
reasons during data collection, a distribution as shown in Figures 2c, 2d is easy to obtain, it would also
be no problem to calculate the stress tensor.

![Figure 2: Stereographic plots of different distributions of measurement directions (\(\varphi, \psi\) pairs)](image)

In a sharply textured specimen the distribution of measurement directions is dictated by the pole figures,
and in a single crystal it is even more restricted to only a discrete number of measurement directions,
see Figure 3a,b. Again there is also no problem to use one of the above-mentioned methods. One can
also deliberately combine measurements with different Miller indices. This is also very helpful for
strongly textured specimens as well as for thin films and virtually a necessity for single crystals (see
again Figure 3).

It also does not matter how the material behaves elastically. The specimen can be a single crystal with
elastic anisotropy, it can be a quasi isotropic polycrystalline material or a polycrystalline material with
any strong texture. The differences among specimens with different elastic behaviors lie only in the
way to get the \(\mathbf{F}\) tensor. For quasi isotropic (see e.g. [4],[5],[6],[7]), as well as for single crystalline
materials the calculation of \(\mathbf{F}\) is quite straightforward ([5]). For materials with a pronounced texture
the calculation is more complicated, but the principal methods are known, programs can be found in the literature. Measurement of \( F \) can also be done, see [5], [8].

With these three equations (Eqs. (1), (7), (10)) it is possible to handle data evaluation of any stress measurement, provided the strains are in the range of linear elasticity and there are no such complications as a stress or composition gradient.

**THE \( \sin^2 \psi \) METHOD**

Probably the strongest arguments to use one of the above-mentioned methods instead of the traditional \( \sin^2 \psi \) method are these: in the \( \sin^2 \psi \) method the measurement directions must be distributed in a way as shown in Figures 2a,b. In all the other distributions shown here, the \( \sin^2 \psi \) method is not applicable. It is also not applicable when different reflection types are needed, and in all cases where there is no elastic isotropy or quasi isotropy.

Nevertheless, one could ask why the \( \sin^2 \psi \) method should be given up also in the cases where it can be used? To answer this question a deeper analysis must be made. In the \( \sin^2 \psi \) method, plots as shown in Figure 4 are done for each azimuth \( \varphi \); from the slopes of the regression lines the in plane stresses \( \sigma(\varphi) \) are calculated (see Eq. (12)). Using further Eq. (13) and with at least three different \( \sigma(\varphi) \) the three unknown components of the stress tensor can be calculated.

\[
m = \frac{1}{2}s_{2a_0}\sigma(\varphi) \quad (12)
\]

\[
\sigma(\varphi) = \sigma_1 \cos^2 \varphi + \sigma_2 \sin^2 \varphi + \sigma_6 \sin 2\varphi \quad (13)
\]

Although in the \( \sin^2 \psi \) method only the slope is used, it must not be forgotten that a regression line (Figure 4) is determined by two parameters, the slope and the intercept at the ordinate axis. For physical reasons, this intercept \( a(\psi = 0) \) cannot be different for different azimuths \( \varphi \). Since, in the \( \sin^2 \psi \) method the regression lines are determined independently from each other, there are usually three different \( a(\varphi, \psi = 0) \). And this is why the \( \sin^2 \psi \) method must be regarded as wrong.
The corrected $\sin^2 \psi$ method

Instead of only calculating the slopes $m$ of the regression lines one could also solve the three overdetermined systems of linear equations, Eqs. (14),(15),(16)

$$
\begin{pmatrix}
\alpha(\varphi_1, \psi_1) \\
\vdots \\
\alpha(\varphi_1, \psi_L)
\end{pmatrix} =
\begin{pmatrix}
1 & \sin^2 \psi_1 \\
\vdots & \vdots \\
1 & \sin^2 \psi_L
\end{pmatrix}
\begin{pmatrix}
\alpha(\varphi_1, 0) \\
\vdots \\
m(\varphi_1)
\end{pmatrix}
$$

(14)

$$
\begin{pmatrix}
\alpha(\varphi_2, \psi_{L+1}) \\
\vdots \\
\alpha(\varphi_2, \psi_M)
\end{pmatrix} =
\begin{pmatrix}
1 & \sin^2 \psi_{L+1} \\
\vdots & \vdots \\
1 & \sin^2 \psi_M
\end{pmatrix}
\begin{pmatrix}
\alpha(\varphi_2, 0) \\
\vdots \\
m(\varphi_2)
\end{pmatrix}
$$

(15)

$$
\begin{pmatrix}
\alpha(\varphi_3, \psi_{M+1}) \\
\vdots \\
\alpha(\varphi_3, \psi_N)
\end{pmatrix} =
\begin{pmatrix}
1 & \sin^2 \psi_{M+1} \\
\vdots & \vdots \\
1 & \sin^2 \psi_N
\end{pmatrix}
\begin{pmatrix}
\alpha(\varphi_3, 0) \\
\vdots \\
m(\varphi_3)
\end{pmatrix}
$$

(16)

These three matrix equations can also be written in only one matrix equation without changing anything, namely:

$$
\begin{pmatrix}
\alpha(\varphi_1, \psi_1) \\
\vdots \\
\alpha(\varphi_1, \psi_\ldots) \\
\alpha(\varphi_2, \psi_\ldots) \\
\vdots \\
\alpha(\varphi_2, \psi_\ldots) \\
\alpha(\varphi_3, \psi_\ldots) \\
\vdots \\
\alpha(\varphi_3, \psi_\ldots) \\
\alpha(\varphi_3, \psi_N)
\end{pmatrix} =
\begin{pmatrix}
1 & 0 & 0 & \sin^2 \psi_1 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & 0 & 0 & \sin^2 \psi_\ldots & 0 & 0 \\
0 & 1 & 0 & 0 & \sin^2 \psi_\ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 1 & 0 & 0 & \sin^2 \psi_\ldots & 0 \\
0 & 0 & 1 & 0 & 0 & \sin^2 \psi_\ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 1 & 0 & 0 & \sin^2 \psi_N
\end{pmatrix}
\begin{pmatrix}
\alpha(\varphi_1, 0) \\
\alpha(\varphi_2, 0) \\
\alpha(\varphi_3, 0) \\
m(\varphi_1) \\
m(\varphi_2) \\
m(\varphi_3)
\end{pmatrix}
$$

(17)

This system is exactly the same as Eqs. (14),(15),(16) and exactly an analytical formulation of the traditional $\sin^2 \psi$ method.

The error which has been shown in Figure 4 is also clearly seen in Eq. (17). Instead of $\alpha(\varphi_1, 0)$, $\alpha(\varphi_2, 0)$, $\alpha(\varphi_3, 0)$, which means that there are too many free parameters, there should be only one ($\alpha(\varphi, 0)$). But this error is easily corrected: the first three columns with 1’s and 0’s are replaced by only one column containing only 1’s, and the three $\alpha(\varphi, 0)$ are replaced by $\alpha(0)$.

![Figure 4: Regression lines for different azimuths $\varphi$, drawn independently from each other.](image-url)
This new system of linear equations can be called the corrected $\sin^2 \psi$ method. As can be shown, it is identical with the correct method, but up to this point only valid for quasi isotropic materials and for measurements distributed as shown in Figures 2a, 2b. Of course, Eq.(17) cannot be solved by graphical methods as the $\sin^2 \psi$ method.

The corrected and generalized $\sin^2 \psi$ method

A single line of Eq. (17) can be written as Eq. (18), whereas for $a(\psi = 0)$ Eq. (19) is valid

$$a(\varphi, \psi) = a(\psi = 0) + \sin^2 \psi \frac{1}{2}s_2a_0\sigma(\varphi)$$  (18)

$$a(\psi = 0) = a_0 + s_1a_0(\sigma_1 + \sigma_2)$$  (19)

Eq. (13) and Eq. (19) inserted into Eq. (18) yields Eq. (20)

$$a(\varphi, \psi) = a_0 + (s_1 + \frac{1}{2}s_2\sin^2 \psi \cos^2 \varphi)a_0\sigma_1 + (s_1 + \frac{1}{2}s_2\sin^2 \psi \sin^2 \varphi)a_0\sigma_2 + \frac{1}{2}s_2\sin^2 \psi \sin(2\varphi)a_0\sigma_6$$  (20)

Eq. (20) is still only valid for quasi isotropic materials, however the restrictions for the distributions of measurement directions according to Figures 1a,b are no longer in force. The factors before $a_0\sigma_i$ are obviously equal to $F_i(\varphi, \psi)$ (e.g. [4],[5],[6],[7]) therefore Eq. (21) can be written instead of Eq. (20).

$$a(\varphi, \psi, hkl) = a_0 + F_1(\varphi, \psi, hkl)a_0\sigma_1 + F_2(\varphi, \psi, hkl)a_0\sigma_2 + F_6(\varphi, \psi, hkl)a_0\sigma_6$$  (21)

Eq. (21) was derived from the corrected $\sin^2 \psi$ method, and it is quite a natural step to extend its validity from quasi isotropic to all materials. Therefore, in a previous paper I called the method using Eq. (21) the generalized $\sin^2 \psi$ method ([9]), since it can be derived either directly from Dölle and Hauk’s equation (Eq. (1) or from the $\sin^2 \psi$ method.

Obviously, in the special case of a uniaxial stress state, the data treatment according to the $\sin^2 \psi$ method is identical with the correct method, see Eq. (9). This is because with only $\sigma_{11}$ as the unknown stress tensor component, only measurements with $\varphi = 0^\circ$ are needed, therefore only one regression line and only one intercept $a_0$.

The Dölle-Hauk method

The Dölle-Hauk method [6] (not to be confused with what was called Dölle-Hauk equation) is a method to calculate all six components of the stress tensor. It needs at least six measurements of lattice plane distances and the exact knowledge of the unstressed lattice parameters. It is also only applicable for quasi isotropic materials, it can also use only one (hkl) and measurement directions have to be distributed in a special scheme, namely that of Figure 2a.

In this method two different types of plots are done for $\varphi = 0^\circ, 45^\circ, 90^\circ$, and as in the $\sin^2 \psi$ method regression lines are drawn or calculated. From the slopes of the regression lines and their intersections with the ordinate axis all information about $\sigma_{ij}$ can be obtained. The equations to calculate $\sigma_{ij}$ from these slopes and intercepts can be found in many textbooks, see e.g. [6], [10], [11].
The method is not only complicated to carry out and restricted to quasi isotropic materials and a special distribution of measurement directions, it also suffers from the fact that independent regression lines mean too many independent variables and therefore it does not comply with the requirements for a correct least-squares method. The consequence is reduced accuracy.

ACCURACIES

Although it is clear that both the sin² ψ and the Dölle-Hauk method are not least-squares methods, it is not clear whether or not this insight has any practical consequences. In other words, the question is: how do the different methods of data treatment influence the accuracy of σ_{ij}.

To quantify accuracy it is usual to look at standard deviations. Since it would be rather impractical to compare all ∆σs extra, I defined one single quantity, this is the mean value of all ∆σ²s: in the case of a stress free surface it is (∆σ²₁ + ∆σ²₂ + 2∆σ²₆)/4, in the case of the full stress tensor to be determined, the sum over all nine components divided by 9 must be taken. The advantage of these quantities lies in the fact that they are invariant, although the matrix ∆σ_{ij} itself is not a tensor.

Furthermore, the comparison of data treating methods should be independent from the accuracy of the x-ray measurements themselves, therefore the mean value is divided by ∆a² or ∆ε², respectively. Here, for the sake of simplicity, the measured data are assumed to be all equally accurate. The new quantity can now be regarded as a quality number of the data treating method as well as of the configuration of the ϕ,ψ pairs.

\[ Q = \frac{\overline{\Delta \sigma^2}}{\Delta a^2} \]  \hspace{1cm} (22)

With this tool it is possible to compare the least-squares method with the sin² ψ method. The comparison is done for different distributions of measurement directions (ϕ,ψ pairs):

A) ϕ = 0°, 45°, 90°
B) ϕ = 0°, 60°, 120°

In both configurations ψ runs from −70° to 70° with an odd number of points for each ϕ and the angles ψ equally distributed over sin² ψ. That means that for each ϕ there is an extra measurement at ψ = 0. Distribution A is one which is most often used, B is the distribution with optimized ϕ angles ([12]) and gives more accurate results in the σs.

The result is shown in Figure 5a: Distribution A (the one most often used) and data treated with the sin² ψ method is the worst one can do. It gives the largest errors in the components of the stress tensor. Configuration B gives much better results although the amount of experimental work is exactly the same as for A. And the correct least-squares method produces better results than the sin² ψ method.

For the Dölle-Hauk method the picture is quite similar (see Figure 5b). The same ϕ,ψ distributions A was taken for the Dölle-Hauk method, and A and B for the least-squares method.

In both cases, the sin² ψ method and the Dölle-Hauk method, the mean standard deviations are significantly higher than after the use of the corresponding least-squares method.

Actually, the results shown in Figure 5 are not absolutely new. The fact that a least-squares method gives better results than the Dölle-Hauk method has been known for 20 years, see [13]. And that it would be an advantage to use the distribution 0°, 60°, 120° instead of 0°, 45°, 90° was not only shown
in the same paper ([13]) and other publications, but can already be found in the well known textbook by Cullity [14]. Unfortunately these insights have been widely forgotten or simply ignored.

Figure 5: Dependencies of the stress tensor’s mean deviation on number and distribution of measurement directions and on the evaluation method. a) \( \sin^2 \psi \) method versus least-squares method. b) Dölle-Hauk method versus least-squares method.

Further special methods

Due to the great success of the \( \sin^2 \psi \) method, but also in order to overcome some of its shortcomings, many other methods for data treatment in x-ray stress measurement have been developed, most of them similar to the \( \sin^2 \psi \) method. An analysis of these methods clearly show that they all are not as generally applicable as the correct methods are, and nearly all of them give less accurate results than their corresponding correct methods. These methods and the correct method to replace them are:

- the \( \sin^2 \psi \) method [6] [10] – Eq. (7)
- the \( \psi \) integral method [15] – Eq. (7)
- The f method [16], [17] – Eq. (10)
- the g method [7][18] – Eq. (7)
- the crystallite group method [6][19] – Eq. (1),(2),(7)
- the \( \cos^2 \psi \) method [20] – Eq. (7)
- the \( \cos \alpha \) method [21] – Eq. (7)

COMPUTING THE STRESS TENSOR

Eqs. (5, 8, 9, 11) can be written in a symbolic form as equations of matrices.

\[
Y = K \cdot X
\]  

(23)

\( Y \) is a Nx1 matrix containing the measured \( a(\varphi, \psi, hkl) \) or \( \epsilon(\varphi, \psi, hkl) \), \( K \) is the Nxn matrix containing \( 1, F_1(\varphi, \psi, hkl) \) and \( X \) is the nx1 matrix for the unknowns \( a_0, \sigma_1, .. \) When using e.g. Mathematica the solution is one single command: \( X := \text{LinearSolve}(K, Y) \)
In all other, similar systems it is in principle the same, just one command.

It would also be an easy task to write one's own program. To calculate the normal equations
\[ K^T \cdot Y = (K^T \cdot K) \cdot X, \]
only matrix multiplications are needed, its solution for \( X \) is then done by an
elimination procedure or something of the sort.

CONCLUSION

The equations Eq. (1), (7), (10) together with the method of least-squares are tools with which all cases
of data treatment in x-ray stress measurements can be handled. These tools are more versatile, easier
to use and more accurate than all traditional methods used so far. In only a few special cases one can
obtain the same accuracy with the \( \sin^2 \psi \) or another one of the older method.

Therefore, all these methods used so far should be given up and instead we should use the equation
discovered by Dölle and Hauk or one of the equations derived from it, together with the least-squares
method.

References

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Tokyo, 1987