The Matrix Method; a - Better - Alternative to the $\sin^2\psi$ and Other Methods

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Abstract. The principle of the matrix method and its many advantages over the $\sin^2\psi$ method and all other traditional methods is described, together with new methods for plotting data and results.

Introduction

The $\sin^2\psi$ method has been known and successfully used for a very long time, but it has some disadvantages. It is not a correct least squares method, therefore the results are not as accurate as they could be and it is not generally applicable. Many other methods have been invented, but most of them suffer from the same flaws as the $\sin^2\psi$ method. With the matrix method we could get rid of all these difficulties.

Principle of the Matrix Method

The method is based on the least squares fit and on Hooke's law in the special form of Dölle-Hauk's equation Eq. 1, [1,2] or one of two equations derived from it [3,4]:

$$\varepsilon(\varphi,\psi,hkl) = [a(\varphi,\psi,hkl) - a_0]/a_0 = F_{ij}(\varphi,\psi,hkl)\,\sigma_{ij} \quad (1)$$

$$a(\varphi,\psi,hkl) = a_0 + F_{11}(\varphi,\psi,hkl)\,\sigma_{11}\,a_0 + F_{22}(\varphi,\psi,hkl)\,\sigma_{22}\,a_0 + F_{12}(\varphi,\psi,hkl)\,\sigma_{12}\,a_0 \quad (2)$$

$$a(\varphi,\psi,hkl) = a_0 + [F_{11}(\varphi,\psi,hkl) + F_{22}(\varphi,\psi,hkl)]\,\sigma\,a_0 \quad (3)$$

Depending on the task one of these equations must be used to establish a system of linear equations which is to be solved with the least squares fit – simply to solve a matrix equation. Therefore the name matrix method or generalized $\sin^2\psi$ method [5].

Advantages of the method

1. Measurement directions (the φ,ψ – pairs) can be distributed in a completely arbitrary way.
2. Different (hkl)s can be used without any problem.
3. The accuracy of results is higher than when the $\sin^2\psi$ or one of the other older methods is used.
4. Calculation of results is clear and simple and always following the same principle.
5. The method is applicable for isotropic, quasi isotropic, textured and single crystalline materials.
6. Error calculation is also clear and simple thanks to the simple calculation of results. This includes error calculation of derived quantities like principal stresses or Mises stress and others.
7. Due to the simple error calculation it is also easy to plan the measurement to obtain the best result.

Plotting of data and results

Due to the versatility of the new method it became necessary to develop also new methods for the depiction of measured data and for the result. For that aim we not only adapted the traditional $\sin^2\psi$ plot, but also developed a completely new plotting scheme. This new type of plot has all the features of the $\sin^2\psi$ plot but it allows the depiction of all data, independent of their parameter triple φ, ψ, (hkl).

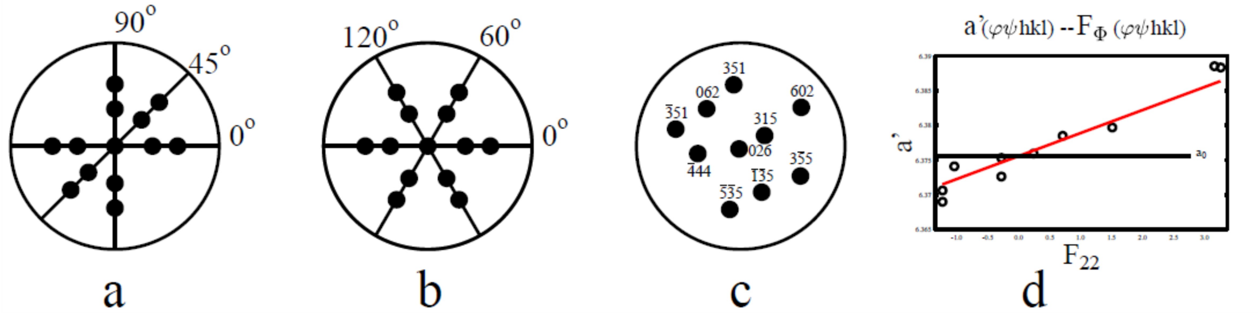

Figure 1: a,b) Distributions of measurement points for a $\sin^2\psi$ measurement. c**)** A distributions (e.g. for a single crystal measurement) as can be used in the matrix method. **c)** The new type of plot as demonstrated for the measurement of Fig. 1c.

Examples to demonstrate the above asserted advantages of the matrix method

Ad 1) Virtually in all the traditional methods the arrangement of measurement directions must comply with a strict scheme, see Fig 1a,b. This is often difficult to follow, for instance if the material to be probed has a strong texture, another example is a thin film measurement. When using the matrix method a distribution like that in Fig. 1c or even the hundreds of data which one obtains in a texture measurement (if a linear detector is used) can easily be used for stress measurement. [5]

Ad 2) In a thin film measurement the grazing incidence method must be used, in which different (hkl)s are to be applied. For only that purpose Baczmanski et al. developed the same method as we did [3]. They called it grazing incidence $\sin^2\psi$ method (g-$\sin^2\psi$ method). Other methods for thin films have been developed [6], but these are all restricted to special cases or are even defective.

Ad 3) In the $\sin^2\psi$ method linear regression lines are calculated (or drawn) for each φ independent from each other. This is wrong for physical and mathematical reasons, therefore the accuracy is not as high as it could be. (Virtually all other older methods have the same flaw as the $\sin^2\psi$ method.) In the matrix method that problem is automatically solved [7].

Ad 4) Two examples for the assertion that the matrix method is much simpler than older methods.: i) In the sin2psi m one has to determine three regression lines, and then a system of linear equations must be solved. ii) In the Dölle-Hauk method [2] - the procedure used when all six components of the stress tensor are to be calculated - six different regression lines must be determined and then six different equations must be solved. In contrast to that, the matrix method needs the solution of only one system of linear equations.

Ad 5) In principle there is no difference whether the material is quasi isotropic or textured or a single crystal. The difference lies only in the calculation of the F-tensor.
Quasi isotropic: $F_{ij}(\varphi,\psi,hkl) = s_1\,\delta_{ij} + \frac{1}{2}\,s_2\,r_i\,r_j$
Textured: $F_{ij}(\varphi,\psi,hkl)$ must be calculated using the o.d.f. and the single crystal elastic parameters S_{ij}.
Single crystal: The calculation consists simply of a tensor reduction and a coordinate transformation.

Ad 6) When solving the matrix equation it is a natural step to use the concept of the (Moore-Penrose) pseudoinverse. Using it, all error calculations become clear and easy, even the seemingly difficult error calculation for the Mises- or Tresca-stress and others.

Ad 7) In some papers dealing with single crystal measurements, published long ago [8,9], we described simple rules for the optimized choice of measurement direction. These rules apply also for polycrystalline specimens.

Example for the new type of data representation.
For a distribution of measurement directions as is often needed is a single crystal measurement (Fig.1c) the usage of the $\sin^2\psi$ plot would not work, but the recently developed a-prime-plot does. See Fig. 1d.

Conclusion

There are many good reasons to replace the $\sin^2\psi$ method and all other traditional methods for data evaluation in x-ray stress measurement by the matrix method.

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