WHY SHOULD WE GIVE UP THE $\sin^2\psi$ AND ALL SIMILAR METHODS?

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The equation

$$\varepsilon\,(r, hkl) = \sum F_{ij}\,(r, hkl)\sigma_{ij} \qquad (1)$$

which has been developed nearly 30 years ago by Dölle and Hauk, together with the well known least squares fit, now about 200 years old, provides us with a perfect tool for accurate data treatment in diffraction stress measurement. Eq. (1) is to be used if all six components of the stress tensor are unknown.

Eqs. (2) and (3) are derived from Eq. (1):

$$a\,(r\,,hkl) = a_0 + F_{11}a_0\sigma_{11} + F_{22}a_0\sigma_{22} + F_{12}a_0\sigma_{12} \qquad (2)$$

$$a\,(r\,,hkl) = a_0 + (F_{11} + F_{22})\,a_0\sigma \qquad (3)$$

Eq. (2) and (3) are well suited for all cases where the unstressed lattice constant is not exactly known but if it is known that $\sigma_{33} = \sigma_{13} = \sigma_{23} = 0$, i.e. that there is a stress free surface. Eq. (2) is used when all in-plane components (σ_{11}, σ_{22}, σ_{12}) of the stress tensor are to be determined, whereas Eq. (3) is to be used if there exists a further extra condition, namely $\sigma_{11} = \sigma_{22}$ and $\sigma_{12} = 0$.

With Eq.(2) a system of simultaneous linear equations can be established which, together with the least squares fit should be used instead of the $\sin^2\psi$ method. But not only the $\sin^2\psi$ method could be replaced by a more sophisticated method, all other methods which have been developed following the principles of the $\sin^2\psi$ method can as well be replaced using one of the abovementioned equations.

It is shown that such a replacement of the $\sin^2\psi$, the Dölle-Hauk, the g, the f and other methods would be quite beneficial for different reasons. One of these benefits is a significant gain in accuracy.

All the advantages of using the proper equation Eq. (1) (2) or (3) will be discussed briefly, the main part of the lecture will be to show the gain in accuracy.

[1] H. Dölle, J. Appl. Cryst. 12 (1979) 489--501