A NEW REGULARIZATION METHOD TO DETERMINE STRAIN/STRESS DEPTH PROFILES FROM DIFFRACTION EXPERIMENTS

Harald Wern, Patrick Klein and Günter Marchand
Laboratory of Computer Aided Applications, HTW des Saarlandes, University of Applied Sciences, Goebenstrasse 40, D-66117 Saarbrücken, Germany

ABSTRACT

Inverse problems which are involved in x-ray or neutron diffraction analysis are known to be extremely ill-conditioned. The reason is that the linear system of equations which has to be solved for the \( \tau \)- or true depth gradients from the measured \( \tau \)-profiles becomes singular. From the mathematical point of view, regularization methods are recommended to overcome the non-uniqueness of the obtained solution. However, all regularization methods reported in the literature are not suitable to the above problem due to several reasons. Therefore, a new method has been developed. In principle it follows the ideas of the Tikhonov regularization but uses a complete different functional to be minimized. Using a matrix decomposition technique, it is shown that the six independent \( \tau \)-gradients can be separated from a usual measurement series. The true depth profiles are then calculated using orthonormal wavelet basis functions.

INTRODUCTION

In x-ray strain/stress analysis, one distinguishes between three different coordinate systems. In the crystallophysical system usually the material properties are defined\(^1\). The measurement is performed in the laboratory system. The measured strain along an \{hkl\} reflection at any point is related to the strain tensor in the user defined specimen system by the well known fundamental equations\(^2\) which are given in equation 1.

\[
< \varepsilon >_{\varphi\psi}(\tau) = \left[ \varepsilon_{11}(\tau) \cdot \cos^2 \varphi + \varepsilon_{12}(\tau) \cdot \sin 2\varphi + \varepsilon_{22}(\tau) \cdot \sin^2 \varphi \right] \cdot \sin^2 \psi
+ \left[ \varepsilon_{13}(\tau) \cdot \cos \varphi + \varepsilon_{23}(\tau) \cdot \sin \varphi \right] \cdot \sin 2\psi
+ \varepsilon_{33}(\tau) \cdot \cos^2 \psi
\]  

(1)

The carrats on the left hand side indicate an averaged information due to the attenuation of the x-rays. In general several \( \varphi \)-rotations and \( \psi \)-tilts are performed in order to detect the full tensor to provide a complete tri-axial analysis. The above system of equations can be rearranged to a linear system for the unknown \( \tau \)-gradients. However, this system of equations becomes singular and, therefore, the uniqueness of the solution is not guaranteed. In order to demonstrate the problems a detailed simulation has been performed.

SIMULATION

With the aid of a random number generator six different highly nonlinear stress gradients as a function of the true depth have been calculated. The results are shown in figure 1. Using Hooke’s law, the stress gradients have been converted to strain gradients. Using equation 2 and assuming the characteristics of a \( \psi \)-goniometer (equation 3) the true strain profiles have
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been converted to the so called \( \tau \)-profiles where three \( \varphi \)-rotations (0, 45, 90) and \( \psi \)-tilts between –60 and +60 degrees have been realized. Using equation 1 the \( \tau \)-profiles have then been superimposed in order to treat them as a measurement series.

\[
e_{ij}(\tau) = \int e^\tau \cdot e_{ij}(z) \, dz
\]

(2)

\[
\tau(\psi, \Theta) = \frac{\sin \Theta \cdot \cos \psi}{2 \cdot \mu}
\]

(3)

**Figure 1:** Simulated normal and shear stresses as a function of depth.
In order to overcome the nonuniqueness of singular systems, from the mathematical point of view, regularization methods are recommended. The Landweber iteration uses a stopping rule for the iterations in order to obtain a regularized solution. However, there is not any a priori information about the stress gradients and the method in fact didn’t work. The method of conjugate gradients is in general well established to solve linear systems of equations or train neural networks, however, for singular systems it cannot be recommended because, again, there is no information to stop the iteration at a certain truncation of the defect. A truncated singular values decomposition (SVD) is a further regularization method. For a given matrix of order N, it calculates the N singular values. To obtain a more or less reliable solution, the singular values must be truncated that means all singular values which are smaller than a certain limit are zeroed. This procedure requires a discrete trade off which in practice lead to ambiguous results. The idea of the Tikhonov regularization is not only to minimize the defect with respect to some norm but also to add a penalty term for the solution as illustrated in equation 4. The relative influence of the penalty term is controlled by a continuous parameter $\gamma$.

$$\| A x - y \|_1^2 + \gamma^2 \| x \|_2^2$$

(4)

The seminorm $\| \cdot \|_2$ is defined by equation 5. The simplest way of choosing the matrix $B$ is the identity matrix. However, in the literature symmetric difference formulas representing the first or higher derivatives are recommended. The principle schema for the first and second derivative is given in equation 6.

$$\| x \|_2^2 = x^T B^T B x$$

(5)

$$B_1 = \begin{pmatrix} -1 & 1 \\ \vdots & \ddots \\ -1 & 1 \end{pmatrix} \quad B_2 = \begin{pmatrix} -1 & 2 & -1 \\ \vdots & \ddots & \vdots \\ -1 & 2 & -1 \end{pmatrix}$$

(6)

In the case of more equations than unknowns one obtains the normal equations as indicated in equation 7.

$$\left( A^T A + \gamma^2 B^T B \right) x_\gamma = A^T y$$

(7)

The solution of equation 7 with the functional $B_2$ is given in figure 2 together with the simulated $\tau$-gradients. The only point which is well defined is epsilon$_{33}$ at $\Psi=0$ which corresponds to the maximum penetration depth. However, the obtained absolute values as well as the slopes are far away from the true solution. The deviation is even more pronounced for functionals representing higher derivatives. For that reason, a new functional has been developed with the property to minimize the deviations from a smooth curve rather than a derivative of first or second kind. The result is shown in figure 3a for the shear components and in figure 3b for the normal components. Whereas the shear components are quite well resolved because of the psi-splitting, there is still a small deviation for the normal components. However, in comparison with $B_2$ of equation 6, there is a considerable improvement in the obtained solution.
Figure 2: Simulated (line) and obtained \( \tau \)-gradients (symbols) from Tikhonov regularization using \( B_2 \).

Figure 3a: Simulated (line) and obtained shear \( \tau \)-gradients (symbols) from Tikhonov regularization using a modified functional to be minimized.
Figure 3b: Simulated (line) and obtained normal τ-gradients (symbols) from Tikhonov regularization using a modified functional to be minimized.

Because the obtained solution is already quite close to the simulated ones, one can use a recurrent neural network with one hidden layer to further improve the solution. This is achieved by a least squares fit of the obtained solution to low order Chebycheff polynomials. The adjustable parameters of the neural network given by equation 8 \( (g_{pk}, w_{ip} \text{ and thresholds } \Theta_p) \) can now be trained very quickly to match the input to the parameters of the Chebycheff polynomials. The Fermi function is used as sigmoidal transfer function \( f \). The number of input neurons corresponds to the number of strain data whereas the output dimension is given by the number of the coefficients \( a_k \) of the polynomials. Now a back loop is introduced in order to minimize the summed squared differences of input strain τ-gradients and calculated strain depth profiles from the parameters of the polynomials as indicated in equation 9. The adjustable parameters are now updated in direction of the steepest gradient descent until a certain stopping criterion holds. In this way all six τ-gradients are separated.

\[
a_k = \sum_{p=1}^{q} g_{pk} f \left( \sum_{i=1}^{n} w_{ip} \epsilon_{i} < \Theta_p \right)
\]

The corresponding techniques and equations have been implemented in the programming language C. A web page will soon be available with some sample code where the user can provide and analyse his own data sets. A link to that page will be found soon at www.htw-saarland.de.
CONCLUSION

Regularization methods reported in literature to overcome the non-uniqueness of inverse and/or singular problems are not suitable to x-ray diffraction depth profile analysis because there exists no a priori information about the depth profiles. Tikhonov regularization together with a matrix decomposition technique in combination with an asymmetric functional to be minimized gives reasonable results. The results are improved by training a recurrent neural network. It is shown that all six τ-gradients from a usual measurement series can be separated. The true depth profiles are then calculated using orthonormal wavelets.

\[ \text{Error function } E = \sum_{i=1}^{n} (\langle \varepsilon \rangle_i - \langle \varepsilon^* \rangle_i)^2 \]  

**Figure 4:** Schematic representation of artificial neural network.

REFERENCES