EVALUATION OF RESIDUAL STRESS GRADIENTS BY DIFFRACTION METHODS WITH WAVELETS; A NEURAL NETWORK APPROACH

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ABSTRACT

The presence of residual stress gradients is often revealed by x-ray diffraction analysis. Because x-rays always detect an averaged information due to absorption, in the past some approaches have been employed to retrieve the true z-profiles from the measured τ-profiles where τ is in general the 1/e information depth of the diffracted intensity. However, all problems which can be described as so called inverse problems like x-ray diffraction analysis are often extremely ill-conditioned. What makes the wavelet basis interesting is that individual wavelet functions are quite localized in space and simultaneously they also are quite localized in frequency. This particular kind of dual localization achieved by wavelets renders operators to be sparse to some high accuracy, when transformed into the wavelet domain. However, the number of required wavelet coefficients for the representation of a residual stress gradients in general still exceeds the number of measurements. Therefore, a multilayer feed forward neural network approach has been investigated. With the implementation of a fast backtracking algorithm, suitable learning rates can be achieved. The advantages of this neural network approach will be discussed.

Keywords: X-ray diffraction, residual stress gradients, wavelets, multilayer feed forward neural network

INTRODUCTION

In the x-ray diffraction technique, three different types of measuring geometries are established: the Ω, Ψ and modified Ψ goniometers.

Figure 1: Angular definitions of the Ω-goniometer with respect to the specimen coordinate system. The tilt axis T lies in the specimen surface and in the diffraction plane but is perpendicular to the diffraction vector (hkI), which is parallel to L.
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The presented results in this paper refer to the \( \Omega \)-goniometer but also can be applied to the other geometries. The angular definitions of the \( \Omega \)-goniometer are shown in figure 1.

A typical experimental setup uses the variation of a rotation angle \( \varphi \) and a tilt angle \( \psi \) with respect to the sample coordinate system. The normal \( L \) refers to the measurement direction which is selected by the Miller indices \((hk)\). Residual strain or stress depth profiles measured with x-rays in the near surface region of polycrystalline materials are always averaged quantities because the counted intensities are averages over the diffracted volume. Therefore, these measured profiles are called \( \tau \)-profiles where \( \tau \) is the \( 1/e \) penetration depth of the x-rays. The measured profiles can be expressed as

\[
< \varepsilon _{\psi_i} (\tau_i) > = \frac{d_\psi \psi_i (\tau_i) - d0}{d0} = \frac{\int_0^Z e^{-i\tau_i} e^{\psi_i} (z) dz}{\int_0^Z e^{-i\tau_i} dz}
\]

(1)

where \( \varepsilon_{\psi_i} \) follows from the usual transformation law of the second rank tensor \( \varepsilon \) from the laboratory system to the specimen system shown in figure 1.

\[
\varepsilon_{\psi_i} (z) = \varepsilon_{11} (z) \cos^2 \varphi \sin^2 \psi + \varepsilon_{22} (z) \sin^2 \varphi \sin^2 \psi + \varepsilon_{33} (z) \cos^2 \psi + \\
\varepsilon_{12} (z) \sin 2\varphi \sin 2\psi + \varepsilon_{13} (z) \cos \varphi \sin 2\psi + \varepsilon_{23} (z) \sin \varphi \sin 2\psi
\]

(2)

For the \( \Omega \)-goniometer \( \tau_i \) is given by

\[
\tau_i = \frac{\sin^2 \Theta_0 - \sin^2 \psi_i}{2\mu \sin \Theta_0 \cos \psi_i}
\]

(3)

where \( \mu \) is the absorption coefficient for the particular wavelength and the material under investigation. \( \Theta_0 \) is the Bragg angle of the stress free lattice spacing \( d0 \). Since the \( z \)-profiles of the residual strains and stresses are generally of more interest in evaluation the effects of surface treatment, analytical and numerical approaches have been employed to retrieve these \( z \)-profiles from the measured \( \tau \)-profiles. From a general point of view one would prefer the analytical method known as Laplace inversion method. This method, however, is very sensitive to measurement errors and additional constraints to the measurement technique must be required to get satisfactorily results. All methods suffer from the fact that the inverse problem of equation 1 is often extremely ill-conditioned making a solution quite difficult. Therefore, an appropriate choice of the trial functions for the representation of the true \( z \)-profiles has considerable influence on the obtained result. In order to avoid redundancy, from a mathematical point of view, orthonormal bases are always the best candidates. The advantages have already been demonstrated in previous papers using trigonometric bases functions. The sensitivity of the obtained solution against measurement errors is unfortunately extremely high for inverse problems resulting in unrealistic error bounds of the obtained solution. In a previous study of the hole drilling method, it was shown that wavelets can lower this sensitivity considerably. Therefore, in this paper wavelets are used for the representation of the strain gradients in order to
provide a robust analysis procedure which is suitable even to industrial applications with automated measuring devices.

WAVELETS

The mathematical background for the construction wavelets cannot be presented here but is referred to the literature\textsuperscript{14,15}. Among the different wavelet families which are available today, the discussion will be restricted to a class of orthonormal wavelets with compact support discovered by Daubechies\textsuperscript{16}. They have build in excellent approximation properties such that a wavelet of order $N$ allows a piecewise exact representation of a polynomial of degree $N-1$. With increasing $N$, the Daubechies wavelets gain any desired order of differentiability. For illustration, in figure 2 four wavelets with the order $N=2, 8, 14, 25$ are shown which make different trade-offs between how compactly they are localized in space and how smooth they are.

For the representation of a strain gradient, a linear superposition of a certain wavelet family of order $N$ is assumed as described by equation 4, e.g.:

$$\varepsilon_{11}(z) = \sum_{j=1}^{k} w_j \cdot \text{wavelet}_j^N(z)$$

(4)
where for computational simplicity and efficiency $k$ should be a power of two. The wavelets in figure 2 have been generated from equation 4 with only one amplitude different from zero. This amplitude is set to unity for the sequences a) $j=8$, b) $j=40$, c) $j=40$, d) $j=80$.

**NEURAL NETWORK**

We had in view to develop a tool to generate the wavelet-coefficients $w_j$ of the strain gradients for a given measured data set as indicated by equation 1. The strain profiles than follow from equation 4 which is nothing more than an inverse wavelet transform (IWT) or wavelet synthesis. A usual neural network is in general trained with a set of known relations\textsuperscript{17}, here that means a set of input data is calculated from a known set of wavelet-coefficients. It is assumed that a more or less complete range of possible relationships can be learned by the network and, thus, provides generalization capabilities in the sense that the input leads to feasible results. Such attempts may be found e.g. for the identification of fluorescence spectra\textsuperscript{18}. Here, a possible occurrence of a single element in the spectrum can only vary between 0 and 100%. However, residual strain or stress profiles cannot be predetermined, they don’t need to be conform to the crystal symmetry like thermal expansion e.g. does. Therefore, a neural network for the determination of residual strain/stress gradients should have to learn an almost infinite set of possible profiles. Such a task would overcharge any net. For that reason we used a modification. A multiple feed forward neural network with one hidden layer was investigated in order to provide capability to allow for a nonlinear relationship between input and output. The principles of the network are summarized in figure 3. The input layer is considered as fan out units. The hidden nodes are considered as formal neurons with the Fermi-function as transfer function. The output layer produces the wavelet-coefficients of the triaxial residual strain gradients where the depth profiles as a function of the true depth below the surface follow from an IWT. Therefore the model design is as follows:

\[
 w_j = \sum_{p=1}^{q} G_{pj} \cdot f \left( \sum_{i=1}^{n} H_{ip} \left< \varepsilon \right>_i - T_p \right) 
\]

where the $T_p$ represent the threshold values.

The obtained strain profiles can be backsubstituted via equation 2 into equation 1, producing again an input vector which is called $\left< \varepsilon^* \right>_i$. If $n$ is the number of input data, the weights and threshold values of the net are trained such that the summed squared residuals are minimized.

\[
 E = \sum_{i=1}^{n} \left( \left< \varepsilon \right>_i - \left< \varepsilon^* \right>_i \right)^2 
\]

where $E$ is called the error function.
Therefore, the net can be viewed as feed forward net with direct feed-back capability. In this sense, the network has to be trained for each individual measurement set. Because of the activation function in terms of the Fermi-function $f$, the inverse problem of equation 1 is mapped onto a nonlinear equation for the weights. Back-propagation of the error is achieved by computing the gradient of the total error with respect to the weights $H_{ip}$, $G_{pj}$ and $T_p$ and adjusting...
the weight proportionally in the direction of the steepest error descent. The error gradient with respect to the $G_{ij}$ is accomplished by application of the chain rule as follows

$$
\frac{\partial E}{\partial G_{pj}} = 2 \sum_{i=1}^{n} \left( <\varepsilon^* >_{ij} - <\varepsilon >_{ij} \right) b_{ji} \cdot f \left( \sum_{i=1}^{n} H_{ip} <\varepsilon >_{ij} - T_p \right)
$$

where $b_{ij}$ takes into account the integrated averages of the wavelets for the individual strain gradients (see eq. 4,2,1).

By similar application of the chain rule, the weights $H_p$ and $T_p$ are updated in the direction of steepest global error descent. In order to guarantee a quick learning algorithm, it is essential to provide suitable initial values of the weights. This is achieved by a preconditioning step in rearranging equation 1 to a linear system of equations for the unknown wavelet-coefficients. This linear system is then solved by a regularization method using singular value decomposition. With this procedure reasonable starting values are obtained. Following back-propagation of error and weight update, the process repeats until the network converges to within the required precision of the global error.

**SIMULATION**

With the aid of a random number generator, a total of 6 different stress gradients have been simulated according to the following formulae

$$
\sigma_{ij}(z) = \left( a_0 + a_1 \cdot z + a_2 \cdot z^2 \right) e^{-a_3 \cdot z}
$$

Boundary conditions were considered by taking into account that a free surface, the orthogonal stress component $\sigma_{33}(0)$ must vanish. Following the idea of the phase compensation hypothesis it is further assumed that the shear stresses $\sigma_{13}$ and $\sigma_{23}$ must also be zero at the surface. The corresponding strain gradients have been calculated from the stress gradients using Hooke’s law. The parameters used are summarized in table 1. The x-ray elastic constants were chosen such to simulate a typical experimental investigation on a steel specimen using an omega-goniometer. The obtained stress gradients are shown in figure 4a and 4b. It is important to note that full triaxial stress/strain gradients are assumed without any simplifications.

<table>
<thead>
<tr>
<th>Table 1: Parameters of simulated data</th>
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<tbody>
<tr>
<td>Young’s modulus</td>
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<td>Poisson’s ratio</td>
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<tr>
<td>Wavelength of the x-rays $\lambda$</td>
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<td>Stress free lattice spacing $d_0$</td>
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<td>$\phi$-orientations [degrees]</td>
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<td>$\psi$-variation [degrees]</td>
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<td>Absorption coefficient $\mu$ [\mu m^{-1}]</td>
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<td>Upper integration limit D</td>
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<td>$\tau(Y=0) = \tau_0$</td>
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Figure 4a: Simulated normal stress gradients versus depth from surface.

Figure 4b: Simulated shear stress gradients as a function of depth from surface.

ANALYSIS RESULTS

For the analysis of the simulated data the Daubechies wavelets of order $N=8$ were used. The choice of the wavelet basis has shown to be uncritical. The x-ray-net has been trained for two different input data sets. In the first data set a total of 93 simulated measurement points were generated according to the data in table 1. In industrial applications, however, in general fewer
data points are available. In order to check the robustness of XRN, a second data set was generated for the same three different \( \varphi \)-orientations where the tilt angle \( \psi \) was varied between \(-45\) and \(+45\) degrees in steps of \(15\) degrees, giving a total of \(21\) data points. In both cases the XRN converged to the simulated profiles within the required global precision of \(10^{-8}\). This value corresponds to the square root of equation 6 where the strains have been normalized to unity. The normalization of the input data is necessary because the nonlinear activation function in terms of the Fermi function only maps an input to the range between zero and unity. In order to provide a suitable relationship between input and output, the wavelet-coefficients which are produced by the output-neurons are multiplied by the rate of the normalized input. The number of input neurons were \(93\), respectively \(21\), the number of neurons in the hidden layer were \(300\) and each strain gradient in the output-layer was represented by \(148\) wavelet-coefficients giving a total of \(888\) neurons. In order to check the sensitivity of XRN against perturbed input data, an error in the simulated d-spacings of \(\Delta d = \pm 5 \times 10^{-6}\) nm was assumed. The resulting error bounds for the stresses are shown in figure 5a for the data set with \(93\) entries and in figure 5b for a reduced data set of \(21\) simulated measurement points. In the first data set the accessible \(\Psi\)-range is up to \(0.933\) in \(\sin^2\psi\) which is very close to the surface. In the second data set, \(\sin^2\psi\) is limited to \(0.5\) which corresponds to a mean penetration depth of \(3.7\) \(\mu\)m in comparison to \(0.5\) \(\mu\)m for the first set. The higher reliability of the first data set can clearly be seen by inspection of figure 5a. Shown are the error bounds for two normal stress gradients as a function of depth. The error estimates are below \(5\) MPa, a value which is often considered as experimental error. The error bounds for the components which are not shown are below \(1\) MPa. The error estimates for the second data set are somewhat larger and reach a maximum of about \(\pm 40\) MPa for the stress component \(\sigma_{11}\). With increasing depth, the bounds are lowered to zero. In a rough estimate one can conclude that the error bounds of data set 2 are amplified by a factor of \(14\) with respect to the first set. In comparison with the absolute values of the gradients in figure 4, in such a representation the error bounds could hardly be seen. This proves that XRN is a very robust neural network in combination with wavelets. The reason is that many of the wavelet-coefficients of the output-neurons are negligible. Therefore, an experimental error propagated through the net also leads to many negligible coefficients.
Figure 5: Error bounds for stresses as a function of depth calculated from strains containing errors with a standard deviation of $5 \times 10^{-6}$ nm in the lattice spacings $d$. a) upper: for data set 1 and b) lower: for data set 2.

CONCLUSIONS

A multiple feed forward neural network has been investigated to evaluate residual strain/stress gradients from x-ray diffraction data. The representation of the full triaxial strain gradients is achieved by an inverse wavelet transform of the results of the output neurons. The excellent approximation properties of wavelets recommend them as state of the art orthonormal bases functions. The result is a very robust network with stable error propagation properties. This is important for industrial applications where in general only few data sets are available. From these results, we conclude that neural network technology in combination with wavelets holds great promise for the difficult arenas of inverse problems. Our work continues in the development of rapid and routine analyses packages for residual stress determination from diffraction experiments. A WINDOWS based software is available.
REFERENCES