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Depth-resolved residual stress evaluation from X-ray diffraction measurement data using the approximate inverse method

The paper deals with the depth determination of residual stress states from diffraction data. First an historical overview of the known approaches is given. Then we apply the approximate inverse method to this problem. This method is known to be very efficient and stable with respect to noise-contaminated data. It is even possible to prove convergence and it allows an error estimate of the calculated depth resolved residual stress profile.

Keywords: X-ray diffraction; Residual stress; Gradient; Regularization; Ceramic; Approximate inverse; Mollifier; Reconstruction kernel

1. Introduction

Nowadays residual stress measurements are usually carried out using the $\sin^2\psi$ method which requires the residual stress to be almost constant within the penetration depth. This condition does not hold true for machined ceramics. To calculate the depth-resolved residual stress state, various methods have already been proposed. In this article, we present a method which is based on the theory of ill-posed problems.

2. Historical overview

The influence of residual stress gradients has been discussed since the end of the 1940s [48Oss]. The first approaches which were published in the beginning of the 80s were linear generalisations of the $\sin^2\psi$ method [80Pei, 84Hau]. They turned out to be numerically stable but yield a linear increasing residual stress which contradicts the mechanical boundary conditions. Nonlinear methods lead to strong instabilities in the solution [89Oet]. The attempt to avoid instability by choosing seemingly realistic functions influences the calculated result strongly [88Hau, 92Rup].

In a first attempt to use a general class of functions, polynomials were used [92Eig]. In this case the instability of the solutions does not lead to satisfying results. Based on this result the AP (Abschnitt-Polynom, spline) method has been developed [96Lev]. Other base functions can be found in [00Beh]. All these methods use a least-square fitting to the model functions (least-squares method, see Section 3). Here, a more general approach is presented.

3. Mathematical base

To calculate the residual stress σ_{ij} as a function of the depth z, the following basic formula of X-ray diffraction (1) is to be inverted.

$$\Delta\theta_{\varphi,\psi}(\tau) = \sum_{i,j} r_{i,j}(\varphi,\psi)\frac{1}{\tau}\int_0^\infty dz\, e^{-\frac{z}{\tau}}\sigma_{ij}(z) \tag{1a}$$

where

$$r_{11}(\varphi,\psi) = -\tan\theta_0\left(\frac{S_2}{2}\cos^2\varphi\sin^2\psi + S_1\right)$$

$$r_{22}(\varphi,\psi) = -\tan\theta_0\left(\frac{S_2}{2}\sin^2\varphi\sin^2\psi + S_1\right) \tag{1b}$$

when the residual stress tensor σ_{ij} is diagonal and $\sigma_{33} = 0$. $\Delta\theta_{\varphi,\psi}$ denotes the stress induced peak shift, ψ the tilt angle, φ is the rotation angle of the measurement device, θ_0 means the peak position of the unstressed probe, and τ is the penetration depth of the X-ray beam which depends on the attenuation of the material. S_1 and S_2 are materials constants and z the depth co-ordinate. Using measurements with varying rotation angles φ, the Laplace transformed function $\breve{\sigma}_{ij}(\tau)$ of $\sigma_{ij}(z)$ can be calculated from Eqs. (1a, b). Using the scattering vector mode yields $\breve{\sigma}_{ij}(\tau)$ in a direct way [94Gen]. The inverse Laplace transform turns out to be the crucial difficulty.

As discussed above many approaches to calculate the residual stress depth profile $\sigma_{ij}(z)$ from measurement data have been published in recent years. The basic concept is always to describe the component functions $\sigma_{ij}(z)$ of the residual stress tensor as functions with free parameters

$$\sigma_{ij}(z) = f_{ij}({}_1a_{ij}, {}_2a_{ij}, {}_3a_{ij}, \ldots) \tag{2}$$

The model function f_{ij} is Laplace-transformed and put in the basic formula of X-ray diffraction [Eq. (1)]. The free parameters are adjusted by a least-squares method minimizing the residuum of the measurement data and the data which result from the calculated solution. These parameters determine the component functions $\sigma_{ij}(z)$ as it follows from Eq. (2). As model functions, which are necessary to apply the least squares method, were proposed e. g. exponential functions [93Pre], Taylor polynomials [94Här], tent functions [94Zhu], Jacobi polynomials [94Gen], piecewise linear functions [95Zhu], trigonometric functions [97Wer], products of polynomials and exponential functions [84Hau, 92Eig], and splines [96Lev].

4. Application of the approximative inverse method (AIM)

The concept of the AIM was developed to solve inverse and ill-posed problems [90Lou, 96Lou]. Here, the equation

$$L\sigma(\tau_i) := \int_0^\infty e^{-\frac{z}{\tau_i}}\sigma(z)\,\mathrm{d}z = \breve{\sigma}(\tau_i)$$

which defines the reciprocal Laplace transform L has to be considered to calculate the residual stress $\sigma(z)$ from a finite number of given measurement data scanning points τ_i. The basic concept is to calculate a mollified version of the solution

$$\sigma_\gamma(z) = \int_0^\infty \sigma(z')\; e_\gamma(z', z)\;\mathrm{d}z' \tag{4}$$

instead of the solution itself. The so-called mollifier e_γ is an approximation to Dirac's delta distribution leading to a smooth approximation σ_γ of σ. This suppresses the influence of noise in the measurement data to the solution. If the equation

$$L^*\vec{\varphi}_\gamma(z) = e_\gamma(z) \tag{5}$$

can be solved the regularized solution is given by

$$\sigma_\gamma(z) = \sum_{\tau_i} \breve{\sigma}(\tau_i)\;\vec{\varphi}_\gamma(\tau_i, z) \tag{6}$$

as follows from

$$\sigma_\gamma(z) = \int_0^\infty \sigma(z')\; e_\gamma(z, z')\;\mathrm{d}z' = \int_0^\infty \sigma(z')\; L^*\vec{\varphi}_\gamma(z, z')\;\mathrm{d}z'$$

$$= \sum_{\tau_i} \breve{\sigma}(\tau_i)\;\vec{\varphi}_\gamma(\tau_i, z) \tag{7}$$

where we used Eqs. (4) and (5) and the definition of the adjoint of an operator. The vector $\vec{\varphi}_\gamma$ solving Eq. (5) is called reconstruction kernel. Its length is equal to the number of scanning points τ_i. For a finite number of data scanning points a collocation method is used to transform Eq. (5) into a system of linear equations, where the collocation points are chosen equal to the data scanning points τ_i:

$$C_m\vec{\varphi}_\gamma(z) = \vec{e}_\gamma(z) \tag{8}$$

Due to the fact that inversion of the Laplace transform is a severely ill-posed problem, the matrix *Cm* is ill conditioned as well. Therefore, an additional regularization is used:

$$(C_m + \rho\mathbf{1})\;\vec{\varphi}^\rho_\gamma(z) = \vec{e}_\gamma(z) \tag{9}$$

where ***1*** denotes the identity matrix and ρ is a small real number. As solution of Eq. (9) we obtain the reconstruction kernels. The multiplication of these reconstruction kernels with the measurement data yields the approximation to σ(z):

$$\sigma^\rho_\gamma(z) = \sum_{\tau_i} \breve{\sigma}(\tau_i)\;\vec{\varphi}^\rho_\gamma(\tau_i, z) \tag{10}$$

5. Properties of the method

The most important difference between this method and the procedures known from literature is that the AIM takes the measurement error into account. It is applicable for a set of arbitrarily distributed tilt angles ψ. Since the system (9) is solved independently from the measurement data it is stable with respect to noise. The main advantage can be seen in the fact that the error in the calculated solution can be estimated.

For a given choice of ρ which depends on the number of scanning points m the error can be estimated with the following equation [03Sch]:

$$\frac{\left|\sigma(z) - \sigma^\rho_\gamma(z)\right|}{\|\sigma(z)\|} \le \delta^\gamma_m(z) + \xi_m(z) \tag{11}$$

The left-hand side of Eq. (11) represents the relative error in the calculated solution. The second summand on the right-hand side represents the discretization error which tends to 0 as m goes to infinity. The other summand δ^γ_m depends first on how exactly the solution of Eq. (9) solves Eq. (5) and second on the approximation accuracy of e_γ to Dirac's delta distribution. δ^γ_m represents an unavoidable error which tends to 0 for $\gamma \to 0$ and $m \to \infty$, but is non-zero in the general case. Thus, the unavoidable error is smaller for a larger number of scanning points. For exact data it is possible to choose $\gamma \approx 0$. In this case the approximate solution (10) converges to the exact solution as long as the exact solution is square integrable. Noisy data require $\gamma > 0$. In this case a certain error in the result is unavoidable.

6. Numerical tests

To test the method two curves were Laplace transformed and recovered. Fig. 1 shows the results. Good accuracy can be obtained even at greater depths $z/\tau_{\max}$ (Figs. 1a and b) and even if the function is not continuously differentiable as shown in Fig. 1a. The reconstruction accuracy is higher when the data points are equally spaced in $1/\tau$ than when equally spaced in the penetration depth τ.

7. Application of the AIM

We used the AIM to calculate the residual stress depth profile of a ground corundum (Al2O3) specimen. The cutting speed was v_c = 35 m/s. The feed rate v_{ft} and the bond type have been varied (Fig. 2). The measurement used a maximum tilt angle of $\psi_{\max}$ = 87° and was carried out with synchrotron radiation at HASYLAB (DESY), Hamburg. The peak positions were determined by fitting the data with Pearson- VII functions using a linear background correction. The evaluation with the AIM yields the residual stress

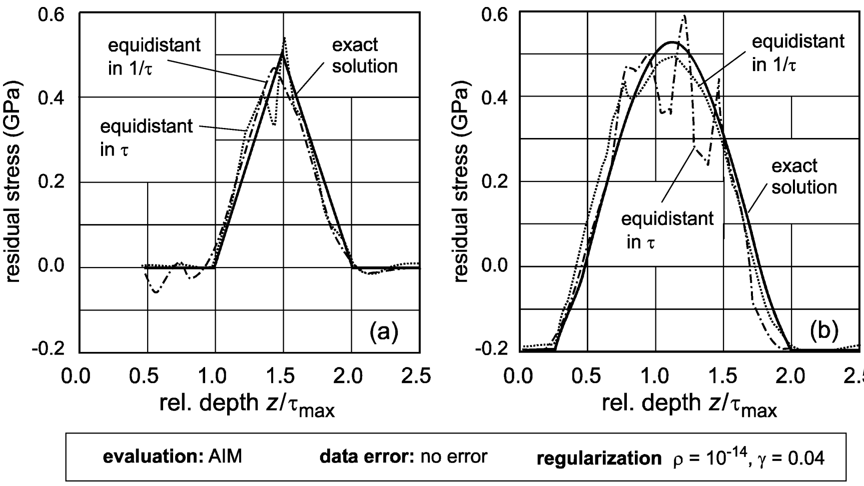

Fig. 1. Achievable accuracy, reconstructions with synthetic data, τ_{max} denotes the maximal penetration depth corresponding to the reflection angle θ_0 . Curves of a continuous function (a) and a continuously differentiable function (b) have been used.

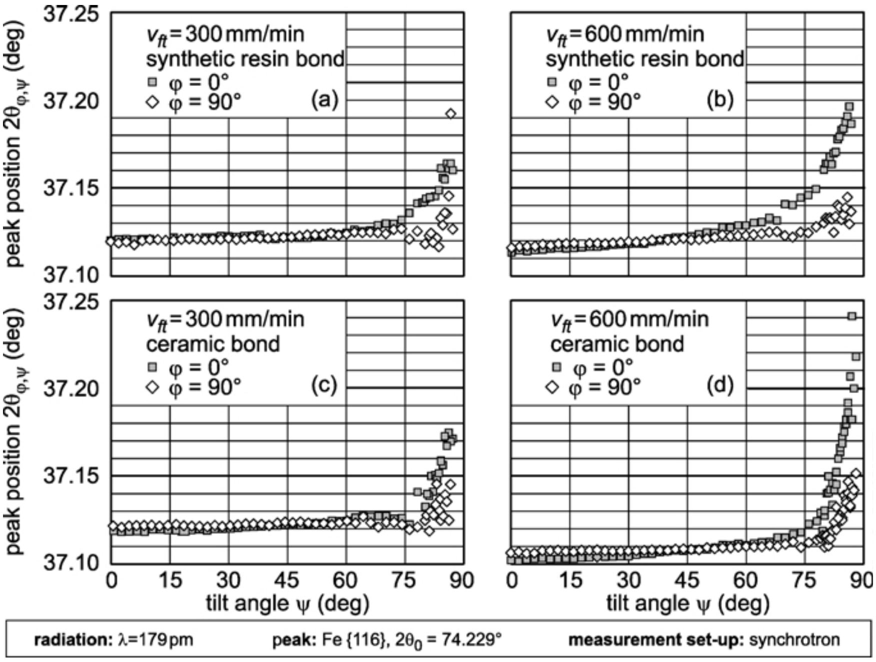

Fig. 2. Measured peak positions using low (a, c) and high feet rates (b, d). The bond types have been varied: (a, b): synthetic resin bond, (c, d): ceramic bond. The peak positions were measured using two rotation angles $\varphi = 0°$ and $\varphi = 90°$. λ denotes the wavelength.

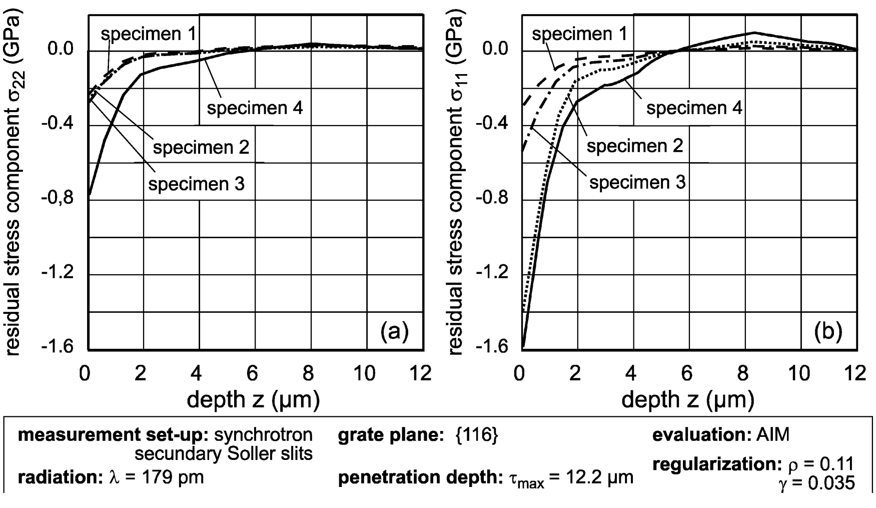

Fig. 3. Calculated residual stress depth profiles depending on the depth z for the stress components σ_{11} (b) and σ_{22} (a) corresponding to the data from Fig. 2. The regularization parameters of the AIM [see Eq. (10)] are chosen as indicated in the box above.

depth profiles shown in Fig. 3. The high feed rate v_{ft} (specimens 2 and 4) leads to higher compressive residual stress states for the component along the moving direction of the diamond grains σ_{11} corresponding to the rotation angle $\varphi = 0°$. This can be explained by lower temperatures in the contact zone. For the component perpendicular to the moving direction σ_{22} (corresponding to $\varphi = 90°$) the high feed rate leads to higher compressive residual stress only for the specimen machined with a grinding wheel having a ceramic bond.

8. Conclusions

The approximate inverse method (AIM) has been used to calculate the residual stress profile from X-ray diffraction data. Since it is based on a regularization approach, the influence of noise in the data to the solution can be damped. Numerical tests show satisfying results even when the data are noisy. The AIM was used to evaluate the residual stress depth profile of a ground corundum specimen. It was found that the residual stress depends on the feed rate. Because of the small number of characterized specimens, further tests are necessary to emphasize the properties of the AIM.

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