Efficient optimisation of initial values for characterising piezoelectric material parameters

Nadine Feldmann[1], Bernd Henning[2]

[1] Elektrische Messtechnik, 33100 Paderborn, Deutschland, Email: feldmann@emt.upb.de

[2] Elektrische Messtechnik, 33100 Paderborn, Deutschland, Email: henning@emt.upb.de

Introduction

The more and more simulation-driven design process of piezoelectric transducers calls for consistent and complete sets of piezoelectric material parameters. Today, the determination of these material parameters requires several differently processed specimen that only allow to measure a subset of parameters each. This can lead to inconsistent sets of parameters that furthermore suffer from uncertainties up to 20 % arising from high fabrication tolerances. Thus, it is essential to calculate the full set of material parameters from a single specimen. The identification process can be done by an inverse optimisation procedure. When considering gradient based optimisation, especially the number of optimisation iterations highly depends on the chosen initial values. Thus, it is crucial to estimate these initial values quite conscientiously. [1] gives a guideline for estimating certain material parameters from simple geometries. Since only one single specimen is to be used, only some of the needed at least 10 parameters can be calculated here. Thus, further considerations have to be made before starting the optimisation.

Overall objective

The overall objective is to develop an inverse measurement set-up that is able to estimate all relevant material parameters using only a unique specimen. The measurand is supposed to be only the frequency-dependent electric impedance $Z(f)$ since it is easy and cheap to obtain. The goal of the inverse method is to find a set of material parameters for a given Finite-Element-Method (FEM) model that best represents the measurement via an optimisation algorithm. Since a simple set-up like common disc-shaped piezoceramics with both faces covered fully with electrodes (full-faced electrodes) lack sensitivity for several material parameters, an optimised triple-ring electrode set-up is proposed [2] (see figure 1). The applied optimisation algorithm is chosen to be gradient-based since it promises to converge using only a moderate number of function evaluation. This is quite important since each function evaluation implies the time-consuming computation of the FEM model. For the determination of the initial optimisation parameters, the simpler full-faced set-up that can be approximated analytically is advantageous. Nevertheless, this causes quite large uncertainties in certain parameters. In order to profit from the possibly fast convergence of the gradient-based algorithms, a fast and easy pre-optimisation of the initial values based on piezoelectric disc with full-faced electrodes is proposed here.

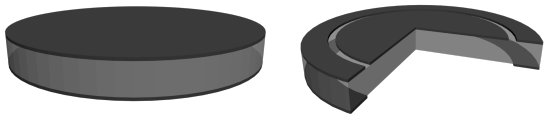

Figure 1: Full-faced and triple-ring electrode set-up

Mathematical description

In piezoelectric materials, the electric (electric field $\boldsymbol{E}$, electric flux density $\boldsymbol{D}$) and mechanical quantities (stress $\boldsymbol{T}$, strain $\boldsymbol{S}$ in Voigt notation) are coupled. In the linear case, the constitutive equations read

$$\boldsymbol{T} = -\boldsymbol{e}^{\mathrm{t}}\boldsymbol{E} + \boldsymbol{c}^{\boldsymbol{E}}\boldsymbol{S} \tag{1}$$

$$\boldsymbol{D} = \boldsymbol{\varepsilon}^{\boldsymbol{S}}\boldsymbol{E} + \boldsymbol{e}\boldsymbol{S}, \tag{2}$$

where $\boldsymbol{c}^{\boldsymbol{E}}$, $\boldsymbol{\varepsilon}^{\boldsymbol{S}}$ and $\boldsymbol{e}$ denote the stiffness, the permittivity and the coupling matrices, respectively. Using the constitutive equations, the differential equations

$$\rho\ddot{\boldsymbol{u}} = \mathcal{B}^{\mathrm{t}}(\boldsymbol{c}^{\boldsymbol{E}}\,\mathcal{B}\,\boldsymbol{u} + \boldsymbol{e}^{\mathrm{t}}\nabla\phi) \tag{3}$$

$$q = \nabla(\boldsymbol{e}\,\mathcal{B}\,\boldsymbol{u} - \boldsymbol{\varepsilon}^{\boldsymbol{S}}\nabla\phi) \tag{4}$$

describe the evolution of the mechanical displacement $\boldsymbol{u}$ and the electric potential ϕ and charge q over time t. $\mathcal{B}$ and ∇ denote the operator for the spacial derivative and the nabla/del operator. The density ρ is assumed to be known by measuring the mass and kept constant at any time in the further considerations. Piezoelectric ceramics typically are transversely isotropic leading to certain symmetries in the material matrices leaving only 10 independent constants to be determined. For the representation of damping, a Rayleigh damping model is chosen introducing two further parameters α_{M} and α_{K}:

$$p_{\mathrm{mat}} = \big[c^E_{11}, c^E_{12}, c^E_{13}, c^E_{33}, c^E_{44}, \varepsilon^S_{11}, \varepsilon^S_{33}, e_{15}, e_{31}, e_{33}, \alpha_{\mathrm{M}}, \alpha_{\mathrm{K}}\big]\,. \tag{5}$$

Impedance calculation

These equations described above are solved for a disc-shaped specimen using the FEM tool CFS++ [3]. For an efficient calculation of the frequency-dependent impedance, a calculation in time domain using an impulse excitation is preferable. From the applied charge impulse

$q(t)$ and the calculated electric potential $\phi(t)$, the impedance $Z(f)$ can be determined by

$$Z(f) = \frac{\mathcal{F}\{\phi(t)\}}{\mathcal{F}\{\dot{q}(t)\}}, \tag{6}$$

where $\mathcal{F}\{\cdot\}$ and $\dot{q}(t)$ denote the Fourier transform and the derivative of the electric charge with respect to time, respectively. An impedance curve of a disc-shaped piezoceramic with an radius of 5 mm and a thickness of 1 mm is depicted in figure 2. The first radial resonance can be seen at around 0.2 MHz followed by its higher harmonics. The thickness resonance that is superimposed by the radial resonances appears at 2 MHz.

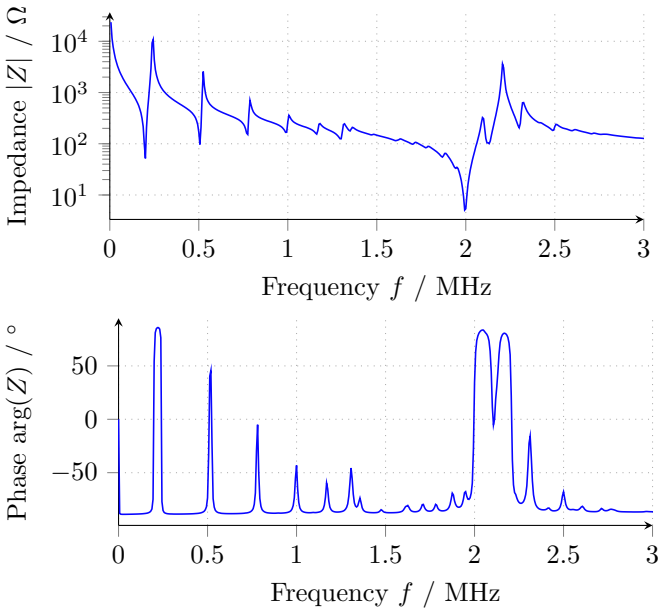

Figure 2: Typical impedance of a piezoelectric disc

Resonance frequency determination

For a first estimate of the material parameters, an approximation based on the resonance and anti-resonance frequencies is applied [1]. In the presence of damping the terms „resonance and antiresonance frequency“ f_{res} and f_{anti} are not well defined since the damped impedance consists of a real and an imaginary part. The concept that is only slightly influenced by the amount of damping present is

$$f_{\text{res}} = \underset{f}{\operatorname{argmax}} \operatorname{Re}\{fZ(f)\} \tag{7}$$

$$f_{\text{anti}} = \underset{f}{\operatorname{argmax}} \operatorname{Re}\left\{\frac{1}{fZ(f)}\right\}, \tag{8}$$

where $\operatorname{Re}\{\cdot\}$ denotes the real part. Other possibilities for defining the resonance frequencies would be the frequency of the minimal absolute value or the zeros of the phase of the impedance [1].

Analytic approximation

For determining an analytic relation between the resonance and anti-resonance frequencies of different modes and the material parameter, an analytic calculation of the impedance for a simplified set-up is used. The approximated impedance is best calculated by splitting the problem into a thickness mode and a radial mode consideration [1, 4, 5]. From considering mainly resonance and anti-resonance frequencies, it is possible to approximate several material constants. Unfortunately, the sensitivity for several parameters resulting from the homogeneous field excitation is very low. Thus, some constants can only be roughly estimated from the single specimen (mostly by assuming isotropy which is not reasonable from a physical point of view). Thus, only relying on the analytic approximation does not always suffice considering the following optimisation.

Sensitivity analysis

The objective for the initial value estimation is to have a simple pre-optimisation using full-faced impedances that gives a better starting point for the following optimisation using triple-ring electrodes. Moreover, the non-physical isotropic model is to be overcome. For simplifying the objective function for this pre-optimisation only the resonance frequencies of single modes are considered. Furthermore, only one parameter is to be adapted at a time. This can lead to fewer optimisation steps and faster convergence. The first step to reach a simple but effective optimisation scheme is a sensitivity analysis. Several simulations changing only one single material parameter around an operational point were calculated in order to learn the influence on the impedance. Figure 3 depicts the simulation results for changing c_{13}^E and c_{33}^E. It can be seen that c_{33}^E changes all the resonance frequencies, but mainly determines the thickness resonance whereas c_{13}^E influences almost only the radial resonances. Thus, for this example it is obvious, that optimising c_{33}^E before c_{13}^E is essential. Table 1 summarises the influences of certain material parameters important for the pursued optimisation. Further sensitivity studies can be found e.g. in [6].

Table 1: Influence of certain material parameters on the electrical impedance

Parameter	Influence
c_{11}^E	all radial resonances
c_{12}^E	first radial resonances
c_{13}^E	all radial resonances
c_{33}^E	all radial and thickness resonances
e_{33}^E	thickness anti resonance
ε_{33}^S	absolute value of the whole impedance
α_{M}	absolute value at lower frequencies
α_{K}	absolute value at higher frequencies

Optimisation of the initial values

The success of the pre-optimisation of the initial values highly depends on choosing an appropriate optimisation sequence and a fitting resonance frequency for each material parameter. Considering table 1, the following op-

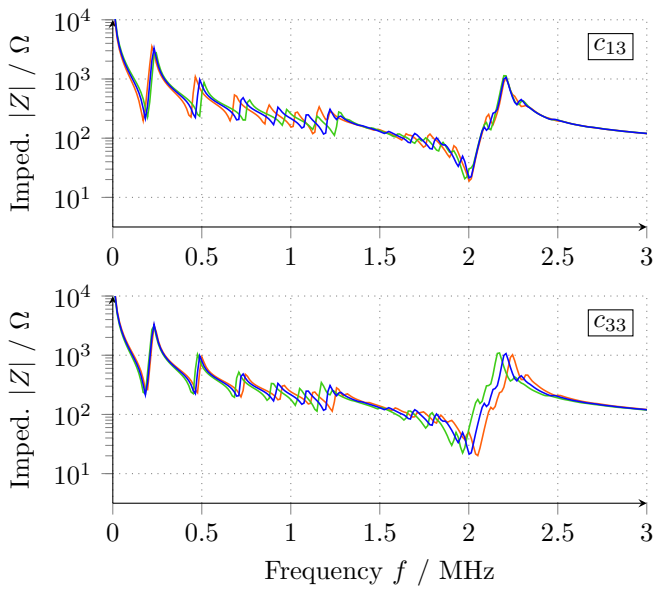

Figure 3: Impedance with changed material parameters c_{13}^E and c_{33}^E (——: +5 %, ——: −5 %, ——: ±0 %)

timisation scheme is considered:

- c_{33}^E using the thickness resonance
- ε_{33}^S using an analytic approximation
- c_{13}^E using the second radial resonance
- c_{12}^E using the first radial resonance
- c_{44}^E using an analytic approximation
- e_{33} using the thickness antiresonance
- e_{31} using an analytic approximation
- α_M using the absolute value at the first radial resonance frequency
- α_K using the absolute value at the thickness resonance frequency

The analytic approximation concerning ε_{33}^S considers the capacitive character outside of the resonance areas and can be calculated by

$$\varepsilon_{33}^S = \frac{A}{2\pi f_\mathrm{cap} \varepsilon_0 h |Z(f_\mathrm{cap})|}, \tag{9}$$

where A, f_cap, ε_0 and h denote the circular area of the disc-shaped ceramic, the frequency outside of the resonance range (e.g. between the first and second thickness resonance), the vacuum permittivity and the hight of the piezoceramic, respectively. c_{44}^E can be approximated using [7] and e_{31} is recalculated from [1]. Since c_{11}^E and c_{13}^E influence the same resonance frequencies only one of the two has been chosen for the optimisation. Because the initial value estimation of c_{11}^E is typically less error-prone, c_{13}^E is included in the optimisation process. ε_{11}^S and e_{15} are not considered in the optimisation process at all since they do not have a reasonable influence on the impedance. For the optimisation itself a simple gradient descent is chosen. The gradient is calculate by finite differences in the operating point of the initial guess. The step width is chosen to be ±5 % of the value in the operating point and changed only if this leads to obviously infeasible results. In order to avoid the time intensive gradient calculation, this gradient is kept fixed for each parameter and not updated during the optimisation process assuming to not change severely.

Results using simulation data

For a first trial of the proposed algorithm, the typically measured impedance to be fitted is replaced by a simulated impedance in order to verify the improvement of the material parameters. A disc with a radius of 5 mm, a thickness of 1 mm, a density of 7800 kg/m^3 and the following material parameters are chosen:

$$\begin{aligned} p_\mathrm{mat} = [&119\,\mathrm{GPa},\ 84\,\mathrm{GPa},\ 83\,\mathrm{GPa},\ 117\,\mathrm{GPa},\ 21\,\mathrm{GPa},\\ &920\varepsilon_0,\ 743\varepsilon_0,\ 12.09\,\mathrm{C\,m^{-1}},\ -6.03\,\mathrm{C\,m^{-1}},\\ &15.49\,\mathrm{C\,m^{-1}},\ 1.267\cdot10^5\,\mathrm{s^{-1}},\ 6.259\cdot10^{-10}\,\mathrm{s}] \end{aligned} \tag{10}$$

Comparing the relative deviation from the chosen parameters in p_mat, table 2 gives an overview of the improvement of material parameters. It is evident that the pre-optimisation made an overall improvement of the guessed parameters, but some still remain far off mainly due to the lack of sensitivity (e.g. ε_{11}^S). In order to test the chosen optimisation strategy, several sets of parameters closely related to real materials are inserted into to the algorithm (e.g. Pz27 and APC855 [8]) and improved the inital guess throughoutly.

Table 2: Comparison of initial guess and optimised material parameters

Parameter	Initial guess	Optimised
c_{11}^E	1.7 %	1.7 %
c_{12}^E	17.8 %	6 %
c_{13}^E	19.3 %	4.1 %
c_{33}^E	3.5 %	2.4 %
c_{44}^E	-47.5 %	-18.7 %
ε_{11}^S	21 %	21 %
ε_{33}^S	50 %	-0.6 %
e_{15}^E	-4.5 %	-4.5 %
e_{31}^E	-42.6 %	-16.1 %
e_{33}^E	11.8 %	-1.8 %
α_M	174 %	-14.6 %
α_K	249 %	67 %

Results using measurement data

For the application on measurements, the impedance of a disc-shaped sample of PIC255 (PI Ceramics GmbH, Lederhose, Germany) has been measured using an E4990A Impedance Analyzer (Keysight Technologies Inc., Santa Rose, USA). The measured impedance is depicted in figure 4, as well as the simulated impedances using the initial and the optimised material parameters. A good

agreement, especially concerning the resonance frequencies, can be seen. Thus, an efficient, non-time-consuming procedure for arriving at useful initial values for the more complex, triple-ring electrode set-up is implemented.

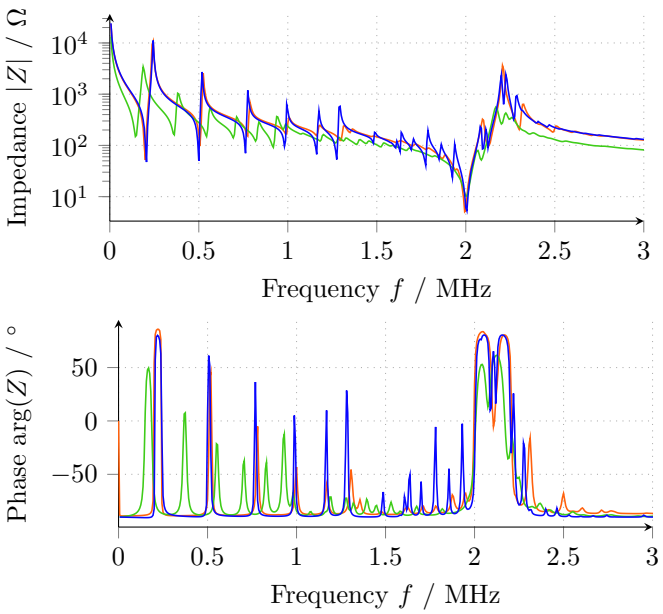

Figure 4: Impedance of the measured impedance (——) and simulation using the initial guess (——) and the optimised (——) material parameters

Conclusions

The presented procedure allows for a fast and easy improvement of the initial values obtained from an impedance measurement of piezoelectric discs with full-faced electrodes. Since the analytic approximation using only a single specimen and an isotropic assumption leads the infeasible material parameter, a pre-optimisation reduces the deviation of the measured and simulated impedances. The pre-optimisation only based on single resonance frequencies leads to an efficient improvement of the material parameters and thus reduced the optimisation time of the following more complex optimisation using triple-ring electrodes. Using simulated data as well as measured data, the described algorithm resulted in an improved agreement of the parameters or the electrical impedance. The determined initial values are now to be used in the main optimisation process using the triple-ring electrode set-up. Since the presented procedure involving a sensitivity analysis and an optimisation adapted to each parameter proved to be quite promising, a similar scheme will be implemented for this more complex set-up as well. Furthermore, the calculation of the derivatives that is up to now realised using finite differences can profit from the implementation of Algorithmic Differentiation [9, 10] which is able to calculate the derivatives accurately to working precision.

Acknowledgement

The authors would like to thank the German Research Foundation (DFG) for financial support of the research project 321120716. Furthermore, we would like to thank Dmitrij Dreiling for extensive testing of the presented algorithm and Lars Meihost for preparing and conducting the measurements.

References

[1] American National Standards Institute, "IEEE Standard on Piezoelectricity," 1987.

[2] K. Kulshreshtha, B. Jurgelucks, F. Bause, J. Rautenberg, and C. Unverzagt, "Increasing the sensitivity of electrical impedance to piezoelectric material parameters with non-uniform electrical excitation," *Journal of Sensors and Sensor Systems*, vol. 4, pp. 217–227, 2015.

[3] M. Kaltenbacher, *Numerical Simulation of Mechatronic Sensors and Actuators*. Springer-Verlag, 2nd ed., 2007.

[4] D. A. Berlincourt, D. R. Curran, and H. Jaffe, "Piezoelectric and piezomagnetic materials and their function in transducers," in *Physical acoustics* (W. P. Mason, ed.), New York: Academic Press, 1964.

[5] A. Meitzler, H. O'Bryan, and H. Tiersten, "Definition and measurement of radial mode coupling factors in piezoelectric ceramic materials with large variations in poisson's ratio," *IEEE Transactions on Sonics and Ultrasonics*, vol. 20, no. 3, pp. 233–239, 1973.

[6] N. Pérez, F. Buiochi, M. Brizzotti Andrade, and J. Adamowski, "Numerical characterization of piezoceramics using resonance curves," *Materials*, vol. 9, no. 2, 2016.

[7] P. Theocaris and D. Sokolis, "Spectral decomposition of the compliance tensor for anisotropic plates," *Journal of Elasticity*, vol. 51, no. 2, pp. 89–103, 1998.

[8] F. Buiochi, C. Y. Kiyono, N. Peréz, J. C. Adamowski, and E. Silva, "Efficient algorithm using a broadband approach to determine the complex constants of piezoelectric ceramics," *Physics Procedia*, vol. 70, pp. 143–146, 2015.

[9] A. Griewank and A. Walther, *Evaluating derivatives: Principles and techniques of algorithmic differentiation*. Philadelphia: Society for Industrial and Applied Mathematics, 2nd ed., 2008.

[10] B. Jurgelucks, L. Claes, A. Walther, and B. Henning, "Optimization of triple-ring electrodes on piezoceramic transducers using algorithmic differentiation," *Optimization Methods and Software*, pp. 1–21, 2018.