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Sensitivity Analysis of Piezoelectric Material Parameters Using Sobol Indices

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Abstract: This computational study examines the sensitivity of the vibrational eigenmodes of a block-shaped piezoelectric test specimen upon variation of the underlying material parameters. The method of Sobol is employed with the calculated resonance positions and their respective electrical impedance as quantity of interest. For this purpose, the FEM-Software COMSOL Multiphysics®in combination with MATLAB® is used to calculate the resonance frequencies and impedance values as well as a mode shape analysis for eigenmode identification.

Keywords: Sobol Indices, Piezoelectric Material Parameters, Mode Selection, COMSOL Multiphysics, MATLAB

Introduction

For finite-element simulations of piezoelectric devices, material parameters are crucial for accurate results. Several methods have been developed to determine these parameters. Traditionally, the IEEE standard [1] suggests using at least four test specimens with isolated vibrations for parameter extraction via impedance measurements, which can be expensive and susceptible to errors [2]. An alternative inverse method, using just two specimens and optimization to match simulated and measured impedance curves, reduces the effort but requires knowledge of material parameter sensitivity. Sobol indices are a common way to quantify this sensitivity [3, 4]. In Ref. [5] the authors examined the applicability of the method of Sobol to the non-smooth, resonant behavior of a vibrational eigenmode of a piezoelectric material for the first time. This work extends the previous study to overlapping resonances. Introducing a mode shape analysis for resonance identification, the Sobol indices are calculated for the specifically selected eigenmodes. The resonance position and its electrical impedance value are considered as sensitivity objective.

Piezoelectric Materials

The effect that occurs in piezoelectric materials can be described by two coupled state equations for the dielectric displacement (D_m) and the mechanical stress (T_{ij}), known as the stress-charge form,

$$D_m = e_{mkl} S_{kl} + \epsilon_{mn}^S E_n, \tag{1}$$

$$T_{ij} = c_{ijkl}^E S_{kl} - e_{ijn} E_n, \tag{2}$$

where E_n is the electric field and S_{kl} the mechanical strain [2]. The material parameters ϵ_{mn}^S (electric permittivity at constant strain), c_{ijkl}^E (elastic stiffness at constant electric field), and e_{ijn} (the piezoelectric stress tensor) are tensor quantities. Symmetries of the crystalline structure reduce the number of independent tensor components which leads (for a crystall class 6mm) to a reduced set of matieral parameters, namely $c_{11}^E, c_{12}^E, c_{13}^E, c_{33}^E, c_{44}^E, c_{66}^E, e_{31}, e_{33}, e_{15}, \epsilon_{11}^S$ and ϵ_{33}^S. Note that the indices are given in the Voigt notation. Which parameters are truly relevant depends on the excited mode shape and/or geometry of the used specimen. When considering the impedance curve of a specimen, it can be observed that resonance frequencies (minima) are not always nicely separated from others. In this work, the so called T1-L-mode and the T1-W-modes of a block shaped sample from [2] are examined. While the T1-L mode shows a nicely isolated frequency, the resonances of the T1-W mode are close together, making them difficult to distinguish when the material parameters are varied [5].

The Method of Sobol

Sensitivity analyses assess how variations in model parameters influence outputs, thereby identifying influential and insignificant parameters. Local methods examine output changes due to small parameter changes in proximity to a fixed value, while global approaches consider the entire parameter space, often using sampling techniques like Latin Hypercube Sampling (LHS) [6]. Sobol indices are commonly employed in global sensitivity analysis to quantify the contribution of each input parameter to the output variance. In this study, the resonance frequency and its associated impedance value, respectively, serve as the model output $y[\mathbf{x}]$ and are calculated upon variation of the

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model parameters $\mathbf{x} = x_1, ..., x_n$, namely the piezoelectric material parameters. The resulting variance is decomposed into the contributions attributable to the individual input parameters.

The first order Sobol index (the so-called main effect) of parameter x_i is defined as [7, 3]

$$S_i = \frac{\mathcal{V}_{x_i}\left[E_{\mathbf{x}_{\sim i}}\left[y|x_i\right]\right]}{\mathcal{V}_{\mathbf{x}}\left[y\right]} \in [0, 1], \tag{3}$$

where $\mathcal{V}_{x_i}\left[y\right]$ is the total variance of the model $y[\mathbf{x}]$ over all input parameters and $E_{\mathbf{x}_{\sim i}}\left[y|x_i\right]$ is the mean value of y with given parameter x_i [8]; the indices x_i and $\mathbf{x}_{\sim i}$ denote which parameters ought to be varied, the latter meaning all but the ith one. With the first order Sobol index, the influence on the variance by one parameter alone can be accessed. To calculate second or higher order interactions S_{ij}, $S_{ijk}, \ldots$, one would have to calculate the resulting model variance when two or more input parameters are varied and subtract the variance of each parameter alone. This procedure is very time consuming, therefore the total Sobol index, which is defined as

$$S_i^T = \frac{E_{\mathbf{x}_{\sim i}}[\mathcal{V}_{\mathbf{x}_{\sim i}}[y|\mathbf{x}_{\sim i}]]}{\mathcal{V}_{\mathbf{x}}[y]} \in [0, 1], \tag{4}$$

is often used [7, 3]. The total Sobol index S_i^T is calculated using the variance of x_i including all higher order interactions that involve x_i. If the first order Sobol index equals the total Sobol index, then no interactions exist between the specified material parameters. The direct calculation of the Sobol indices by solving the variance integral is not feasible. Instead, the integrals are approximated by estimators using a statistical approach with only $m \cdot (n + 2)$ model evaluations [3]. Here, m denotes the sample size while n is the number of parameters. With the Latin Hypercube Sampling (LHS) two $m \times n$ matrices A and B containing independent samples are generated. These matrices are rearranged into cross matrices AB_i by inserting the ith column of matrix B at the position of the ith column of matrix A. In this way, the dependencies among individual variables are represented.

Simulation Model and Methods

This study focuses on the vibrational eigenmodes of block-shaped piezoelectric specimens, characterized by an increased vibration at resonance. In this work, the eigenfrequencies are calculated using the eigenfrequency study in COMSOL followed by a frequency domain study to calculate the associated impedance values. This approach combines the computationally cheap eigenfrequency study with the costly frequency domain study, which itself is only executed for the identified eigenfrequencies.

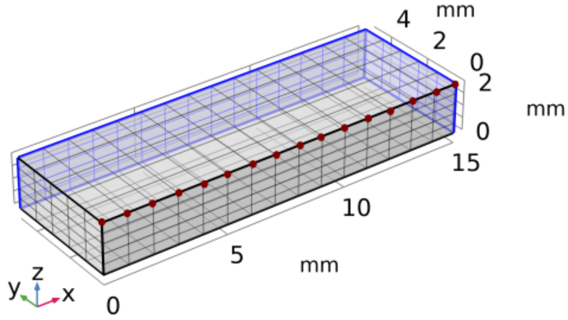


Fig. 1: Model geometry and mesh of the block-shaped test specimen considered in this work. Highlighted are the symmetry planes used to reduce the model size and the evaluation points for the displacement.

For our analysis, a block of length 30 mm, width 10 mm, and thickness 2 mm from [2] is used. The block is polarized in the thickness (z-)direction and made of the material PIC255 for which optimized material parameters can be found in Ref. [2]. Furthermore, as a loss and damping model, the loss factor damping is used, for which the tensors ϵ^S and c^E from Eq. (1) and Eq. (2) are supplemented with an imaginary part, that represents a loss or damping factor.

In COMSOL Multiphysics®, piezoelectricity is modelled using the Solid Mechanics and Electrostatics interfaces coupled via the Piezoelectricity interface. A 1 V voltage boundary condition is applied to the top surface, with the bottom grounded. Two symmetry planes are used to reduce computational cost (see Figure 1). The mesh consists of 15 x 5 x 5 cubic elements. The frequency domain study is configured to search for eigenfrequencies whose real part is larger than a specified value, 40 kHz for the T1-L-mode and 130 kHz for the T1-W-mode. For the last mentioned mode, a difficulty arises, as two resonances very close in frequency exist. Therefore, seven eigenfrequencies are identified followed by a post processing step, where the eigenfrequencies are matched using their mode shape. This is necessary as the eigenfrequencies shift with varying material parameters. For this purpose, a reference mode (with fixed material parameters) that shows the desired eigenfrequencies and has well distinguishable mode shapes is used to calculate the correlation

$$r_{xy} = \frac{\frac{1}{n}\sum_{i=1}^{n} x_i y_i - \overline{xy}}{\sqrt{\left(\frac{1}{n}\sum_{i=1}^{n} x_i^2 - \bar{x}^2\right)\left(\frac{1}{n}\sum_{i=1}^{n} y_i^2 - \bar{y}^2\right)}}. \tag{5}$$

The correlation of two variables $\mathbf{x}$ und $\mathbf{y}$ is limited between -1 and 1 with -1 indicating a negative linear, 1 a positive linear and 0 no relationship. It is evaluated for every reference mode paired with every calculated mode, which leads to a matrix of 7x7 entries, similar to a correlation matrix. Then, using the exclusion principle, the modes are matched according to the highest correlation. Fig. 3a shows the reference modes, the desired modes are highlighted. In this case, the mode shape was evaluated using the absolute displacement of the test specimen along an edge in x-direction. The evaluation points are marked in Fig. 1.

To check that the right eigenfrequencies are identified, two visualizations are utilized. The histogram in Figure 2 shows the distributions of the distance between the 1^{st} and 2^{nd} eigenfrequencies of the T1-W mode; it has a continuous behavior and is always positive - as it should be. Similarily, the mode shapes themselves, cf. Figures 3b and 3c, form only one family of curves for each mode with no outliers.

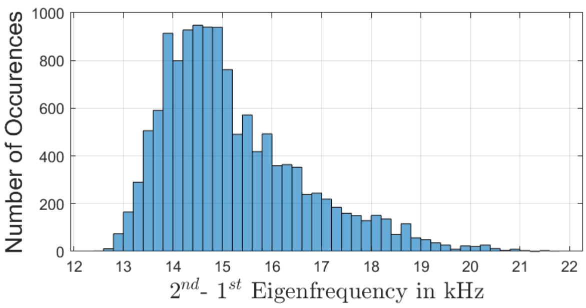
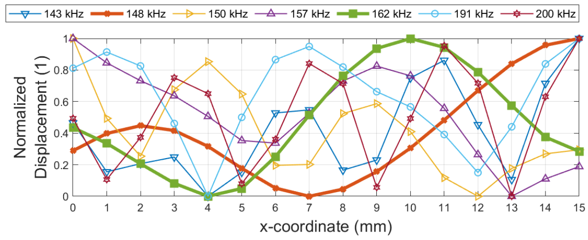
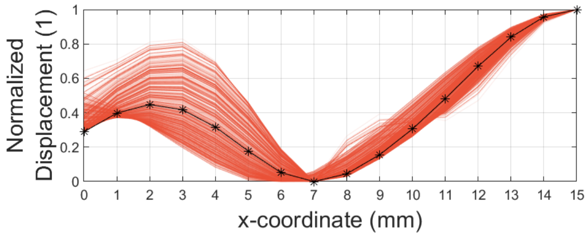


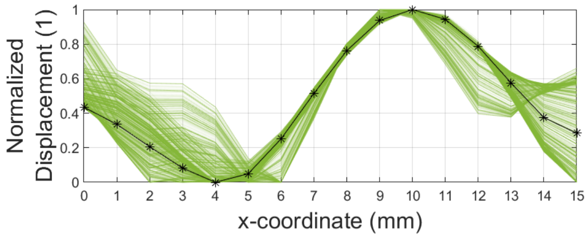
Fig. 2: Histogram of the distance between the 1^{st} and 2^{nd} eigenfrequencies.



(a) Computed Eigenfrequencies. The desired eigenfrequencies at 148kHz and 162kHz are highlighted as bold lines.



(b) 1^{st} Eigenfrequency



(c) 2^{nd} Eigenfrequency

Fig. 3: (a) Min-Max-normalized displacement along an edge of the block shaped sample. (b, c) Family of mode shapes of identified eigenfrequencies for a sample size of $m = 100$.

Computational Approach

The LHS sampling and COMSOL model creation are performed using MATLAB® and the COMSOL LiveLink™ for MATLAB®, followed by simulations in COMSOL Multiphysics®. Post-processing and statistical analysis are conducted in MATLAB®.

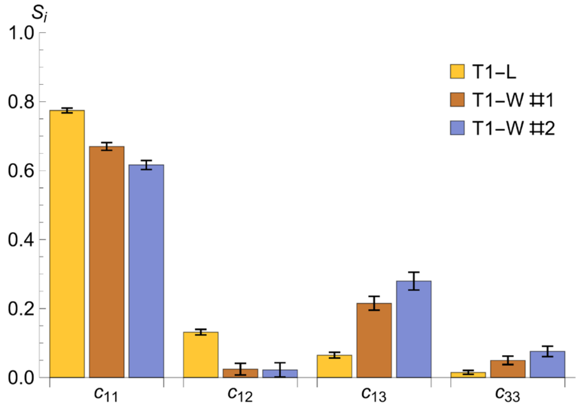
Material parameters are sampled in 5 % intervals from literature values using MATLAB's lhsdesign() function, with sample sizes up to $m = 5000$. Additionally, a statistical approach is implemented to calculate the mean Sobol indices over a sampling using different random seeds. Details of this approach can be found in [5]. It is important to calculate different sample sizes to access the convergence of the mean Sobol indices. In the following, the converged values with a sample size of $m = 5000$ are considered.

Results

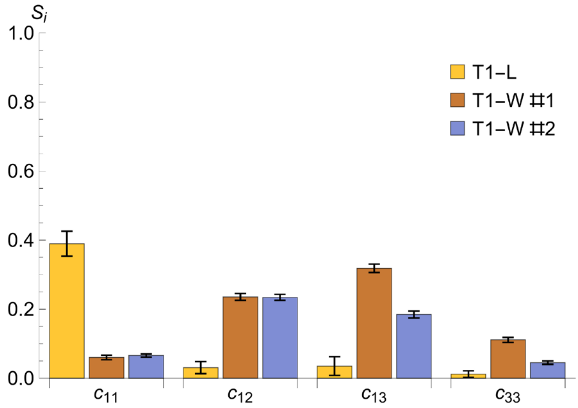
Figures 4a to 4d show the first order and total Sobol indices for the eigenfrequency and the associated impedance value. Only material parameters identified as important are considered. The remaining Sobol indices are close to zero. Different Sobol indices can be observed for the eigenfrequency and impedance values, indicating that the same material parameter can exert a different degree of influence on the eigenfrequency and the associated impedance. When comparing the first-order and total Sobol indices, it is evident that the values are within the same range for the eigenfrequencies, indicating minimal interaction with other material parameters. Conversely, the total Sobol indices are bigger for the impedance, meaning that there are more interactions.

Conclusion and Outlook

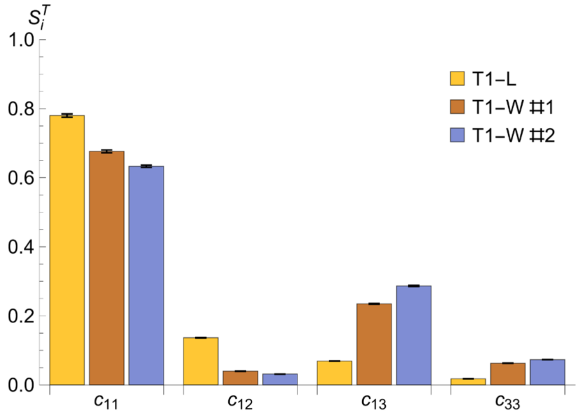
In this work, the first order and total Sobol indices were calculated for two modes, one showing two eigenfrequencies. A method for identifying the wanted eigenmodes from the multitude of computed eigenfrequencies was implemented using their mode shape. In conclusion, the results indicate, that the same material parameter can have more influence on the resonance



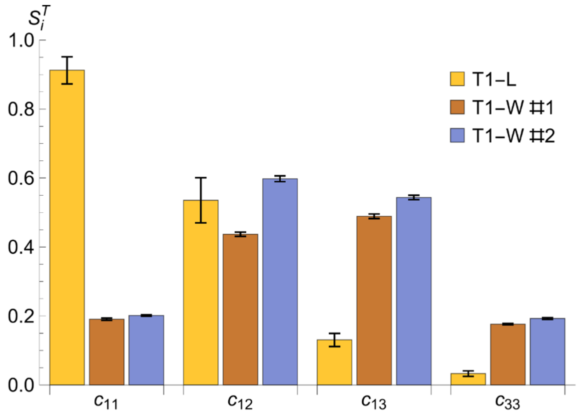
(a) 1^{st} order Sobol index for the eigenfrequency.



(b) 1^{st} order Sobol index for the impedance.



(c) Total Sobol index for the eigenfrequency.



(d) Total Sobol index for the impedance.

Fig. 4: Mean values and 95 % confidence intervals of first order and total Sobol indices for selected material parameters.

frequency than on the impedance and vice versa, as well as interactions with other material parameters can appear for the impedance value alone. This warrants further investigation in future works.

References

[1] "Publication and Proposed Revision of ANSI/IEEE Standard 176-1987 "ANSI/IEEE Standard on Piezoelectricity"". In: *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control* 43.5 (Sept. 1996). Conference Name: IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, pp. 717–. ISSN: 1525-8955.

[2] S. J. Rupitsch. *Piezoelectric Sensors and Actuators: Fundamentals and Applications*. Topics in Mining, Metallurgy and Materials Engineering. Berlin, Heidelberg: Springer, 2019. ISBN: 978-3-662-57532-1.

[3] C. Prieur and S. Tarantola. "Variance-Based Sensitivity Analysis: Theory and Estimation Algorithms". en. In: *Handbook of Uncertainty Quantification*. Ed. by R. Ghanem, D. Higdon, and H. Owhadi. Cham: Springer International Publishing, 2016, pp. 1–23. ISBN: 978-3-319-11259-6.

[4] B. Iooss and A. Saltelli. "Introduction to Sensitivity Analysis". en. In: *Handbook of Uncertainty Quantification*. Ed. by R. Ghanem, D. Higdon, and H. Owhadi. Cham: Springer International Publishing, 2016, pp. 1–20. ISBN: 978-3-319-11259-6.

[5] F. Anderl and M. Mayle. "Sensitivity analysis of piezoelectric material parameters using Sobol indices". In: *tm - Technisches Messen* 92.6 (2025), pp. 234–242.

[6] M. D. McKay, R. J. Beckman, and W. J. Conover. "A comparison of three methods for selecting values of input variables in the analysis of output from a computer code". In: *Technometrics. A Journal of Statistics for the Physical, Chemical and Engineering Sciences* 21.2 (1979), pp. 239–245. ISSN: 0040-1706,1537-2723.

[7] I. M. Sobol. "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates". In: *Mathematics and Computers in Simulation*. The Second IMACS Seminar on Monte Carlo Methods 55.1 (Feb. 2001), pp. 271–280. ISSN: 0378-4754.

[8] A. Saltelli et al. "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index". en. In: *Computer Physics Communications* 181.2 (Feb. 2010), pp. 259–270. ISSN: 00104655.