Piezoceramic linear parameters calculation from the Thickness Shear mode of, thickness poled, thin plate excited along its length

Introduction

For the fundamentals and definitions of the resonance method for piezoceramic characterization in the linear range the user of this software is addressed to the standards in the matter: "IEEE Standard on piezoelectricity". ANSI/IEEE Std. 176-1987, and "Piezoelectric properties of ceramic materials and components. Part 2: methods of measurement – Low power". European Standard CENELEC, EN 50324-2.

This software offers a solution to the limitations of the standard calculation method concerning characterization in the linear range of high loss and low sensitivity ferro-piezoelectric ceramic materials.

Besides, this software analyzes measurements at resonance of a thickness-poled shear plate, excited along one of the longest directions. The Standard, in-plane poled, plate offers problems both in poling, which requires high electric fields, and in the measurement, when strong coupling of modes is often found and cannot be avoided. Also, the parameters calculation from Standard shear plate leads to underestimation of the piezoelectric parameters due to the dynamic clamping at resonance. For information on this topic see:
L. Pardo, M. Algueró and K. Brebøl. " *Resonance modes in Standard piezoceramic shear geometry: a discussion based on Finite Element Analysis*". J. Physique IV France **128** 207 (2005), L. Pardo, M. Algueró and K. Brebøl. "*Resonance modes in Standard characterization of piezoceramics: a discussion based on Finite Element Analysis*". Ferroelectrics 336, 181 (2006) and L. Pardo, F. Montero De Espinosa and K. Brebøl. "*Study by laser interferometry of the resonance modes of the shear plate used in the Standards characterization of piezoceramics*". J. Electroceramics 19(4), 437-442 (2007).

This software allows determining a number of material coefficients in complex form, thus including losses, from the measurement of the frequency dependence of the complex impedance or admittance at the thickness shear electromechanical resonance mode of, thickness poled, thin plates excited along its length.

In the first stage of the program, it creates the needed file for the calculation that will be stored with the extension "xxx.SHR", which the program will recognize in future calculations as appropriated.
This file is created from density and dimensions of the sample and from a file of the measured complex admittance ($Y^* = /Y/\cos\theta + i\ /Y/\text{sen}\theta$) with the format:
frequency$_1$(kHz), /Y_1/(Siemen), θ_1(rad)
frequency$_2$, /Y_2/, θ_2
etc., where a point is used to separate decimals.

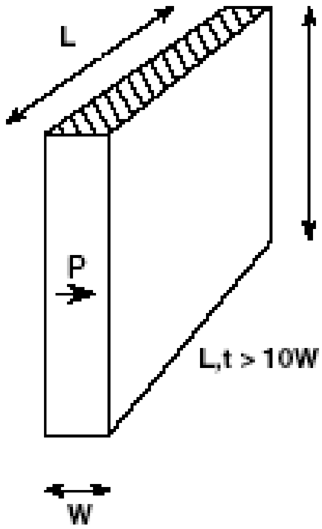
The calculation

The material coefficients are here determined by solving a set of non-linear equations that results when experimental impedance data at a number of frequencies are introduced into the appropriate analytical solution of the wave equation. This set of equations is established for as many frequencies, which are automatically selected by the program, as unknown coefficients.

Solution is carried out by an iterative numerical method, fully automatic, similar to the one described for the thickness extensional mode of, thickness poled, thin plates in: C. Alemany, L. Pardo, B. Jiménez, F. Carmona, J. Mendiola and A.M. González. "*Automatic iterative evaluation of complex material constants in piezoelectric ceramics*". J. Phys. D: Appl. Phys. 27, 148-155 (1994).

This software solves for the **thickness shear mode of a, thickness poled, thin plate excited along its length**, the following analytical solution:

$$Y = G + iB = i\frac{2\pi f w L \varepsilon^{s}_{11}}{t} + i\frac{2we^{2}_{15}}{t}\sqrt{\frac{s^{E}_{55}}{\rho}}\tan\left(\pi f L\sqrt{\rho s^{E}_{55}}\right) \qquad (1)$$



Where ρ is the ceramic density, *w* is the thickness for poling and *L.w* is the area of the electroded surfaces used for electrical excitation, which takes place along the longest direction, *t*. For more details see L. Pardo, M. Algueró and K. Brebøl. "*A non-Standard shear sample for the matrix characterization of piezoceramics and its validation study by finite element analysis*". J. Phys. D: Appl. Phys. 40 2162 (2007).

Accurate measurement of the dimensions and density of the samples are required for the accurate determination of the complex material parameters.

In order to evaluate the frequency dependence of the material parameters, this software allows calculation of the coefficients, not only for the fundamental resonance, but also for the overtones, taking place at odd multiples of the fundamental frequency (A.M. Gonzalez and C. Alemany.
Fig.1. Thickness-poled shear plate.
"*Determination of the frequency dependence of characteristic constants in lossy piezoelectric materials*". J. Phys. D: Appl.Phys. 29, 2476-2482 (1996)). To do so, information on the measured overtone is asked when the data file used for the calculation is created.

This software also carries on the reconstruction of the spectra (R and G versus frequency curves, where Y=G+iB=1/Z = 1/(R+iX)) using the above mentioned analytical expression and the material parameters obtained. Reconstructed curves are plotted together with the experimental ones as an accuracy test of the final set of calculated coefficients. This accuracy is also quantitatively characterized by the regression factor (R^2) of such reconstruction to the experimental data.

The above mentioned analytical solution is valid for thickness poled shear plate geometries with given aspect ratios, with t ,L>> w, which in principle will allow exciting uncoupled modes. Recently, it was also observed that for the high aspect ratios (L,w/t=15/1) mode coupling was still found (L. Pardo, A. Garcia, F. Montero De Espinosa and K. Brebøl. "*Choosing the best geometries for the linear characterization of lossy piezoceramics: Study of the thickness poled shear plate*". Appl. Phys. Lett. 92 , 172907 (2008)). This means that, inherently to this resonator geometry, two types of modes of resonance are driven simultaneously. Due to the studied mechanism, shear and other plate waves couple necessarily in a periodic manner as a function of the ratio L,w/t.

Instead of a threshold aspect ratio (L,t>10w, as recommended by stds.) to be able to measure uncoupled modes, we must speak about the optimum length and thickness of the shear plate for each material to obtain uncoupled modes. The minimum length should be the one where the distance between two plate resonances is the same as the distance between the maximum of the conductance and the maximum of the resistance for the shear resonance. Such distance is determined by the shear electromechanical coupling factor of the material. Optimum thicknesses are the ones that place both maximums between given overtones of the plate resonances.

In practical use, for this measurement the plate must be thickness-poled and afterwards re-electroded and measured. When coupling of modes is found upon measuring, the thickness must be finely decreased in steps of 0.02mm, measuring the resonance at each step and monitoring the minimization of the secondary modes. The calculation has the maximum precision when R^2 is maximum.

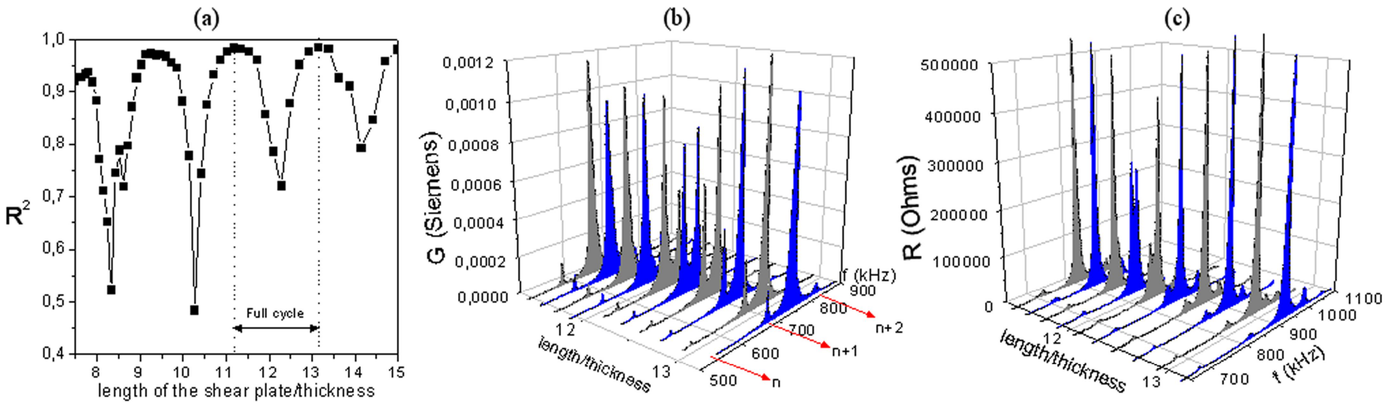


Figure 2. (a) Regression factor of the recalculated spectra to the experimental one in thickness-poled shear plates (15x15mm) of PZ27 as a function of the aspect ratio; (b) evolution of G curve and (c) of the R curve for a full cycle between two spectra with low mode coupling (corresponding R values marked in plot (a)).

Directly and indirectly calculated material properties

The **directly calculated parameters** for this mode are: the elastic compliance, at constant E, $\mathbf{s^E_{55}}$, the dielectric permittivity $\boldsymbol{\varepsilon^S_{11}}$ and the direct piezoelectric coefficient $\mathbf{e_{15}}$**.**

This program uses also the following relations that allows, additionally, the indirect calculation of other interesting parameters of the material:

the direct piezoelectric coefficient h_{15} and the inverse (charge and voltage) piezoelectric coefficients, d_{15} and g_{15}

$$e_{15} = h_{15}\varepsilon_{11}{}^{S} \qquad d_{15} = e_{15}s_{55}{}^{E} \qquad g_{15} = \frac{d_{15}}{\varepsilon_{11}{}^{T}} \tag{2}$$

the latter, after determining the dielectric permittivity ε^T_{11} from

$$\varepsilon_{11}{}^{T} = \frac{\varepsilon_{11}{}^{S}}{1 - h_{15}{}^{2}s_{55}{}^{D}\varepsilon_{11}{}^{S}} \tag{3}$$

The program also calculates the elastic compliance and stiffness, at constant D, s^D_{55} and c^D_{55} and at constant E, $c^E{}_{55}$ from

$$s_{55}{}^{E} = \frac{1}{c_{55}{}^{E}} \qquad s_{55}{}^{E} = \frac{s_{55}{}^{D}}{1-k_{15}{}^{2}} \qquad c_{55}{}^{D} = \frac{1}{s_{55}{}^{D}} \tag{4}$$

A loss factor is calculated and displayed for each material complex parameter $P^*=P'- i P''$, defined as $Q_i(P) = P'/P''$(i=p for piezoelectric, i=m for elastic and i=e for dielectric coefficients).

Values of the relative width of the peak at half-height ($Q=f/\Delta f$) are provided for the G and R peaks, Q_s and Q_p, respectively, from both the experimental data and reconstructed spectra.

The following parameters, useful in many engineering connections, are also calculated:
the length extensional electromechanical coupling factor k_{15} (ratio between converted and input energies) from

$$d_{15} = k_{15}\left(\varepsilon_{11}{}^{T}s_{55}{}^{E}\right)^{1/2} \tag{5}$$

and the frequency number $N_{15} = w(mm).f_s$ (kHz) (6)
where f_s is the frequency for the G_{max}.

Practical notes on the software

The LabView window
On the top of the LabView Window there are two buttons. Use the red button to stop the program at any point and the arrow to re-start it.

The button "Readme first"
The button "Readme first" will automatically open this information file.

The button "GENERATE FILE TO CALCULATE"
Any measurement file can be converted into a file for calculation using the button "GENERATE FILE TO CALCULATE" of the software when the corresponding density, distance in between electrodes, surface of these and if the measurement corresponds to the fundamental mode or to a given overtone is known. This is possible provided that the file has the correct format.

As an exercise, you can convert the file "raw_data.txt" that is provided here and contains in the correct format the measurement of the fundamental mode of a BNBT6 ($(Bi_{0.5}Na_{0.5})_{0.94}Ba_{0.06}TiO_3$) ceramic square plate that has thickness= 0,83mm, distance between electrodes= 9,53 mm, electrode area=7,83 mm^2 and density of 5,49 $g.cm^{-2}$. This is the same measurement as the one in the file "BNBT6.SHR" and, when the generation of the calculation file is done correctly, the results must be identical.

Note that, when creating the calculation file, a comma is used to separate decimals for all the inputs. Use 0 to identify the fundamental mode measurement and 1 for the first overtone (3^{rd} harmonic), 2 for the second (5^{th} harmonic) and so on.

The file to convert will be shown in three columns at the right window of this page in the same way as the calculation program will read it. Only those files that can be correctly shown here will give place to correct calculations.

Pressing the "GENERATE" button will allow you to provide the calculation file name and choose the folder to save it. Then the software will create the file and automatically bring you to the "CALCULATE WITH EXISTING FILE" page. The software adds the correct extension to the typed calculation file name.

The original programs in which the present ones are based were designed to be used while the measurement of the admittance took place. At each iteration of the calculation, the program asked the measuring equipment to measure the admittance at two auxiliary frequencies, that may be far away from the narrow interval of the resonance (away from f_s or f_p).

Note, also, that, when calculations are done with this software from a formatted measurement file, the measured interval must be wide enough to contain the experimental data that the program will ask for. It is suggested to take data in an interval that covers at least $5(f_p\text{-}f_s)$. If the calculation program needs data at a frequency outside the measured interval it will stop and an error message explaining this will appear in the screen.

The button "CALCULATE WITH EXISTING FILE"
The calculation window will open when pressing the button "CALCULATE WITH EXISTING FILE".
First, navigate in your folders to choose the "File to open". This is the formatted file including the information on the sample density, dimensions, complex admittance measurement and overtone.

When the file is open, you must "PLOT", by pressing the corresponding button, the measured impedance, as R and G peaks, which will appear in the window "Experimental data". In the right upper corner of this window there are some LabView graphic utilities that can be used to see sections of the plot in detail. Full use of the utilities is obtained from the menus that you can get by the right-click of the mouse when the cursor is on the graphic area.

To carry on the calculation press the "CALCULATE" button. Results of the calculus will appear at the right part of the window. The reconstructed spectra using the analytical solution and the calculated material coefficients will be now plotted together with the experimental data in the window re-named as "Final result". Calculations are carried out from the complete experimental data and are independent of the previously chosen view with the plot utilities.

After calculation, the program stores the four following files:
"xxx.DAT"= G(Siemens) and R(Ohms) experimental data vs. frequency (calculated from the measured Y^*),
"xxx.DAR"= " " reconstructed " " . These can be used to create plots.
"xxx.txt" = text file with the results of the calculation, and
"xxx.html" = html " " " . These can be used to create tables of calculated coefficients.
Plots and tables are useful when writing reports or manuscripts, create presentations etc.
This files are saved by default in the same folder and with the same name (just with a change of the extension) as the calculation file.
The "SAVE RESULTS" button will open a window that will allow you to rename these files and store them in the folder of your choice. At the same time, the previous files are erased.

On the calculations from overtones
Calculations from measurements at the overtones are done in the same way as those at the fundamental resonance. The information on this is part of the formatted file. As mentioned above, when creating a calculation file you must correctly identify the measurement.

On the files provided as examples
The material data provided with this software corresponds to various types of ceramics. You can check the references quoted below to know more about them.

KNN is a lead-free material under research. Information on its ceramic properties can be found in:
B. Malic, J. Bernard, A. Bencan and M. Kosec, "*Influence of zirconia addition on the microstructure of* $(K_{0.5}Na_{0.5})NbO_3$ *ceramics*". J.Eur.Ceram.Soc.28(6), 1191 (2008).

BNBT6 is a lead-free solid-solution under research. Information on its ceramic properties can be found in:
E. Mercadelli E, C. Galassi, A.L. Costa, S.Albonetti and A. Sanson. "*Sol-gel combustion synthesis of BNBT powders*" J. Sol-Gel Sci. and Technol., 46(1), 39 (2008).

Erratum:
Since thickness for poling (*w*) is the leading dimension for the shear resonance of this sample, the correct equation (1) to be used is:

$$Y = G + iB = i\frac{2\pi f w L \varepsilon_{11}^{s}}{t} + i\frac{2we_{15}^{2}}{t}\sqrt{\frac{s_{55}^{E}}{\rho}}\tan\left(\pi f w\sqrt{\rho s_{55}^{E}}\right)$$

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