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Iterative evaluation of the complex constants of piezoceramic resonators in the radial mode

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Abstract

An iterative method is presented for the characterization of lossy piezoelectric materials in the radial resonant mode, which provides a new formula to calculate the frequencies at which the electrical admittance is to be measured. This new method considerably reduces the measurement time by separating the programs for data acquisition and for calculus. The accuracies of the material constants for several soft and hard piezoceramic materials, covering a wide range of values of the planar coupling factor and mechanical quality factor, were tested and it was evidenced that they depended on the type of the piezoelectric material. The new method proved to be as accurate as, or in some cases even more accurate than, the other iterative methods. This new method can also be applied whenever the standard method does not allow the determination of the material constants. \odot 2002 Elsevier Science Ltd. All rights reserved.

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1. Introduction

There are several standard methods used to determine the material constants of piezoelectric ceramics, $1-3$ but they ignore, to a great extent, the dielectric, piezoelectric and elastic losses, considering these constants as real quantities. Such an approach is accurate enough for materials with low losses, as sometimes is the case for PZT type materials. However, the development of sophisticated transducers using new lossy materials or composites, requires alternative methods for material characterization which take into account the losses, regardless of how low they are. Such a characterization becomes useful even for low lossy materials, when used at higher temperatures, since losses become important with increasing temperature. It is also important when resolution between series and parallel resonances is very poor and standard methods become difficult, or even impossible to apply. The losses of the piezoelectric materials were taken into account by treating the material constants as complex quantities.⁴ The first attempts to

measure them were made by Holland et al.5,6 The actual methods used to determine the material constants, in complex form, can be clasified as iterative^{$7-9$} and noniterative. $10,11$ The iterative ones use the frequency spectrum of the electrical immittance, within the range of the resonance–antiresonance of the fundamental mode only, to determine all material constants, while the noniterative methods require some more measurements, away from fundamental resonance, to determine the dielectric constants at constant stress, or strain. They also need the measurement of a set of ''critical'' frequencies, in the range of the first or higher overtones, and sometimes, even a second set, for materials with low coupling factors (lower than 0.3), or high dielectric dispersion.¹¹ For radial mode, the noniterative method is valid only for materials with intermediate mechanical quality factors.¹⁰

The most accurate iterative methods were elaborated by Smits⁷ and Alemany et al.^{8,9}

Smits' method requires a judicious choice of three frequencies where admittance (impedance) is measured, in order to avoid the determination of the constants with large errors. Since the frequency selection is a difficult task when measurements are performed on a large number of samples, Smits suggested calculating these

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frequencies by using the coupling factor estimated by standard methods.¹ However, such a procedure has the impediment of being impossible to apply for poor resolution between series and parallel resonances (as is the case of lead metaniobate, for example).

Alemany's method eliminates this difficulty by using another iteration to calculate the frequencies in which the immittance is measured. This has the advantage of being applied to any type of piezoceramic material, even to those with very poor resolution between resonance and antiresonance. But it has the disadvantage of being rather slow, due to the impossibility of separating the programs for data acquisition and for calculus, since the frequencies at which immittance is to be measured, during the iteration process, are calculated in the same process. Therefore, a more rapid method seems to be necessary, especially when measurements are carried out as a function of temperature, since the temperature cannot be maintained constant for a long time.

The present work proposes a new improved iterative method to determine the material constants, in complex form, for radial mode, which provides a new formula to calculate the frequencies at which the electrical admittance is to be measured and considerably reduces the measurement time, by separating the programs for data acquisition and for calculus. This new method is comparatively tested with Smits' and Alemany's methods on several soft and hard piezoceramic materials, covering a wide range of values of the planar coupling factor and mechanical quality factor.

2. Measurements

The measurement technique consists in generating a radial mode of vibration in a disc shaped piezoceramic resonator, by sinusoidal electrical stimulation and frequency sweep, by means of an HP-4194A impedance gain/phase analyzer, controlled by a computer.

The real (conductance G) and imaginary (susceptance B) parts of the complex electrical admitance Y are measured as a function of frequency within the range of resonance and antiresonance of the fundamental radial mode and these data are stored as input resonance spectrum, in order to check only the agreement with output data calculated with the constants provided by this method.

The series and parallel resonance frequencies f_s and f_p corresponding to the maxima of G and R (resistance), respectively are determined and stored together with their corresponding values of complex admittances, Y_s and Y_p . The frequencies f_{Bmax} and f_{Bmin} of maximum and minimum of B around f_s and their corresponding admittances Y_{Bmax} and Y_{Bmin} are also determined and stored. The frequencies $f_{1,2}$ eff are calculated with the formula:

$$
f_{1,2\text{eff}} = \frac{f_s}{\sqrt{1 \pm k_{\text{perf}}}}
$$
 (1)

where k_{perf} is given by:

$$
k_{\rm eff} = \sqrt{\frac{f_{\rm p}^2 - f_{\rm s}^2}{f_{\rm p}^2}}
$$
 (2)

The values $Y_{1,2}$ eff of the electrical admittance, measured at these frequencies, are also stored. Then, the frequency range is changed so as to include the first overtone of the radial mode, in order to determine its series resonance frequency f_{s2} .

For materials with small k_p and low Q_m , when f_s and f_p may coincide, or even may be in a reversed order, $f_{1,2eff}$ cannot be calculated. Therefore, they will be replaced by $f_{1,2mn}$ given by:

$$
f_{1,2mn} = \frac{f_s}{\sqrt{1 \pm k_{mn}}} \tag{3}
$$

where k_{mn} is defined as:

$$
k_{\rm mn} = \sqrt{\frac{f_{\rm n}^2 - f_{\rm m}^2}{f_{\rm n}^2}}\tag{4}
$$

with the frequencies f_m and f_n corresponding to the maxima of absolute admittance and absolute impedance respectively, the relationship $f_m < f_s < f_p < f_n$ between the frequencies f_m , f_n , f_s and f_p being well known.¹

As one can see, the measurement procedure does not involve the results of the iterative method, thus being completely independent of that. It requires only the measurement of some frequencies and admittances from the input resonance spectrum, even for determining the frequencies $f_{1,2eff}$ (or $f_{1,2mn}$ whenever necessary), which is an easy task for any acquisition program. The separation between data acquisition and processing considerably reduces the measurement time, to a few seconds and allows the use of a more performant ''soft'' for processing. This is the main difference between our method and Alemany's, which requires new measurements of the admittance during the iteration process, so that the measurements and the processing cannot be separated and the whole program takes place in minutes.

3. Description of the method

This new method uses the following expression for the electrical admittance Y , as a function of the oscillating frequency f :⁹

$$
Y = i\frac{2\pi^2 f a^2}{t} \left[\varepsilon_{33}^T + 2d_{31}^2 \frac{c_{11}^p}{\frac{1}{2 - j_i \left[2\pi f a \sqrt{\rho/c_{11}^p} \right]}} - \frac{1}{1 + \sigma} \right]
$$
(5)

where a, t and ρ are the radius, thickness and density of where *a*, *t* and ρ are the radius, thickness and density of the sample, respectively and $i = \sqrt{-1}$. The dielectric permitivity ε_{33}^T , the piezoelectric constant d_{31} , the Poisson's ratio σ and the elastic constant c_{11}^p , given by:

$$
\sigma = -\frac{s_{12}^E}{s_{11}^E} \tag{6}
$$

$$
c_{11}^p = \frac{s_{11}^E}{\left(s_{11}^E\right)^2 - \left(s_{12}^E\right)^2} \tag{7}
$$

are complex quantities. The last two constants are defined with the elastic compliances s_{11}^E and s_{12}^E at constant field E. The complex function $j_1(z)$ of complex variable z is given by:

$$
j_1(z) = zJ_0(z)/J_1(z)
$$
 (8)

where J_0 and J_1 are Bessel functions of first kind and zeroth and first order, respectively.

The relationship (5) is derived from Eq. (117) of the IEEE $Std.,¹$ by substituting the planar coupling factor k_p with the formula:

$$
k_{\rm p} = \frac{\sqrt{2}d_{31}}{\sqrt{\varepsilon_{33}^T\left((s_{11}^E + s_{12}^E\right)}}\tag{9}
$$

in order to evidence the explicite contributions of the dielectric, piezoelectric and elastic constants, which are complex quantities, written, following Holland,⁴ as: real part— $i \times$ imaginary part.

Table 1 The values of the input constants for materials A, B, C, and D respectively

The iterative procedure requires initial estimations of the elastic constants c_{11}^p and σ . It also requires the value of η_{lin} which is the first positive root of the equation:

$$
j_1(z) + \sigma - 1 = 0 \tag{10}
$$

representing the condition of radial resonance in a lossless piezoceramic resonator with all material constants as real quantities, including the function $j_1(z)$. The Poisson's ratio σ is initially estimated as a real quantity, σ_{in} , with no imaginary part, and is calculated, as well as η_{lin} , by a polynomial fit⁹ of the data given in Table 10 of IEEE Std.:¹

$$
\sigma_{\rm in} = \sum_{i=0}^{4} a_i r^i \tag{11}
$$

$$
\eta_{\text{lin}} = \sum_{i=0}^{3} b_i r^i \tag{12}
$$

with a_i and b_i given by Table 1 of Ref. [9] and $r = f_{s2}/f_s$. The real part of c_{11}^p is initially estimated from the relationship: $¹$ </sup>

$$
c_{11\text{in}}^p = \rho \left(\frac{\pi d f_s}{\eta_{1\text{in}}}\right)^2 \tag{13}
$$

and the imaginary part of c_{11}^p , from:

$$
c_{11\text{in}}^{p''} = -\frac{f_{\text{Bmin}} - f_{\text{Bmax}}}{f_{\text{x}}} c_{11\text{in}}^{p'} \tag{14}
$$

Our method, as well as Smits', is based on the measurement of the electrical admittance Y at three different frequencies f_1 , f_2 and f_3 , in order to determine four material constants: ε_{33}^T , d_{31} , c_{11}^p and σ , from Eq. (5). It consists in two successive iterations, which both follow the same algorithm, but the values of f_1, f_2 and the initial estimations of c_{11}^p and σ are different. Thus, in the first iteration f_1 , f_2 are substituted by f_{Bmax} and f_{Bmin} , respectively, and the initial estimations for σ and c_{11}^p are

given by (11)–(14), whereas in the second iteration, $f_{1,2\text{eff}}$ becomes $f_{1,2}$ and the initial guess for c_{11}^p and σ are the final values provided by the first iteration. The first iteration is the central iteration of the method described in details by Alemany et al., 9 except the correction of the piezoelectric constant d_{31} , by using the admittance measured at f_p , since in some circumstances the iteration is not convergent.

The algorithm will be further described. With initial estimations of c_{11}^p and σ , the electrical admittance from (5) becomes linear in ε_{33}^T and d_{31}^2 . Measuring Y at frequencies f_1 and f_2 , a linear system of two equations is obtained. By solving it, ε_{33}^T and c_{11}^p , are determined. Then, better aproximations of c_{11}^p and σ are obtained, by using the experimental value of Y measured at f_3 which is f_s in both iterations. First, c_{11}^p is determined from:

$$
c_{11}^p = \rho \left(\frac{\pi df_s}{\eta_1}\right)^2 \tag{15}
$$

after calculating the complex argument η_1 of the complex function $j_1(\eta_1)$, by using the preceeding values of the four constants. Second, a better approximation of σ is obtained at the same frequency f_s , with the new values of c_{11}^p , and $j_1(\eta_1)$ and the previous ones of ε_{33}^T and d_{31} . With the new values of c_{11}^{p} and σ , (as initial guess) the iterative procedure restarts and is repeated until the cut-off criterion:

$$
\frac{\left|c_{11f}^p - c_{11i}^p\right|}{\left|c_{11f}^p\right|} \leq 10^{-8} \tag{16}
$$

is fulifiled. Here, c_{11i}^p is the value of c_{11}^p , used at the beginning of the algorithm, and c_{11f}^p is provided by the algorithm.

Constants c_{11}^p and σ are calculated from (5) at f_s since they determine this frequency, according to (10) and (13). The series resonance frequency corresponds to mechanical resonance and, therefore, it is naturally to calculate the elastic constants at this frequency. If k_p is large, than a large amount of input energy is converted to elastic energy, thus allowing an accurate determination of the elastic constants around f_s , which is not possible for dielectric constant, since the dielectric energy is small compared to the elastic energy. This happens even at small k_p and high mechanical quality factor Q_m , when mechanical losses are very small. Therefore, it is necessary to determine the dielectric constant far from f_s , where the dielectric energy becomes dominant. This is accomplished in the second iteration, where ε_{33}^T is calculated at frequencies $f_{1,2}$ eff, with high accuracy, after it was determined with large errors, at f_{Bmax} and f_{Bmin} in the first iteration. The accuracy of the piezoelectric constant is situated between those of the dielectric and elastic constants. The reason of using two iterations is that the first iteration provides only the elastic constants with relative high accuracy and therefore a second iteration is necessary to improve the accuracy of the dielectric and piezoelectric constants.

The algorithm of this method was written in Mathematica 3.0, which allows an easy manipulation of complex functions with complex variables.

4. Results and discussion

The new method was tested on the following types of materials: soft PZT (denoted material A), lead metaniobate (material B), hard PZT (material C) and bismuth niobat (material D), covering a wide range of values of the planar coupling factor $(k_p = 2.5-57%)$ and mechanical quality factor (Q_m =20–3000). Each type of material was simulated by giving complex values to material constants $\varepsilon_{33}^T, d_{31}, c_{11}^p$ and σ , considered as input constants, and then by generating the admittance data using Eq. (5). The new method, together with Smits' and Alemany's were applied to the generated admittance data, considered as experimental (input) resonance spectrum, in order to calculate the material constants and to compare them with their input values.

The accuracies of the real and imaginary parts of each material constant were calculated by the following relationships:

$$
\varepsilon_{\text{const'}} = \frac{|\text{const}'_i - \text{const}'_c|}{|\text{const}'_i|} \tag{17}
$$

and

$$
\varepsilon_{\text{const}} = \frac{|\text{const}'_i - \text{const}'_i|}{|\text{const}'_i|} \tag{18}
$$

where subscripts "i" and "c" designate the input and calculated constants, respectively and single and double primes signify the real and imaginary parts, respectively.

The resonance spectra were generated for disc shaped resonators of 20 mm in diameter and 1mm thickness, by using a program in Mathematica 3.0. The frequencies $f_s, f_p, f_{Bmax}, f_{Bmin}$ and f_{s2} were determined with high accuracy $(10^{-8}\%)$ by this program. The programs for the three methodes were also made in Mathematica 3.0.

Table 1 shows the input constants for materials A–D and input k_p and Q_m calculated with input constants by formula (9) and the following one:

$$
Q_{\rm m} = -\frac{c_{11}^{p'}}{c_{11}^{p''}}\tag{19}
$$

Input constants were chosen in agreement with the following constraints, found by Holland:4

$$
\begin{aligned}\n\left(\varepsilon_{33}^T\right)'' &\geq 0 \\
\left(s_{11}^E\right)'' &\geq 0 \\
\left(s_{11}^E\right)'' &\geq \left|\left(s_{12}^E\right)''\right| \\
\varepsilon_0\left(s_{11}^E\right)''\left(\varepsilon_{33}^T\right)'' &\geq \left(d_{31}\right)^2\n\end{aligned}
$$
\n(20)

Material constants determined by the new method were also in agreement with constraints (20). They were substituted in Eq. (5) to obtain calculated (output) admittance data, in the range of resonance–antiresonance of fundamental radial mode, in order to compare them to generated admittance data. The aim of the method is that output data reproduce as much as possible the input data.

Figs. 1A–D show the real and imaginary parts of the generated and calculated admittance and impedance, as a function of frequency, in the range of resonance and antiresonance of the fundamental radial mode, for materials A–D, respectively. One can see that output and input data are in very good agreement, for all materials.

Table 2A–D shows the accuracies of the material constants, of the radial mode, determined by the three

mentioned methods, for materials A–D, respectively. The coupling factors k_p and k_{31} , the piezoelectric constant g_{31} and the elastic compliances $s_{11}^{E,\overline{D}}$ and $s_{12}^{E,\overline{D}}$ at constant E (electric field) and constant \overline{D} (dielectric displacement) were determined from the previous constants.

Since the accuracy of Smits' method is drasticaly influenced by the choice of frequencies $f_{1,2}$, we used three pairs of such frequencies to test it: $f_{1,2eff}$ [see Eq. (1)] and $f_{1,2st}$ and $f_{1,2d}$, given by:

$$
f_{1,2st} = \frac{f_s}{\sqrt{1 \pm k_{\text{pst}}}}
$$
\n(21)

and

$$
f_{1,2d} = \frac{f_s}{\sqrt{1 \pm |k_{\rm pd}|}}\tag{22}
$$

where k_{pst} is the planar coupling factor calculated according to IEEE Std.¹ and k_{pd} is the input planar coupling factor given in Table 1. We have found practicaly the same accuracy for all these frequencies. This was valid for each of materials A–D. We have also

Fig. 1A–D. Resonance (a) and antiresonance (b) generated and calculated spectra of the fundamental mode for materials A, B, C and D, respectively.

Fig. 1A–D (continued).

chosen some other frequencies to test the accuracy of Smits' method and we found larger errors than for $f_{1,2eff}$, $f_{1,2st}$ and $f_{1,2d}$, which seem to give the best accuracies. This could be explained by the analogy of their definitions with the formula for the frequencies associated with maximum piezoelectric energy content.⁷ Therefore, we selected only the frequencies $f_{1,2}$ and use as $f_{1,2}$ in Smits' method, since they are easier determined, thus simplifying the use of this method.

As one can see from Table 2A–D, the new method as well as Alemany's have almost the same accuracy for all investigated materials. This accuracy is also the same with Smits', only for materials A and B, with moderate and low Q_m . For material C, with large k_p and high Q_m , the two methods are more accurate than Smits', providing lower errors for the imaginary parts of the piezoelectric and elastic constants and coupling factors. For material D, with very small k_p and high Q_m , Smits' method seems to be more accurate, especially for the imaginary parts of the constants and coupling factors. The results proved that all three methods have similar accuracies. This is natural, since they are all based on the same algorithm. Even if our method proved to be as accurate as the others, or even more, for materials with large k_p , it has the main advantage of being easier to use, by providing a simple and rapid technique of measurement, which can be completely separated from the program for determining the material constants. The principle of this method can be also used for other resonant modes.

The imaginary parts of the material constants were usualy obtained with larger errors, up to one order of magnitude, than the real parts. The imaginary part of σ was given with very large errors, by all three methods, for materials A and B. This is due to the fact that the imaginary part of this constant, which is determined from the elastic term of the admittance [Eq. (5)], has a very small contribution to this term, thus being difficult to be accurately determined. For material B, with high losses, c_{11}^p as well as the other elastic constants, is given with rather large errors, probably due to the initial estimation of its imaginary part, by Eq. (14), which is no longer valid for high mechanical losses, as one can see in Table 1, where the difference between input Q_m and the ratio $f_s/(f_{\text{Bmin}} - f_{\text{Bmax}})$ is about 40%. For each of the other materials, with low losses, the two quantities have almost the same values, differing by less than 1% . Sherrit et al.¹⁰ explained this by giving a new definition of these frequencies. They defined the series and parallel resonance frequencies as the frequencies corresponding to maxima of the real parts of $Y(f)/f$ and $f\cdot Z(f)$, Table 2

A–D. The accuracies of the material constants of the radial mode determined by the new method and comparatively by Smits' and Alemany's methods, for the four materials A, B, C and D, respectively

(continued on next page)

Table 2(continued)

respectively and not to the real parts of $Y(f)/f$ and $fZ(f)$ as in IEEE Std.¹ They also defined f_{Bmax} and f_{Bmin} as the extrema of $Y(f)/f$ The difference between the two definitions is only significant for materials with low Q_m , which is defined as the ratio of the real to imaginary part of the elastic constant. If the frequencies are defined according to Sherrit et at, for material B, the values of Q_m , and of the ratio $f_s/(f_{Bmin}-f_{Bmax})$ will be almost equal and thus the relationship (14) becomes valid again. Besides, using the new definitions of the frequencies, in formulas (11) – (14) , for the initial estimations of σ and c_{11}^p , the errors of the real parts of calculated constants and coupling factors are about one order of magnitude lower than in the case of using the standard defined frequencies. Therefore, when low Q_m materials are characterized, the frequencies used for initial estimations of the elastic constants are recommended to be chosen according to their new definitions.

5. Conclusions

A new iterative method, for determining the dielectric, piezoelectric and elastic constants, in complex form, for the piezoceramic materials, in the radial mode, was proposed. This new method is valid even for materials with very poor resolution between resonance and antiresonance. It consists in two successive iterations, based on the measurement of the electrical admittance at five properly chosen frequencies, determined by the program for data acquisition. Two of these frequencies are calculated using only the other ones, by a new simple relationship, provided by this method, without requiring intermediate results of the iterations, as Alemany's method does. This allows the separation between the programs for data acquisition and processing, thus reducing the acquisition time. This separation is also possible, since no further measurements are necessary,

during the calculation of the material constants and this is the main benefit from this new method.

The new method was compared with other iterative methods, by determining their accuracies for several types of materials. It was found that all methods have similar accuracies, but ours is more rapid and easiear to apply and it provides higher accuracy for materials with large planar coupling factors.

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