Letters

A Novel Method for Characterization of Piezoelectric Material Parameters by Simulated Annealing Optimization

Yangyang Dong, Zhengbin Wu, Hong Hu, Bo Wu, and Guoqing Xu

***Abstract*—A novel, accurate characterization method for piezoelectric materials, based upon a simulated annealing optimization algorithm, is developed. The theoretically calculated complex material constants of lossy piezoelectric materials with precisely fitted electrical impedance resonant characteristics by this method are reported.**

I. Introduction

High-loss piezoelectric materials, such as piezoelectric composites and highly damped piezoelectric ceramics, have attracted much interest for use in the manufacture of wide band ultrasonic transducers. It was found that an elevated work temperature is able to further enhance the loss characteristics of piezoelectric materials [1]. Therefore, accurate characterization of piezoelectric materials, including loss characteristics, is crucial. The IEEE standard method [2], only calculates real material constants and is thus applicable for low-loss materials like lead zirconate titanate (PZT). Other methods that consider the elastic, piezoelectric, and dielectric losses as the imaginary part of a complex material constant were suggested by Smits [3], Sherrit *et al.* [4], and Kwok *et al.* [5], respectively. The calculated result by the method of Sherrit *et al.* is not as accurate as the others with loss characteristics [5]. The methods developed by Smits and Kwok *et al.* are both sensitive to the selection of the initial material parameter values, and thus results are not necessarily convergent. In this report, a new method based on the simulated annealing (SA) [6] optimization algorithm is suggested. It is able to accurately determine complex piezoelectric material characteristics with arbitrarily selected initial material parameter values. Material constants calculated by this method for a lossy piezoceramic and a PZT5A/epoxy piezoelectric composite are also reported.

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II. Experiments

The thickness extensional vibration mode piezoelectric samples investigated in this report were a lead metaniobate ceramic plate (PZ35, Ferroperm Piezoceramics A/S, Kvistgård, Denmark) and a 1–3 PZT5A/epoxy composite disc. The square lead metaniobate plate had a side length of 10 mm, a thickness of 1.1 mm, and a density of 4750 kg/m^3. The 1–3 composite sample was prepared by the dice-and-fill method. The volume fraction of PZT5A (Shanghai Jinmao Industrial Co. Ltd, Shanghai, China) in the composite was 60%. The epoxy was low viscosity two-part adhesive 2058A/B (Wuxi Huayue Epoxy Materials Co. Ltd, Wuxi, China). The density, diameter, and thickness of the piezocomposite sample were 5395 kg/m^3, 17.2 mm, and 1.6 mm, respectively. The electrical impedance of the samples was measured with an Agilent HP4294 impedance analyzer combined (Agilent Technologies, Santa Clara, CA) with a 16034H test fixture. All impedance measurements were conducted in air at ambient temperature. It should be noted that the maximum root mean square (RMS) output voltage from the impedance analyzer is approximately 1 V. Therefore, the experimental results reported here only represent small-signal material characteristics and are thus not applicable to devices for high-electric-field applications such as actuators. The effect of the electrodes (thickness less than 10 μm for the lead metaniobate and 0.1 μm for the composite samples) on the electrical impedance characteristics is neglected here.

III. Theory

For a piezoelectric vibrator subject to one specific vibration mode, an analytical expression can be derived that relates the electrical impedance characteristics to the motion and boundary conditions. The elastic, piezoelectric, and dielectric constants of the piezoelectric material can be obtained by fitting the theoretically calculated electrical impedance around resonance to the measured data.

For the thickness mode piezoelectric samples investigated in this report, the resonant electrical impedance characteristics can be described as [5, Eq. (1)]

$$Z(f) = \frac{t}{i2\pi f A \varepsilon_{33}^{S*}} \left[1 - k_t^{*2} \frac{\tan\left(\pi f t \sqrt{\rho / c_{33}^{D*}}\right)}{\pi f t \sqrt{\rho / c_{33}^{D*}}} \right], \qquad (1)$$

where t is the thickness of the piezoelectric resonator, f the frequency, A the lateral electrode area, and ρ the density. The complex material parameters, clamped dielectric permittivity ε_{33}^{S*}, thickness vibration electromechanical coupling coefficient k_t^*, and elastic stiffness coefficient under constant electric displacement c_{33}^{D*}, are defined as [5]

$$\varepsilon_{33}^{S*} = \varepsilon_{33}^{S}(1 - i \tan \delta_e) \qquad (2)$$

$$k_t^* = k_t(1 + i\tan\delta_{\mathrm{k}}) \tag{3}$$

$$c_{33}^{D*} = c_{33}^{D}(1 + i\tan\delta_{\mathrm{c}}). \tag{4}$$

Here, $\tan\delta_{\mathrm{e}}$, $\tan\delta_{\mathrm{k}}$, and $\tan\delta_{\mathrm{c}}$ are the elastic, dielectric, and electromechanical coupling factor loss tangents, respectively. Eq. (1) can also be represented by

$$Z(f) = R(f) + iI(f) \tag{5}$$

$$\varphi(f) = \arctan\left(\frac{I(f)}{R(f)}\right), \tag{6}$$

where $R(f)$ and $I(f)$ are the resistance and reactance, respectively, and $\varphi(f)$ is the phase angle.

For piezoelectric transducers, equivalent circuit models are more convenient than algebraic expressions of impedance [e.g., (1)] when trying to predict device behavior. Two commonly used circuit models are the Van Dyke model, which is recommended by the IEEE standard [2], and the complex circuit model proposed by Sherrit *et al.* [7]. Sherrit *et al.* identified that the Van Dyke model (with four real-value circuit constants), cannot accurately represent the functional relationship shown in (1), particularly for materials with significant losses. Therefore they proposed a complex circuit model [7], containing three complex-valued elements, (6 variables in total: 3 real, 3 imaginary) to be consistent with the components calculated directly from the material constants.

SA, independently introduced by Kirkpatrick *et al.* in 1983 [6], is a probabilistic method used to find the global minimum of a cost function with more than one local minimum. The whole process of the SA optimization algorithm imitates the physical process whereby a solid is slowly cooled from high temperature until eventually the structure is frozen with a minimum energy configuration. This report proposes the use of an SA optimization algorithm to calculate complex piezoelectric material constants. This approach may avoid the dependency of the calculation convergence on the choice of the initial material parameter values (a problem reported for other methods for precise characterization of lossy piezoelectric materials [3], [5]). The optimization objective function $\min F(x)$ is the nonlinear function of the vector x as

$$\min F(x) = \sum_{i=1}^{N}\left[\sqrt{R^2(x,f_i) + I^2(x,f_i)} - Z(f_i)\right]^2, \tag{7}$$

where $x = (\varepsilon_{33}^{S}, \tan\delta_{\mathrm{e}}, k_t, \tan\delta_{\mathrm{k}}, c_{33}^{D}, \tan\delta_{\mathrm{c}})$, ranging from $(0, -1, 0, -1, 0, -1)$ to $(10, 1, 1, 1, 10^{15}, 1)$ based on the practical physical conditions. N is the fitted data number in the frequency range between $2f_n - f_m$ and $2f_m - f_n$, and f_n and f_m are the frequencies where impedance magnitude has the maximum and minimum around resonance, respectively. The calculation of SA algorithm was realized by coding MATLAB. The optimization process of SA algorithm is shown as the flowchart in Fig. 1. $T(n)$ are the control factors that mimic the temperature condition in the annealing process. $x(n)$ and L represent the randomly generated solutions and the maximum iteration time for each $T(n)$ value, respectively. To study the effect of various initial values on the calculated result, the initial values of $x(0)$, $T(0)$ used in this report were defined manually. The solutions $x(n)$ were judged to be accepted or abandoned by the Metropolis criterion, which is related to $F(x)$ and $T(n)$ [8]. Within the maximum iteration time for each $T(n)$ value, each accepted solution was tested to see if it satisfies the terminal condition, (i.e., $\min F[x(n+1)] - \min F[x(n)] < \varepsilon$, where ε is a user-specified constant) and then used to generate the final optimization result accordingly. If this test was failed, the control factor $T(n)$ was reset and the iterative process was restarted. Because it optimizes over the full range of available values, the result of SA algorithm is not dependant on the selection of initial values.

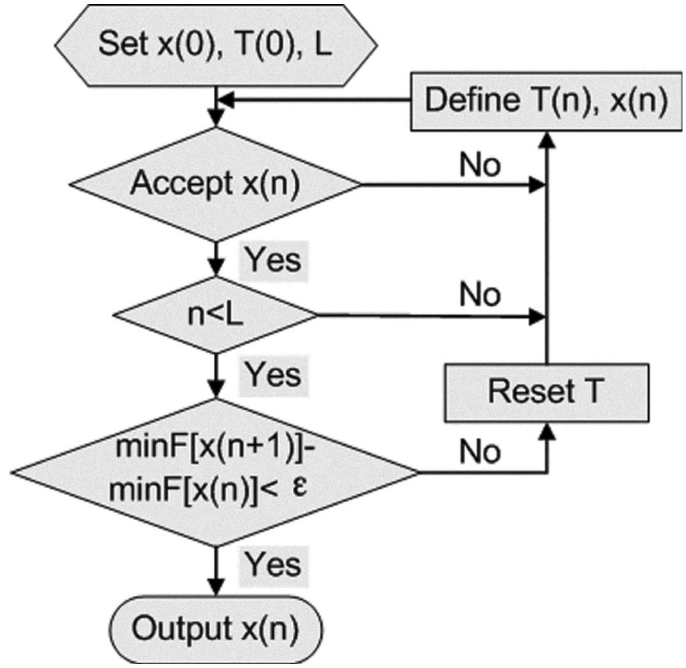


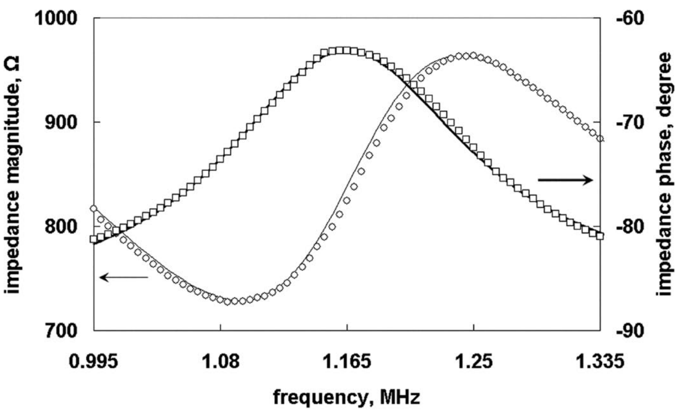
Fig. 1. Simulated annealing optimization algorithm process flowchart.

IV. Results

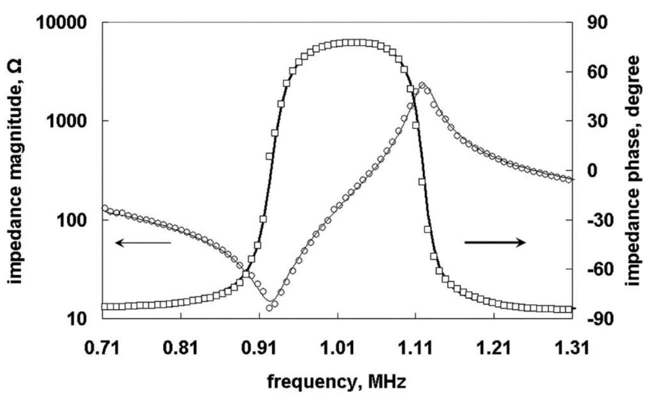
Once the SA algorithm has been used to determine the material constants for a given piezo-sample, these values can then be used in (1) to predict the electrical impedance. A comparison between the theoretical impedance (based on the fitted coefficient) and the original experimental data for the lead metaniobate sample can be found in Fig. 2(a). A similar plot for the PZT5A/epoxy composite sample is shown in Fig. 2(b). As can be seen, there is a very good visual agreement between the theoretically predicted impedance data and the experimental results. To characterize the matching between the predicted and measured electrical impedance data, and thereby determine the calculation accuracy of the material constants, a matching coefficient R_1 is introduced; R_1^2 can be calculated as

TABLE I. Some Piezoelectric Material Parameters Calculated With the Simulated Annealing Optimization Algorithm.

	PZT/epoxy composite			Lead metaniobate		
Material parameter	Initial value 1	Initial value 2	Result	Initial value 1	Initial value 2	Result
ε_{33}^{S}, 10^{-9} F/m	3	1	5.556	6	1	1.670
$\tan\delta_{\mathrm{e}}$	−0.5	0.1	0.0800	−0.5	0.1	0.0473
κ_t	0.5	0.1	0.602	0.5	0.1	0.290
$\tan\delta_{\mathrm{k}}$	0.5	0.1	−0.0129	0.5	0.1	−0.0100
c_{33}^{D}, 10^{10} N/m^2	5	1	6.926	6	1	3.252
$\tan\delta_{\mathrm{c}}$	0.9	0.1	0.0220	0.9	0.1	0.167



(a)



(b)

Fig. 2. Electrical impedance resonant characteristics of (a) lead metaniobate and (b) PZT5A/epoxy composite. Hollow circle is the measured impedance magnitude. Thin line is the calculated impedance magnitude. Hollow square is the measured impedance phase. Thick line is the calculated impedance phase.

$$R_{\mathrm{I}}^{2} = 1 - \frac{\sum_{i=1}^{N} [Z_{\mathrm{m}}(i) - Z_{\mathrm{c}}(i)]^{2}}{\sum_{i=1}^{N} [Z_{\mathrm{m}}(i) - \bar{Z}_{\mathrm{m}}]^{2}}. \tag{8}$$

Here, Z_{m}, Z_{c} are the measured and calculated impedance data, respectively. $\bar{Z}_{\mathrm{m}}$ is the average value of Z_{m}. R_1, in the range between 0 and 1, is the positive function of the fitting of simulated impedance resonant characteristics to the measured results. The calculated values of R_{I}^2 are 0.997 and 0.998 for the magnitude and phase of the lead metaniobate sample. The piezocomposite sample had R_{I}^2 values of 0.993 and 0.998 for magnitude and phase. All values of R_{I}^2 are very close to the maximum, 1, and confirm the high level of correlation between the measurement and prediction by SA.

Some calculated material parameters are listed in Table I. Two different initial values were defined and used to calculate each parameter. The final optimized results converge to the same value, which verifies that the result of the SA optimization algorithm is independent of the initial value.

V. Conclusion

A novel, accurate characterization method based on the SA optimization algorithm for high-loss piezoelectric materials has been presented. Very good matching between the theoretical calculation and the experimental data verifies that this method can generate precise material parameters independent of initial values.

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References

[1] Z. Wu, S. Cochran, and A. Hurrell, “Material parameter variations of lead metaniobate piezoceramic in elevated temperature applications,” *Electron. Lett.*, vol. 44, pp. 940–941, 2008.

[2] *IEEE Standard on Piezoelectricity*, ANSI/IEEE Std. 176–1987, 1987.

[3] J. G. Smits, “Iterative method for accurate determination of the real and imaginary parts of the materials coefficients of piezoelectric ceramics,” *IEEE Trans. Sonics Ultrason.*, vol. SU-23, pp. 393–402, 1976.

[4] S. Sherrit, H. D. Wiederick, and B. K. Mukherjee, “Non-iterative evaluation of the real and imaginary material constants of piezoelectric resonators,” *Ferroelectrics*, vol. 134, pp. 111–119, 1992.

[5] K. W. Kwok, H. L. W. Chan, and C. L. Choy, “Evaluation of the material parameters of piezoelectric materials by various methods,” *IEEE Trans. Ultrason. Ferroelectr. Freq. Control*, vol. 44, pp. 733–742, 1997.

[6] S. Kirkpatrick, C. D. Gelatt, and M. P. Vecchi, “Optimization by simulated annealing,” *Science*, no. 4598, vol. 220, pp. 671–680, 1983.

[7] S. Sherrit, H. D. Wiederick, B. K. Mukherjee, and M. Sayer, “An accurate equivalent circuit for the unloaded piezoelectric vibrator in the thickness mode,” *J. Phys. D Appl. Phys.*, vol. 30, pp. 2354–2363, 1997.

[8] W. Xing and J. Xie, *Modern Optimization Calculation Method*, Beijing, China: Tsinghua University Press, 1999, pp. 90–136.