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Short communication

Crystallographic approach to obtain intensive elastic parameters of k_{33} mode piezoelectric ceramics

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ABSTRACT

This paper presents an advanced piezo-material characterization method to obtain intensive elastic parameters of the k_{33} vibration mode from the k_{31} geometry through crystallographic approach with canted polarization. Three effective k_{31} bars with 0, γ, and π/2-γ degree angled polarization is needed where $0 < \gamma < \pi/4$. Eliminating $s_{13}{}^{E,*}$ and $s_{55}{}^{E,*}$ components from the effective elastic parameters, the k_{33} mode elastic parameters could be derived. $Pb\{(Zr_{0.56}Ti_{0.44})_{0.99}Nb_{0.01}\}O_3$ with 0, 15, 30, 45, 60, 75° angled polarization were prepared and characterized under constant vibration velocity to obtain the effective elastic parameters for the k_{31} mode. The intensive elastic compliance $s_{33}{}^{E}$ and elastic loss $\tan\phi'_{33}$ are derived and compared to the measured value from the conventional methods Due to the low structural impedance of the measured geometry (i.e., large sample capacitance), the reliability on the proposed method is extraordinary, and the implicit relative error in the conventional methods could be avoided.

1. Introduction

For the past century, piezoelectric materials and applications have been widely studied for transducers, sensors and actuators [1]. With enhanced computation technology, finite element analysis has become indispensable for designing and optimizing piezoelectric devices [2]. It is obvious that accurate intensive parameters are essential for the simulation, in particular around the resonance and antiresonance frequency range [3]. In general, the elastic properties are obtained from the sound velocity. For practicality, the sound velocity is calculated from the resonance frequency of k_{31} vibration mode and the antiresonance frequency of k_{33} vibration mode where the half-wave is generated along the vibration. However, by structural constraint, a significant difficulty is experienced occasionally in determining intensive elastic compliance $s_{33}{}^{E}$ and the corresponding loss $\tan\phi'_{33}$ in the k_{33} mode; that is, the mode with elastic vibration along the polarization direction. [4–6] This paper is to provide a solution to this experimental problem.

The k_{33} mode samples works under mechanically-free condition along the 3 axis (stress X_3 constant) or electrically-open circuit (electric displacement D_3 constant) condition of a piezoelectric sample. The intensive dielectric permittivity $\varepsilon_{33}{}^{X}$ and the piezoelectric constant d_{33} could be directly obtained from other geometry such as k_{31} mode bar or k_p mode disk. However, the intensive elastic compliance $s_{33}{}^{E}$ should be calculated indirectly with the measured extensive elastic compliance $s_{33}{}^{D}$ and electromechanical coupling factor k_{33}, as [7];

$$s_{33}^{E} = \frac{s_{33}^{D}}{1 - k_{33}^{2}} \tag{1}$$

Though both $s_{33}{}^{D}$ and k_{33} can be derived from measured resonance and antiresonance frequencies of a long rod sample with polarization along the length direction, large measurement error necessarily comes from its structure with a very small capacitance compared to k_{31} mode samples. The high structural impedance from the low capacitance induces large measurement error in overall electrical response and the relative error becomes as;

$$\frac{\Delta s_{33}^{E}}{s_{33}^{E}} = \frac{\Delta s_{33}^{D}}{s_{33}^{D}} + 2\left(\frac{\Delta k_{33}}{k_{33}}\right)\left(\frac{k_{33}^{2}}{1 - k_{33}^{2}}\right) \tag{2}$$

Note that the error in the k_{33} value dramatically enhances the error in $s_{33}{}^{E}$ value.

Now, we consider the loss factors. In our previous paper [8], we reported the relationship of the mechanical quality factors at the resonance (Q_A) and at the antiresonance (Q_B) with intensive

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dielectric ($\tan\delta'$), elastic ($\tan\phi'$) and piezoelectric ($\tan\theta'$) loss factors as

$$Q_B = \frac{1 - k_{33}^2}{\tan\phi'_{33} - k_{33}^2\left(2\tan\theta'_{33} - \tan\delta'_{33}\right)} \tag{3}$$

$$\frac{1}{Q_A} = \frac{1}{Q_B} + \frac{2\left(2\tan\theta'_{33} - \tan\delta'_{33} - \tan\phi'_{33}\right)}{k_{33}^2 - 1 + \left(\frac{\Omega_A}{k_{33}}\right)^2} \tag{4}$$

Here, the normalized resonance angular frequency Ω_A is given from the following relations:

$$\Omega_A = k_{33}^2 \tan\Omega_A;\ \Omega_A = \frac{\omega_A L}{2}\sqrt{\rho s_{33}^D} = \frac{\pi f_A}{2 f_B} \tag{5}$$

where ω_A, L, ρ, f_A and f_B are resonance angular frequency, length, density, resonance frequency and anti-resonance frequency, respectively. The electro-mechanical coupling factor k_{33} can be obtained from Eq. (5) by knowing the resonance and antiresonance frequencies. From Eqs. (3)–(5), the intensive elastic loss $\tan\phi'_{33}$ can be obtained as;

$$\tan\phi'_{33} = \frac{1}{Q_B} - \frac{1}{1-k_{33}^2}\left[\frac{k_{33}^2}{\tan\delta'_{33}} + \tan\delta'_{33} + \frac{k_{33}^2}{2}\left(\frac{1}{Q_B} - \frac{1}{Q_A}\right)\left(k_{33}^2 - 1 + \frac{\pi^2 f_A^2}{4 f_B^2 k_{33}^2}\right)\right] \tag{6}$$

Accordingly, the relative error of elastic loss could be approximated as;

$$\frac{\Delta\tan\phi'_{33}}{\tan\phi'_{33}} \approx -\frac{\Delta\tan\delta'_{33}}{\tan\delta'_{33}} - 2\left(\frac{\Delta k_{33}}{k_{33}}\right)\left(\frac{1}{1-k_{33}^2}\right) \tag{7}$$

Note that the relative errors from the electro-mechanical coupling factor in real and imaginary parameters are in opposite sign. Although the relative error must be accepted inevitably at present using the conventional rod geometry, higher accuracy in the real and imaginary parameters is appreciated for the computational optimization on piezoelectric devices.

2. Proposed method

Since the high measurement error comes from its sample geometry, it could be eliminated by using measurements of effective k_{31} mode with a sufficiently large capacitance. We propose a new methodology based on the measurement using three different k_{31} bars with angled polarization where $0 < \gamma < \pi/4$ as illustrated in Fig. 1.

Considering polycrystalline structure (P∞mm symmetry), and using a rotation transformation matrix A, the effective elastic compliance with the angled polarization in k_{31} mode can be expressed as Eq. (9).

$$A = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} \tag{8}$$

$$s_{11,\mathrm{eff}}^E(\theta) = \cos^4\theta s_{11}^E + \cos^2\theta\sin^2\theta\left(2s_{13}^E + s_{55}^E\right) + \sin^4\theta s_{33}^E \tag{9}$$

From the difference of Fig. 1(b) and (c), the elastic compliance $s_{13}{}^E$ and $s_{55}{}^E$ can be canceled out remaining only $s_{11}{}^E$ and $s_{33}{}^E$. The $s_{11}{}^E$, $s_{11,\mathrm{eff}}{}^E(\pi/2-\gamma)$ and $s_{11,\mathrm{eff}}{}^E(\gamma)$ can be obtained from measured resonance frequencies of the effective k_{31} modes and the elastic compliance $s_{33}{}^E$ becomes as;

$$s_{33}^E = s_{11}^E + \frac{\left[s_{11,\mathrm{eff}}^E\left(\frac{\pi}{2}-\gamma\right) - s_{11,\mathrm{eff}}^E(\gamma)\right]}{\cos2\gamma} \tag{10}$$

By assuming Eq. (11) and integrating the rotation matrix A, the effective elastic loss with angled polarization can be expressed as Eq. (12)

$$s_{\mathrm{eff}}^{E,*}(\theta) = s_{\mathrm{eff}}^E(\theta)\left(1 - j\tan\phi'_{\mathrm{eff}}(\theta)\right) \tag{11}$$

$$tan\phi'_{11,\mathrm{eff}}(\theta) = \frac{1}{s_{11,\mathrm{eff}}^E(\theta)}\left[\cos^4\theta s_{11}^E \tan\phi'_{11} + \cos^2\theta\sin^2\theta\left(2s_{13}^E\tan\phi'_{13} + s_{55}^E\tan\phi'_{55}\right) + \sin^4\theta s_{33}^E\tan\phi'_{33}\right] \tag{12}$$

Accordingly, from Fig. 1(b) and (c) samples, $\tan\phi'_{13}$ and $\tan\phi'_{55}$ can be canceled out and the intensive elastic loss in k_{33} mode $\tan\phi'_{33}$, (E-constant elastic loss), can be derived from measured effective parameters as in Eq. (13)

$$\tan\phi'_{33} = \frac{1}{s_{33}^E}\left[s_{11}^E tan\phi'_{11} + \frac{1}{cos2\gamma}\left\{s_{11,\mathrm{eff}}^E\left(\frac{\pi}{2}-\gamma\right) tan\phi'_{11,\mathrm{eff}}\left(\frac{\pi}{2}-\gamma\right) - s_{11,\mathrm{eff}}^E(\gamma)\, tan\phi'_{11,\mathrm{eff}}(\gamma)\right\}\right] \tag{13}$$

Therefore, the real and imaginary intensive elastic parameters of k_{33} vibration mode are obtainable from measurements of effective k_{31} samples.

3. Experimental procedures

To check the feasibility of the proposed method and compare the level of experimental error in the conventional method, effective k_{31} samples and conventional k_{33} samples with the size of 15 × 3 × 1 (L × w × t, mm) were prepared by PI Ceramic GmbH from a material with a nominal composition of $Pb\{(Zr_{0.56}Ti_{0.44})_{0.99}Nb_{0.01}\}O_3$. The sample capacitance of k_{31} mode structure, 0.24 nF, is L^2/t^2 times higher than 1.0 pF of the k_{33} mode sample. Sintered blocks were poled and cut with a precision saw in a direction to have desired polarization angle, followed by low temperature electroding. The polarization angles were designed as $\theta = 0$, 15, 30, 45, 60 and 75° for $\gamma = 15°$ and 30° in the proposed method. Frequency vs voltage/current response was observed with our high-power characterization system (HiPoCS^{TM}) under constant vibration velocity of 5 mm/sec where the heat generation is low enough to prevent peak distortion near the resonance and antiresonance frequencies. The effective elastic compliance and loss were derived from the measured resonance frequency and corresponding 3 dB bandwidth on the voltage spectrum. In addition, the properties from the conventional methods (a long rod k_{33} geometry) were obtained using impedance spectrum from impedance analyzer HP4294A (Agilent Technologies, CA, USA).

4. Results and discussions

The predicted effective elastic compliances by angled polarization in 95% confidence intervals are plotted in Fig. 2(a) (b) and (c) with the measured parameters in Fig. 2(b). The $s_{33}{}^E$ calculated with IEEE standard is plotted in Fig. 2(d) for comparison. The $s_{33}{}^E$ derived from proposed method and IEEE standard is 14.82 $\mu m^2/N \pm 0.13\%$ and 13.59 $\mu m^2/N \pm 0.43\%$, respectively. The relative error found in the real parameter was −8.3%; the IEEE Standard underestimates the elastic compliance.

Fig. 3(a), (b) and (c) shows the predicted effective elastic loss with angled polarization in 95% confidence intervals. In comparison with, the loss calculated from the k_{33} geometry is plotted in Fig. 3(d). The $\tan\phi'_{33}$ derived from proposed method is $0.0096 \pm 2.6\%$ where the loss with the conventional method is $0.017 \pm 9.1\%$. The relative error found in the imaginary parameter was 74%; the conventional method overestimates the elastic loss.

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