Electromechanical coupling coefficient k_{31}^{eff} for arbitrary aspect ratio resonators made of [001] and [011] poled $(1-x)Pb(Mg_{1/3}Nb_{2/3})O_3$–$xPbTiO_3$ single crystals

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The dependence of k_{31}^{eff} on the aspect ratio $G=l_1/l_2$ has been calculated for resonators made of [001] poled $0.67Pb(Mg_{1/3}Nb_{2/3})O_3-0.33PbTiO_3$ (PMN-0.33PT) and [011] poled $0.71Pb(Mg_{1/3}Nb_{2/3})O_3-0.29PbTiO_3$ (PMN-0.29PT). Based on the derived unified formula, the lateral electromechanical energy conversion efficiency $|k_{31}^{eff}|^2$ decreases with G for [001] poled PMN-0.33PT but increases with G for [011] poled PMN-0.29PT.
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I. INTRODUCTION

For a piezoelectric vibrator, such as vibrators made of $Pb(Zr,Ti)O_3$ (PZT) ceramic, if a positive electric field is applied along its poling direction, the vibrator will expand in that dimension and shrink in the lateral dimensions because of the Poisson's ratio effect. Therefore, generally, the piezoelectric coefficients d_{31} and d_{32} will have opposite sign to d_{33}. The [001] poled $(1-x)Pb(Mg_{1/3}Nb_{2/3})O_3-xPbTiO_3$ (PMN-xPT) single crystals have similar behavior as PZT ceramic because $d_{31}=d_{32}$ for tetragonal symmetry.[1] However for [011] poled PMN-xPT single crystals, d_{33} and d_{31} are both positive, while only d_{32} is negative. This means that one of the perpendicular dimensions will expand together with the poling direction expansion under a positive field, while the other perpendicular dimension will shrink. Owing to the Poisson's ratio effect, the amplitude of d_{32} becomes very large.[2,3]

The square of the electromechanical coupling coefficient k_{31}^2 is used to characterize energy conversion efficiency between electrical and mechanical energies for a given mode of vibration. Based on experience, the effective electromechanical coupling coefficients will change for different geometric designs of piezoelectric vibrators. However, in related textbooks on piezoelectricity and in the IEEE piezoelectric standard, the electromechanical coupling coefficients are defined using one-dimensional (1D) equivalent circuit models as fixed constants,[4,5] which cannot accurately reflect the true electromechanical energy conversion efficiency when the geometry of the resonators do not satisfy the assumed boundary conditions. Focused on this issue, Kim *et al.*[6–8] studied the effect of aspect ratio dependence of the electromechanical coupling coefficients by solving two-dimensional coupled vibration equations and derived explicit analytical expressions for the aspect ratio dependence of the electromechanical coupling coefficient k_{33} and k_{31} for PZT vibrators, which has ∞m (same as $6mm$) symmetry.

In this work, we have extended the aspect ratio dependence discussion to systems having other crystallographic symmetries and apply these unified formulas to calculate PMN-xPT single crystals poled along two different directions; in particular, our focus is on the change in k_{31}^{eff} with aspect ratio for piezoelectric vibrators made of [001] poled PMN-0.33PT and [011] poled PMN-0.29PT single crystals, which are now being used in making ultrabroadband medical ultrasonic imaging transducers.

II. THEORETICAL MODEL

The aspect ratio in this paper is defined as $G=l_1/l_2$ for a vibrator shown in Fig. 1. We assume $l_3 \ll l_1, l_2$, so that for a given G value, the following conditions always hold: $T_1 \neq 0$, $T_2 \neq 0$, $T_3=0$, $S_1 \neq 0$, $S_2 \neq 0$, and $S_3 \neq 0$. The shear strains and stresses are all zero under an electric field along the poling direction x_3. For such a situation, the electric conditions are $E_1=E_2=0$, $E_3 \neq 0$, $D_1=D_2=0$, and $D_3 \neq 0$. Based on these electric and mechanic conditions, we can write out relevant constitutive relations,

$$S_1 = s_{11}^E T_1 + s_{12}^E T_2 + d_{31} E_3, \tag{1a}$$

$$S_2 = s_{12}^E T_1 + s_{22}^E T_2 + d_{32} E_3, \tag{1b}$$

$$S_3 = s_{13}^E T_1 + s_{23}^E T_2 + d_{33} E_3, \tag{1c}$$

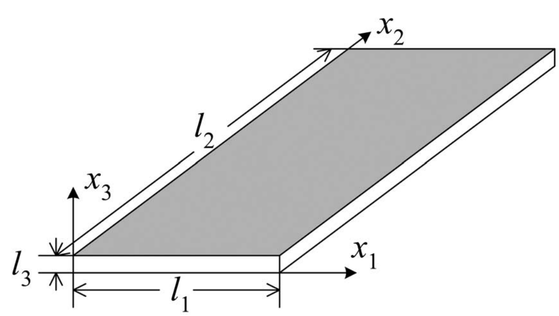

FIG. 1. Geometry and coordinates of the piezoelectric vibrator.

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$$D_3 = d_{31}T_1 + d_{32}T_2 + \varepsilon_{33}^T E_3. \tag{1d}$$

When l_2 is very small compared to l_1, i.e., $G\to\infty$, $S_2\neq 0, T_2=0$; when l_2 is very large compared to l_1, i.e., $G\to 0$, $S_2=0, T_2\neq 0$. We define a function $g(G)$ to reflect the general situation, which satisfies the following boundary condition:

$$g(G) = \begin{cases} 0, & G\to 0 \\ 1, & G\to\infty. \end{cases} \tag{2}$$

Using this function $g(G)$, for an arbitrary aspect ratio k_{31} resonator S_2 can be written as

$$S_2 = g(G)[s_{12}^E T_1 + d_{32}E_3]. \tag{3}$$

Considering $S_2=s_{12}^E T_1 + s_{22}^E T_2 + d_{32}E_3$, we can write the stress T_2 in terms of $g(G)$,

$$T_2 = \frac{g(G)-1}{s_{22}^E}[s_{12}^E T_1 + d_{32}E_3]. \tag{4}$$

Substituting Eqs. (3) and (4) into Eq. (1), we have

$$S_1 = \left\{ s_{11}^E + [g(G)-1]\frac{(s_{12}^E)^2}{s_{22}^E} \right\} T_1 + \left\{ d_{31} + [g(G)-1]\frac{s_{12}^E}{s_{22}^E} d_{32} \right\} E_3. \tag{5}$$

The internal energy density of this vibrator is given by

$$U = \tfrac{1}{2}S_n T_n + \tfrac{1}{2}D_i E_i = \tfrac{1}{2}S_1T_1 + \tfrac{1}{2}S_2T_2 + \tfrac{1}{2}D_3E_3. \tag{6}$$

Substituting Eqs. (3)–(5) into Eq. (6), we get

$$\begin{aligned} U &= \frac{1}{2}\left\{ s_{11}^E + \frac{(s_{12}^E)^2}{s_{22}^E}[g^2(G)-1] \right\} T_1^2 + \left\{ d_{31} + [g^2(G) - 1]\frac{s_{12}^E d_{32}}{s_{22}^E} \right\} T_1E_3 + \frac{1}{2}\left\{ [g^2(G)-1]\frac{d_{32}^2}{s_{22}^E} + \varepsilon_{33}^T \right\} E_3^2 \\ &= U_d + 2U_m + U_e, \end{aligned} \tag{7}$$

where U_d, U_m, and U_e are the elastic, mutual, and dielectric energies, respectively. The electromechanical coupling coefficient k_{31}^{eff} can be formally written as

$$k_{31}^{\mathrm{eff}} = \frac{U_m}{\sqrt{U_eU_d}} = \frac{d_{31} + [g^2(G)-1]\dfrac{s_{12}^E d_{32}}{s_{22}^E}}{\sqrt{\left\{ s_{11}^E + \dfrac{(s_{12}^E)^2}{s_{22}^E}[g^2(G)-1] \right\}\left\{ \varepsilon_{33}^T + [g^2(G)-1]\dfrac{d_{32}^2}{s_{22}^E} \right\}}}, \tag{8}$$

where k_{31}^{eff} stands for the effective coupling coefficient for a vibrator with arbitrary aspect ratio G.

When l_1 is very large compared to l_2, i.e., $G\to\infty$, $g(G)\to 1$, Eq. (8) becomes the textbook definition, i.e.,

$$k_{31}^{\mathrm{eff}} = \frac{d_{31}}{\sqrt{s_{11}^E \varepsilon_{33}^T}} = k_{31}. \tag{9}$$

When l_2 is very large compared to l_1, i.e., $G\to 0$, $g(G)\to 0$, Eq. (8) changes into

$$k_{31}^{\mathrm{eff}} = \frac{d_{31} - \dfrac{s_{12}^E d_{32}}{s_{22}^E}}{\sqrt{\left[s_{11}^E - \dfrac{(s_{12}^E)^2}{s_{22}^E} \right]\left[\varepsilon_{33}^T - \dfrac{d_{32}^2}{s_{22}^E} \right]}}. \tag{10}$$

This corresponds to the textbook definition of k_{31}'. One can see this more clearly by applying the formula to the PZT ceramic case, for which $d_{31}=d_{32}$, $s_{11}^E=s_{22}^E$, and $s_{13}^E=s_{23}^E$, so that Eq. (10) becomes

$$k_{31}^{\mathrm{eff}} = \frac{k_{31}}{\sqrt{1-k_{31}^2}}\sqrt{\frac{1+\sigma}{1-\sigma}}, \tag{11}$$

which is exactly the expression of k_{31}' for a PZT ceramic resonator in the IEEE standard for piezoelectricity.

One can simplify the expression of k_{31}^{eff} in Eq. (8) for a vibrator made of PZT ceramic or [001] poled PMN-PT (or PZN-PT) using symmetry arguments to become

$$k_{31}^{\mathrm{eff}} = \frac{d_{31}\left\{ 1 + [g^2(G)-1]\dfrac{s_{12}^E}{s_{11}^E} \right\}}{\sqrt{\left\{ s_{11}^E + \dfrac{(s_{12}^E)^2}{s_{11}^E}[g^2(G)-1] \right\}\left\{ \varepsilon_{33}^T + [g^2(G)-1]\dfrac{d_{31}^2}{s_{11}^E} \right\}}}. \tag{12}$$

If there is no coupling between different dimensions, the resonance frequencies for x_1 and x_2 dimensions are given by

$$f_x = \frac{1}{2l_1}\sqrt{\frac{c_{11}^E}{\rho}} = \frac{v_1}{2l_1}, \tag{13a}$$

$$f_y = \frac{1}{2l_2}\sqrt{\frac{c_{22}^E}{\rho}} = \frac{v_2}{2l_2}. \tag{13b}$$

Based on Eq. (13), in a small time interval Δt, the ratio of displacements along the two directions may be written as

$$\frac{\xi_2}{\xi_1} \propto \frac{v_2\Delta t}{v_1\Delta t} = \frac{l_2f_y}{l_1f_x}, \tag{14}$$

so that the strains have the following relationship:

$$S_2 = \frac{\xi_2}{l_2} \propto \frac{f_y}{f_x}\frac{\xi_1}{l_1} = \frac{f_y}{f_x}S_1. \tag{15}$$

For an arbitrary aspect ratio G, S_1 is always treated finite in order to study the coupling coefficient k_{31}^{eff}. Considering $S_2=g(G)(s_{12}^E T_1 + d_{32}E_3)$, Eq. (15) tells us that $g(G)$ should be a function of f_x and f_y. When there is coupling between these two dimensions, both frequencies will be shifted, for which we can rewrite $g(G)$ as a function of the ratio between f_1 and f_2, the two eigenfrequencies to be obtained by solving the coupling vibration equation[7]

$$g(G) = \kappa(G)\frac{f_2}{f_1}, \tag{16}$$

where $\kappa(G)$ is a function of G, which should satisfy the following limiting conditions:

$$\lim_{G\to 0} \kappa(G) = 0, \tag{17a}$$

and

$$\lim_{G\to\infty} \kappa(G) = \frac{f_1}{f_2}. \tag{17b}$$

For the coupled piezoelectric system, the equation of motion is given by

$$\frac{\rho\partial^2 u_1}{\partial t^2} = \left(c_{11}^E - \frac{c_{13}^E c_{13}^D}{c_{33}^E}\right)\frac{\partial^2 u_1}{\partial x_1^2} + \left(c_{12}^E - \frac{c_{13}^E c_{23}^D}{c_{33}^E}\right)\frac{\partial^2 u_2}{\partial x_1\,\partial x_2}, \tag{18a}$$

$$\frac{\rho\partial^2 u_2}{\partial t^2} = \left(c_{12}^E - \frac{c_{13}^D c_{23}^E}{c_{33}^D}\right)\frac{\partial^2 u_1}{\partial x_1\,\partial x_2} + \left(c_{22}^E - \frac{c_{23}^E c_{23}^D}{c_{33}^D}\right)\frac{\partial^2 u_2}{\partial x_2^2}. \tag{18b}$$

Based on the symmetry of the resonance modes in consideration, the harmonic solutions for the displacements along the x_1 and x_2 directions may be written as

$$u_1 = A_1 \sin(k_1x_1)\cos(k_2x_2)\cos(\omega t), \tag{19a}$$

$$u_2 = A_2 \cos(k_1x_1)\sin(k_2x_2)\cos(\omega t). \tag{19b}$$

Substituting Eq. (19) into Eq. (18) leads to an eigenvalue problem for the angular frequency ω.

Because $\omega=2\pi f$, $k_1=\omega_1/v_1=\omega_1\sqrt{\rho/c_{11}^E}$, $k_2=\omega_2/v_2=\omega_2\sqrt{\rho/c_{22}^E}$, the final derived two eigenfrequencies are

$$l_1^2 f_1^2 = \frac{1}{8\rho}(ac_{11}^E + bc_{22}^E G^2) + \frac{1}{8\rho}\sqrt{a^2(c_{11}^E)^2 + b^2(c_{22}^E)^2 G^4 - 2c_{11}^E c_{22}^E(ab-2c^2)G^2}, \tag{20a}$$

$$l_1^2 f_2^2 = \frac{1}{8\rho}(ac_{11}^E + bc_{22}^E G^2) - \frac{1}{8\rho}\sqrt{a^2(c_{11}^E)^2 + b^2(c_{22}^E)^2 G^4 - 2c_{11}^E c_{22}^E(ab-2c^2)G^2}, \tag{20b}$$

where $a=1-c_{13}^E c_{13}^D/(c_{11}^E c_{33}^D)$, $b=1-c_{23}^E c_{23}^D/(c_{22}^E c_{33}^D)$, and $c^2=(c_{12}^E-c_{13}^D c_{23}^E/c_{33}^D)(c_{12}^E-c_{13}^E c_{23}^D/c_{33}^D)/(c_{11}^E c_{22}^E)$.

From Eq. (20) we have

$$\lim_{G\to\infty}\frac{f_2^2}{f_1^2} = \frac{c_{11}^E(ab-c^2)}{c_{22}^E b^2 G^2}. \tag{21}$$

Because

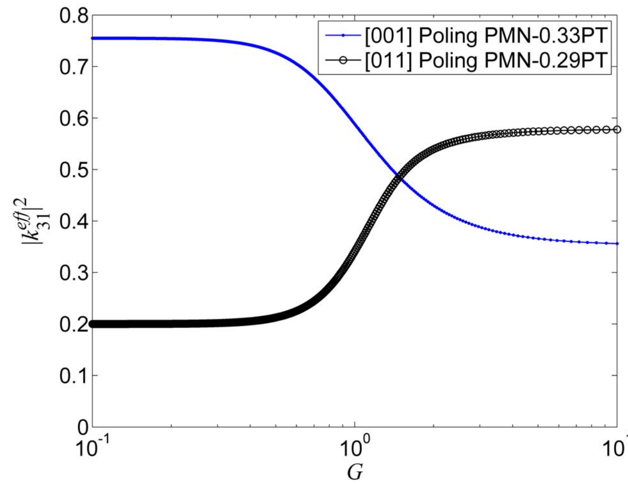

FIG. 2. (Color online) Aspect ratio dependence of the electromechanical energy conversion efficiency for [001] poled PMN-0.33PT and [011] poled PMN-0.29PT single crystal vibrators.

$$\lim_{G\to\infty} g(G) = \lim_{G\to\infty} \kappa(G)\frac{f_2}{f_1} = \kappa(G)\frac{1}{bG}\sqrt{\frac{c_{11}^E(ab-c^2)}{c_{22}^E}} = 1, \tag{22}$$

one can easily derive the form of the function $\kappa(G)$,

$$\kappa(G) = bG\sqrt{\frac{c_{22}^E}{c_{11}^E(ab-c^2)}}. \tag{23}$$

Finally, for a general aspect ratio k_{31} resonator, the function $g(G)$ is given by

$$g(G) = bG\sqrt{\frac{c_{22}^E}{c_{11}^E(ab-c^2)}}\frac{f_2}{f_1}. \tag{24}$$

III. RESULTS AND DISCUSSION

The aspect ratio dependences of k_{31}^{eff} for [001] poled PMN-0.33PT and [011] poled PMN-0.29PT single crystals have been calculated using Eqs. (8) and (12) and the $g(G)$ function [Eq. (24)]. The k_{31}^{eff} values are all negative for [001] poled PMN-0.33PT vibrator but all positive for [011] poled PMN-0.29PT single crystal vibrators. Interestingly, the electromechanical energy conversion efficiency $|k_{31}^{\mathrm{eff}}|^2$ of vibrators made of these two types of materials shows very different trend as shown in Fig. 2. For [001] poled PMN-0.33PT vibrator, the $|k_{31}^{\mathrm{eff}}|^2$ value decreases with G, while for [011] poled PMN-0.29PT vibrator, $|k_{31}^{\mathrm{eff}}|^2$ increases with G.

One can see from Fig. 2 that the variation in $|k_{31}^{\mathrm{eff}}|^2$ mainly happens for the aspect ratio from $G=0.4$ to 4, in which the k_{31}^{eff} value deviates significantly from the textbook 1D definition. In order to get a better feeling of the deviation, in Fig. 3 we have plotted the relative errors $\delta k/k_{31}^{\mathrm{eff}}=|(k_{31}-k_{31}^{\mathrm{eff}})/k_{31}^{\mathrm{eff}}|$ and $\delta k/k_{31}^{\mathrm{eff}}=|(k'_{31}-k_{31}^{\mathrm{eff}})/k_{31}^{\mathrm{eff}}|$ produced by using the textbook definitions of k_{31} and k'_{31} to describe the lateral electromechanical coupling. One can see that the k_{31} formula works better for very large aspect ratio, while the k'_{31} formula works better for very small aspect ratio. Neither one will work when the aspect ratio is in the range of $G=0.4-4$. The worst situation for the [001] poled PMN-0.33PT happens at

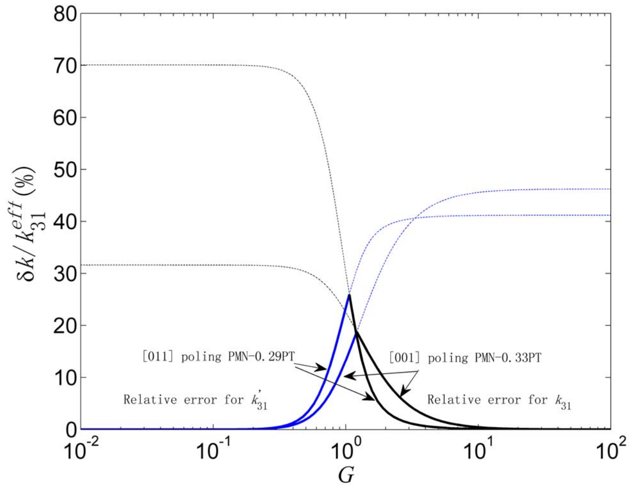

FIG. 3. (Color online) Percentage error of k_{31} and k'_{31} for different aspect ratio vibrators made of [001] poled PMN-0.33PT and [011] poled PMN-0.29PT single crystals.

$G=1.21$ for which the minimum deviation is 18.78% no matter which formula being used. For the [011] poled PMN-0.29PT, the worst deviation occurs at $G=1.06$, reaching a relative error of about 25.9%.

Another interesting phenomenon worth further discussion is for crystals with $mm2$ symmetry, like the [011] poled PMN-0.29PT, its d_{31} value is positive, while d_{32} value is negative and usually much larger than the magnitude of d_{31}. The coupling coefficient is positive when l_2 is very large compared to l_1, i.e., $G \to 0$, $g(G) \to 0$, the k_{31}^{eff} value have the form in Eq. (10). The sign of d_{31}^{eff} is determined by the numerator $d_{31}-s_{12}^E d_{32}/s_{22}^E$; because d_{31} and s_{22}^E are positive, d_{32} and s_{12}^E are negative, $s_{12}^E d_{32}/s_{22}^E$ is also positive. Hence, there is a possibility that the d_{31}^{eff} value may become negative for some crystals. For such a case, d_{31}^{eff} will change from positive to negative with decreasing $G=l_1/l_2$. When this happens, k_{31}^{eff} could equal to zero for a certain G value. This is significant because if such condition satisfied, one may design a resonator without x_1 direction displacement! It could provide an innovative design that could eliminate lateral coupling in a transducer array. In fact, when using the data of PMN-0.32PT given in Ref. 9, a negative d_{31}^{eff} value in deed appears. Following this idea, we have fabricated several resonators using the [011] poled PMN-0.32PT single crystal, but unfortunately could not reproduce the reported data that gave such negative d_{31}^{eff}. In order to find the geometry design of a resonator that has no lateral displacement based on Eq. (8), more accurate data sets are needed.

IV. SUMMARY AND CONCLUSION

In summary, textbook formulas for electromechanical coupling coefficients were all derived for extreme geometries, which cannot describe resonators having arbitrary aspect ratio. In this work we have derived the general formula for the aspect ratio dependence of the effective electromechanical coupling coefficient k_{31}^{eff} to account for piezoelectric systems having $4mm$ and $mm2$ symmetries. The formulas can recover the textbook definitions for limits for extreme geometries.

Based on our calculations, in order to achieve very large lateral electromechanical energy conversion efficiency, the aspect ratio of the k_{31} vibrator should be designed to have a very small aspect ratio G for vibrators made of [001] poled PMN-0.33PT single crystals, while for [011] poled PMN-0.29PT single crystal resonators, the G value should be very large.

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