Uniform behavior of the electromechanical coupling factor in piezoelectric resonators

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Abstract
The coupling of mechanical and electrical energies in piezoelectric materials is a problem extensively studied by many researchers. A precise determination of this coupling is an essential aspect of the theory and performance evaluation of the piezoelectric transducers utilized in multiple medical and industrial applications. In this article, the derivation of the electromechanical coupling factor in dynamic regime, $k$, of four of the most common piezoelectric resonators vibrating under lossless conditions is reviewed. It is explicitly demonstrated that the frequency spectrum of $k$ is uniform through the resonators with respect to their fundamental mechanical resonance frequencies, regardless the vibration mode considered. This uniformity can be described by a simple mathematic expression with the ‘same form’ for all the vibration modes studied. The outcomes presented are in the hope to shed some new light on the basic functional theory of the piezoelectric resonator.

1. Introduction

The characterization of piezoelectric materials and devices is currently an active field of investigation. In ultrasound transducers, frequently a piezoelectric resonator is used to generate or detect the acoustic waves utilized in dissimilar applications, including SONAR projectors, food industry, ultrasonic welding and cleaning, sonochemistry and diverse diagnostic and therapeutic medical interventions [1–7]. Piezoelectric resonators operate based on the direct conversion of electrical polarization to mechanical stress or vice versa [8].

A dimensionless figure of merit that characterizes the electromechanical coupling in a piezoelectric resonator excited mechanically or electrically is the so-called electromechanical coupling factor, $k$. The parameter has been studied by numerous researchers since the early 20th century [9].

Using an energy description, the square of the electromechanical coupling factor of a piezoelectric resonator, $k^2$, can be defined as the ratio of the convertible electrical (mechanical) energy stored in the resonator, to the total input mechanical (electrical) energy supplied to it. For example, strictly speaking, the convertible electrical energy is that part of the electrical energy stored in the resonator that can be released through its electrodes in the process of energy conversion [10]. This bidirectional definition is applicable for both quasistatic and dynamic regimes. In general, $k$ expresses the capacity of a piezoelectric resonator to transform energy between the mechanical and the electrical domains [11–13].

Under quasistatic conditions, the IEEE Std. (176) defines the quasistatic material coupling factor, $k_{ms}$, corresponding to a number of simple one-dimensional geometries (1D), as a particular combination of the real elastic, piezoelectric and dielectric coefficients of the piezoelectric material under consideration [14]. The standard correlates the meaning of the parameter, to a process that seems to be equivalent to the general energy definition above specified [1]. Frequently, $k_{ms}$ is employed as a comparative indicator of piezoelectric materials in defined electric field and stress configurations, independently of the specific values of the corresponding real
coefficients of the materials. Usually, a high $k_m$ is desirable for better electromechanical conversion capacity and improved bandwidth of the piezoelectric transducer [15].

On the other hand, in several applications it is especially important to account the capacity of a piezoelectric resonator to transfer energy between the electrical and mechanical domains in dynamic regime [11]. It is reported that the electromechanical coupling factor in such regime is, in general, less than the associated quasistatic material one [16].

Different researchers have investigated the coupling factor in dynamic regime [17, 18]. In this sense, expressions to calculate the electromechanical coupling factor in dynamic regime were obtained in [17], for a number of simple piezoelectric resonators. In this work, the calculated frequency behavior of the parameter was not comparatively uniform through all the resonators. Particularly, it looks contradictory that the computed magnitude of $k$ for the thickness-extensional mode, based on its energy definition, does not converge to the corresponding quasistatic material one, when the operational regime of the resonator converges to a quasistatic process. It is worth noting that the expression reported in [17] to compute $k$ for this mode of vibration is currently used in the literature [19]. Following a different approach, an expression to determine $k$ in the length-extensional mode was developed in [18], consistently with the outcome reported in [17], for the same vibration mode.

Therefore, it seemed that the frequency spectrum of the electromechanical coupling factor of these common piezoelectric resonators needed to be reviewed, in order to develop a coherent theory, and probably to avoid miscalculations in the literature. Considering in addition, that an accurate quantification of the electromechanical coupling phenomenon in dynamic regime is an essential aspect of the theory and performance evaluation of the piezoelectric resonator, this article presents an analysis conducted with the aim of reviewing the derivation of the electromechanical coupling factor in lossless piezoelectric resonators vibrating in thickness-extensional ($k_1$), length-extensional ($k_{33}$), thickness-shear extensional ($k_{15}$) and length-thickness extensional ($k_{31}$) modes, when the resonators are driven in the mathematic models by harmonic-time excitation fields.

2. Materials and methods

In this work, low-excitation fields in harmonic regimes are considered and calculations are conducted basically in frequency domain. The reduced matrix notation is utilized for physical tensorial magnitudes represented by their amplitudes [20]. Piezoelectric materials considered in calculations are characterized by a 6mm (equivalent to $\infty$mm) symmetry. Additionally, the materials coefficients are supposed to be independent of frequency, and the effects of the temperature and the magnetic fields are ignored. A superscript in a material coefficient indicates the independent variable that is held constant in its experimental evaluation.

In this article, the symbols $k_m$ and $k$ will represent the electromechanical coupling factors of the piezoelectric resonators in quasistatic and dynamic regimes, respectively, indistinctly of the vibration mode considered.

The study of the electromechanical coupling factor will be conducted in some detail first in the thickness-extensional mode for uniform and nonuniform deformations, in order to obtain some of the basic expressions reported. After that, for the rest of the vibration modes, only the nonuniform deformation is considered in the aim of simplifying this exposition. Mode of vibrations will be classified according to [21].

2.1. Thickness-extensional mode

2.1.1. Uniform deformation

Let us consider a piezoelectric plate of thickness $l$ along the polarization direction ($x_3$) with both major faces electroded and located at $x_3 = 0$ and $x_3 = l$, figure 1. In the resonator $l \ll a, b$. In this case the physical problem is reduced to 1D, and the piezoelectric behavior of the element can be properly described by the h-form of the linear piezoelectric constitutive equations [22]:

$$T_j = c_{33}^{D} S_3 - h_{33} D_3,$$  \hspace{1cm} (1)

$$E_3 = -h_{33} S_3 + \beta_{33}^{S} D_3,$$  \hspace{1cm} (2)

where $S_3$ is the strain, $T_j$ is the stress, $E_3$ is the electric field and $D_j$ is the dielectric displacement; $c_{33}^{D}$, $h_{33}$ and $\beta_{33}^{S}$ are the elastic stiffness (at constant dielectric displacement), piezoelectric stiffness and inverse permittivity (at constant strain) coefficients of the piezoelectric material, respectively.

For the analyzed situation, the change in the stored energy density in the piezoelectric element produced by applying to it increments of the strain and the dielectric displacement is [23]:

$$W_{\text{str}} = \frac{1}{2} (S_3 \cdot c_{33}^{D} \cdot S_3 - h_{33} S_3 \cdot D_3 - h_{33} D_3 \cdot S_3 + \beta_{33}^{S} D_3 \cdot D_3).$$
If a mechanical excitation is supplied to the piezoelectric element by an increment of the strain with open-circuit electrical boundary condition, \( dD = 0 \) (additionally \( \partial D / \partial x_3 = 0 \) [22]) and from equations (1) and (3) the supplied mechanical energy density is:

\[
W_m = W_m^D = \frac{1}{2} \varepsilon_{33}^D S_3^2,
\]

where \( W_m = W_m^D \) is the mechanical energy density provided to the element with the electrodes open-circuited, or the mechanical energy density supplied to it at constant \( D \).

On the other hand, the electrical energy density stored in the piezoelectric element mechanically stimulated is:

\[
W_e = \frac{1}{2} \varepsilon_{33} E_3^2.
\]

In this case, the electric field \( E_3 \) is internally generated by the direct piezoelectric effect. Consequently, from equations (2) and (5) the convertible electrical energy density is:

\[
W_c = \frac{1}{2} \varepsilon_{33} h_{33} S_3^2.
\]

From the energy definition of the electromechanical coupling factor from [10] and equations (5) and (6) we have:

\[
k^2 = \frac{W_c}{W_m} = \frac{W_c}{W_m^D} = \frac{\varepsilon_{33} h_{33} S_3^2}{\varepsilon_{33} S_3^2} = \frac{h_{33}^2 S_3^2}{\varepsilon_{33}^2 S_3^2} = k_3^2,
\]

as it is well-known [22].

### 2.1.2. Nonuniform deformation

The wave equation for this mode of vibration is the following [22]:

\[
\frac{\partial^2 u_3}{\partial t^2} = \frac{c_{33}^D}{\rho} \frac{\partial^2 u_3}{\partial x_3^2},
\]

where \( u_3 \) is the particle displacement in \( x_3 \) direction and \( \rho \) is the material density.

For electric excitations described as \( V = V_0 e^{i \omega t} \), the general solution of equation (8) is of the form:

\[
u_3 = \left[ A \sin \left( \frac{\omega x_3}{v_3^D} \right) + B \cos \left( \frac{\omega x_3}{v_3^D} \right) \right] e^{i \omega t},
\]

where \( v_3^D = (c_{33}^D / \rho)^{1/2} \) is the acoustic wave propagation velocity in the \( x_3 \) direction (at constant dielectric displacement).

Evaluating constants \( A \) and \( B \) considering free mechanical boundary conditions \( T_{3}(0) = T_{3}(l) = 0 \) and taking into account that \( S_3 = \partial u_3 / \partial x_3 \) in frequency domain the strain distribution in the resonator becomes [21]:

\[
S_3 = \left[ \cos \left( \gamma_{3} x_3 \right) + \tan \left( \frac{\gamma_{3} l}{2} \right) \sin \left( \gamma_{3} x_3 \right) \right] V_0,
\]

\[
\frac{\omega}{v_3} = \frac{\omega}{v_3^D} = \gamma_3 \coth \left( \frac{\gamma_3 l}{2} \right).
\]
where \( \gamma = \omega / v^D \) is the propagation constant of the acoustic waves, and \( A_1 \) is an expression that depends on the piezoelectric material characteristic parameters, the distance between the electrodes, and the angular frequency, \( \omega \).

For harmonic-time mechanical excitation fields with open-circuit electrical boundary condition in the resonator, the reciprocity principle may be applied [23, 24]. Then, equation (10) can be used to calculate \( W_m^D \) and \( W_e \) accordingly.

In this case:

\[
W_m^D = \frac{c^D_{33}}{2l} \int_0^l S_3^1 dx_3, \tag{11}
\]

and

\[
W_e = -\frac{s^S_{33} h^D_{33}}{2l^2} \left[ \int_0^l S_3^1 dx_3 \right]^2.
\tag{12}
\]

Equation (11) is obvious; but equation (12) is not really so evident. Nevertheless, it can be easily obtained if one considers that the electric field intensity that effectively represents an electrical energy that can be released through the resonator electrodes in the process of energy conversion is:

\[
E_3 = -h_{33} \frac{1}{l} \int_0^l S_3^1 dx_3.
\tag{13}
\]

This idea can be deduced from the work of Ulitko [10]. But if it is explicitly stated, avoids resolving once again the implicit electrostatic problem, at least for the piezoelectric resonators investigated in this work.

Employing equations (11) and (12) the electromechanical coupling factor in dynamic regime results:

\[
k^2 = \frac{W_e}{W_m^D} = k_1^2 \left[ \int_0^l S_3^1 dx_3 \right]^2. \tag{14}
\]

From above equation it follows:

\[
k^2 = k_1^2 \frac{8 \sin^2 \frac{\pi \omega}{2 \omega_0}}{\pi \omega / \omega_0 \left[ \sin \left( \frac{\pi \omega}{\omega_0} \right) + \frac{\pi \omega}{\omega_0} \right]} = k_1^2 \times FDC,
\tag{15}
\]

where \( \omega_0 = \pi v^D_3 / l \) is the fundamental mechanical resonance frequency, and obviously:

\[
FDC = \frac{8 \sin^2 \frac{\pi \omega}{2 \omega_0}}{\pi \omega / \omega_0 \left[ \sin \left( \frac{\pi \omega}{\omega_0} \right) + \frac{\pi \omega}{\omega_0} \right]}, \tag{16}
\]

is a frequency dependent coefficient (FDC) of the square of the electromechanical coupling factor in dynamic regime.

2.1.3. Length-extensional mode

Consider now a piezoelectric bar of length \( l \) along the polarization direction (\( x_3 \)) with both end faces electroded and located at \( x_3 = 0 \) and \( x_3 = l \), figure 2. In the resonator \( l \gg a, b \).

In this case, the g-form of the linear piezoelectric constitutive equations can be used to describe the 1D problem [22]:

\[
S_3 = s^D_{33} T_3 + g_{33} D_3, \tag{17}
\]

\[
E_3 = -g_{33} T_3 + \beta^S_{33} D_3, \tag{18}
\]

where in addition to the physical magnitudes above defined, \( s^D_{33}, \beta^S_{33} \) and \( g_{33} \) are the elastic compliance (at constant dielectric displacement), inverse permittivity (at constant stress) and the piezoelectric voltage constant of the material, respectively.

Alternatively, equations (17) and (18) can be rewritten in the equivalent h-form as follows:

\[
T_3 = e^D_{33} S_3 - \tilde{h}_{33} D_3, \tag{19}
\]

\[
E_3 = -\tilde{h}_{33} S_3 + \beta^T_{33} D_3, \tag{20}
\]

where, \( e^D_{33} = 1 / s^D_{33}, \tilde{h}_{33} = g_{33} / s^D_{33} \) and \( \beta^S_{33} = \beta^T_{33} + g^2_{33} / s^D_{33} \).
The wave equation of the problem is [22]:

$$\frac{\partial^2 u_3}{\partial t^2} = \frac{1}{\rho_s \beta_3^2} \frac{\partial^2 u_3}{\partial x_3^2},$$

(21)

where $u_3$ is the particle displacement in the $x_3$ direction.

For electrical excitations expressed as $V = V_0 e^{j\omega t}$ and free mechanical boundary conditions ($T_3(0) = T_3(l) = 0$), considering the solution of equation (21), the strain distribution in frequency domain is evidently:

$$S_3 = \left( \cos (\gamma_3 x_3) + \tan \left( \frac{\gamma_3 l}{2} \right) \sin (\gamma_3 x_3) \right) A_{33} V_0,$$

(22)

where $\gamma_3 = \omega/\beta_3^0$ is the propagation constant of the acoustic waves and $V_0 = (1/\rho_s \beta_3^2)^{1/2}$. $A_{33}$ is the corresponding expression for the $k_{33}$ mode.

Analogously to the $k_1$ vibration mode, using equations (19), (20), it can be shown that:

$$k^2 = \frac{W_0}{W_m} = k_{33}^2 \frac{\int_0^l S_3^2 dx_3}{l \int_0^l S_3 dx_3} = k_{33}^2 \times FDC,$$

(23)

where for the FDC, $\omega_0 = \pi \nu_3^D / l$ is the corresponding fundamental mechanical resonance frequency.

2.1.4. Thickness-shear mode

Let us assume a plate poled in its plane ($x_3$ direction) with thickness $l$ ($x_1$ direction) with both major faces electroded and located at $x_1 = 0$ and $x_1 = l$, figure 3. In the resonator $a \gg l; b$ is arbitrary [12].

For this 1D problem the h-form of the linear piezoelectric constitutive equations can be used too for its description [22]:

$$T_5 = \frac{D}{\varepsilon_{55}} S_5 - h_{15} D_1,$$

(24)

$$E_i = -h_{15} S_5 + \beta_{51}^E D_1,$$

(25)

where $S_5$ is the shear strain around $x_5$ direction, $T_5$ is the corresponding shear stress, $E_i$ is the electric field, $D_1$ is the dielectric displacement; $\varepsilon_{55}^D$, $h_{15}$ and $\beta_{51}^E$ are the elastic stiffness (at constant dielectric displacement), piezoelectric stiffness and dielectric impermeability (at constant strain) coefficients of the piezoelectric material, respectively.
The wave equation of the problem is:

$$\frac{\partial^2 u_3}{\partial t^2} = \frac{1}{\rho E_{31}} \frac{\partial^2 u_3}{\partial x_3^2},$$

(26)

where $u_3$ is the particle displacement in the $x_3$ direction, with wave propagation direction along $x_3$.

Employing an analogous procedure to that used in the analysis of the $k_0$ mode, and considering also electrical excitations expressed as $V = V_0 e^{i\omega t}$ under free shear mechanical boundary conditions ($T_3(0) = T_3(l) = 0$), we have:

$$S_5 = \left[ \cos (\gamma x_1) + \tan \left( \frac{\gamma l}{2} \right) \sin (\gamma x_1) \right] \frac{V_0}{A_{15}},$$

(27)

where $\gamma = \omega / \sqrt{E}$ is the propagation constant of the acoustic waves and $\sqrt{E} = (1/\rho E_{31})^{1/2}$. $A_{15}$ is the corresponding expression for the $k_{15}$ mode.

Analogously:

$$k^2 = \frac{W_d}{W_{m0}} = k_{31}^2 \left[ \frac{\int_0^l S_5 d\xi}{\int_0^l S_3^0 d\xi} \right]^2 = k_{31}^2 \times FDC,$$

(28)

where for FDC, $\omega_0 = \pi \sqrt{E} / l$ is the corresponding fundamental mechanical resonance frequency.

### 2.1.5. Length-thickness extensional mode

Let us suppose a piezoelectric bar in $x_3$ direction with electroded faces normal to the poled direction ($x_3$). In addition, the length of the bar ($l$) is long enough compared with its cross-sectional dimensions ($a$, $b$), figure 4.

Then, the d-form of the linear piezoelectric constitutive equations are the appropriated ones [22]:

$$S_1 = \varepsilon_{31}^E T_1 + d_{31} E_3,$$

(29)

$$D_3 = d_{31} T_1 + \varepsilon_{33}^E E_3,$$

(30)

where $S_1$ is the strain, $T_1$ is stress, $E_3$ is the electric field and $D_3$ is the dielectric displacement. In addition, $\varepsilon_{31}^E$, $d_{31}$ and $\varepsilon_{33}^E$ are the elastic compliance (at constant electric field), piezoelectric strain and permittivity (at constant stress) coefficients of the piezoelectric material, respectively.

For this vibration mode the wave equation is:

$$\frac{\partial^2 u_3}{\partial t^2} = \frac{1}{\rho \varepsilon_{31}^E} \frac{\partial^2 u_3}{\partial x_3^2},$$

(31)

where $u_3$ is the particle displacement in the longitudinal dimension of the resonator.

For sinusoidal stimulations of the form $V = V_0 e^{i\omega t}$ [25]:

$$S_1 = \left[ \cos (\gamma_1 x_1) + \tan \left( \frac{\gamma_1 l}{2} \right) \sin (\gamma_1 x_1) \right] \frac{V_0}{A_{31}},$$

(32)

where $\gamma_1 = \omega / \sqrt{E}$ is the wave propagation constant and $\sqrt{E} = (1/\rho \varepsilon_{31}^E)^{1/2}$. $A_{31}$ is the corresponding expression for the $k_{31}$ mode.
Since each resonator electrode is an equipotential surface, once again analogously:

\[
\frac{k^2}{k_{mn}} = \frac{8}{\pi^2} \frac{W_0}{W_m} = k_{31} \left[ \int_0^l S_1(\alpha) \, d\alpha \right]^2 = k_{31}^2 \times FDC,
\]

where for the \( FDC \) \( \omega_0 = \pi v F / l \) is the fundamental mechanical resonance frequency.

3. Numerical results

Figure 5 shows the frequency spectrum of \( k^2/k_{mn} \) for all the piezoelectric resonators investigated, considering a common fundamental mechanical resonance frequency of 1 MHz. In it, \( f = \omega / 2\pi \).

It is evident that the frequency spectrum of \( k^2 \) (or \( k \)) is uniform through the resonators with respect to their fundamental mechanical resonance frequencies, regardless the vibration mode considered.

From the common \( FDC \) expression (16) for all the resonators, it can be easily computed that the square of the coupling factor evaluated at the respective fundamental mechanical resonance frequencies is:

\[
k^2 = \frac{8}{(2n + 1)^2 \pi^2} k_{mn}^2,
\]

where \( n = 0, 1, 2, 3, \ldots \), in agreement with [26]. In addition, the common \( FDC \) expression (16) \( \rightarrow 1 \) when \( \omega \rightarrow 0 \). Note that the electromechanical coupling goes to zero when \( f = mf_0 \), where \( m = 2, 4, 6, \ldots \), i.e., for the even modes of vibrations.

4. Discussion

In this paper the relationship between the electromechanical coupling factor in dynamic regime, \( k \), and the corresponding material quasistatic one, \( k_{mn} \), is described by a simple mathematic expression with the ‘same form’ for all the vibration modes analyzed. In this way, it is uncovered for the first time explicitly and without any ambiguity, the uniform behaviour of this physical quantity in the piezoelectric resonators investigated. Additionally, it is presented a conceptual theoretical approach that simplified the derivation of the mathematic expressions reported.

In the analyses of the electromechanical coupling factor in dynamic regime, power or thermal loss in the piezoelectric material was excluded. Power loss can be included in the mathematic model of the piezoelectric resonator, by assuming the coefficients of the piezoelectric material as complex quantities [27]. In this case, different physical magnitudes involved in the model become complex. But, some caution must be exercised when the method is utilized in the mathematic model of the piezoelectric resonator to account for power loss. First, complex material coefficients are approximations valid for small signal excitation fields in a limited range of frequencies. Besides, the approach implies some subtle analyses when it is utilized to describe the electromechanical coupling phenomenon in piezoelectrics with the inclusion of power losses [28, 29].

Nevertheless, a good approximation to account for power loss in the model presented herein for piezoelectric resonators with a mechanical quality factor \( Q_m > 50 \), is just taking the real part of square of the
resulting complex material coupling factor, as a valid magnitude to be used in substitution of $k_m^2$ \cite{30,31}, while the common FDC expression (16) for all the resonators remains real.

Additionally, the reciprocity principle was used in order to simplify the mathematic procedures utilized to obtain the mathematic expressions presented. This principle is a relatively simple but powerful technique for the piezoelectric transducer analysis \cite{24,32}. Accordingly, the resonators were considered mechanically excited in open-circuit electrical boundary condition, or alternatively, electrically excited in free mechanical boundary conditions.

In the frame of this paper, a unique criterion of the electromechanical coupling factor is utilized, which is represented by the symbol $k$. In this criterion, for example, the so-called effective coupling factor for the fundamental resonance mode, defined in some literature as: $k_{eff} = (8/\pi^4)k_m$ \cite{26,33}, is just the value of the electromechanical coupling factor in dynamic regime evaluated at the fundamental mechanical resonance frequency (see expression (34), for $n = 0$).

Finally, the results presented were obtained for simple 1D piezoelectric resonators, but these configurations are utilized in several theoretical models, and as good approximations for numerous practical applications.

5. Conclusions

The derivation of the electromechanical coupling factor of lossless piezoelectric resonators vibrating in the common stiffened and unstiffened 1D modes $k_1$, $k_{33}$, $k_{15}$, and $k_{31}$ was reviewed. It was theoretically demonstrated that the electromechanical coupling factor in dynamic regime for all the resonators investigated in this work can be calculated by:

$$k = k_m \sqrt{FDC},$$

(35)

where the frequency dependent coefficient, $FDC$, is given by expression (16), in which $\omega_0$ is calculated and $k_m$ is selected according to the specific piezoelectric resonator considered.

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9