Ambiguous definitions of the piezoelectric coupling factor

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Abstract
When a piezoelectric material is subjected to a quasi-static electric (or mechanical) load, part of the input energy is converted to the mechanical (or electric) domain. The piezoelectric coupling factor $k^2$ is defined as the ratio between the converted energy and the supplied energy. This factor is often considered as a measure of the transduction efficiency of the material. Another definition of the coupling factor is a non-dimensional ratio of material coefficients. To examine the compatibility between these two different definitions, we consider several quasi-static loading cycles of a simple one-dimensional problem. We show that in some specific cases, the two definitions are equivalent, but that in other cases they are incompatible. In addition, we show that in specific quasi-static loading cycles, the converted energy may be increased by a slight modification of the unloading part of the cycle.

Keywords
Piezoelectric transduction, piezoelectric coupling factor

I. Introduction
Piezoelectric transducers are used as actuators (Farghaly et al., 2017; Grinberg et al., 2017), sensors (Marrison, 1948; Muralt et al., 2005), and energy harvesters (Blystad et al., 2010; Erturk and Inman, 2011). When a piezoelectric material is subjected to a quasi-static electric (or mechanical) load, part of the input energy is converted to the mechanical (or electric) domain. The piezoelectric coupling factor $k^2$ is defined as the non-dimensional ratio between the converted energy and the supplied energy (ANSI/IEEE Std 176-1987, 1988; Ikeda, 1996; Wolf, 2000)

$$k^2 = \frac{U_{\text{converted}}}{U_{\text{supplied}}} \quad (1)$$

There are many different definitions of the electromechanical coupling factor $k^2$, and they are often assumed to be compatible. For example, in Section 2 of Ikeda's book (Ikeda, 1996), there are seven different definitions. One definition is the ratio between the converted and the supplied energies (equation (1)). Another definition is the mathematical ratio between the square of a relevant piezoelectric coupling coefficient, and the product of a mechanical coefficient (i.e. stiffness or compliance) and permittivity (which is a dielectric coefficient) (Ikeda, 1996; Roscow et al., 2019). From here on, we mark this mathematical ratio of coefficients as $\kappa^2$ (using the Greek kappa to distinguish it from the Latin "k" used for the first definition). The physical interpretation of $\kappa^2$ is the ratio between the material's ability to convert energy from one domain to the other, and its ability to store energy in the mechanical and electric domains. In the following, we show that the two measures, $k^2$ and $\kappa^2$, are equivalent for some specific problems. However, we also show that for other problems, they are incompatible. The conflict between the two definitions is the source of some confusion, which we hope to alleviate.

Often the piezoelectric coupling factor is considered as a universal measure for comparing the effectiveness of piezoelectric materials, whether they are used as actuators or sensors, or for energy harvesting. The present study aims to raise the awareness that the mathematical ratio of coefficients $\kappa^2$ may not always be a relevant measure.

2. A simple one-dimensional problem
In the present study, we consider a piezoelectric patch with poling in $e_3$, which is coated by electrodes on top and bottom surfaces (Figure 1). The width, $w$, and length, $L$, are assumed to be sufficiently large relative...
to the thickness, \( d \) \( (w \gg d, L \gg d) \), so that fringing fields can be neglected, and there is no electric flux or field in these transverse directions

\[
D_1 = D_2 = 0, \quad E_1 = E_2 = 0
\]  

(2)

The piezoelectric layer may be subjected to a uniform mechanical strain in the \( e_3 \) direction or to a uniform electrostatic displacement (i.e. electrostatic flux) in \( e_3 \). Since the load and response are both in the \( e_3 \) direction, we will consider the two definitions of \( k_{33}^2 \) and \( \kappa_{33}^2 \). For example, if the loading was in the \( e_1 \) direction, then the two relevant definitions would have been marked as \( k_{31}^2 \) and \( \kappa_{31}^2 \) (ANSI/IEEE Std 176-1987, 1988; Bowen et al., 2016).

In the following sections, we will consider either plane-stress or plane-strain conditions. We will use the \( T-E \) form of the piezoelectric constitutive equations for plane-stress conditions, and the \( S-E \) form for plane-strain conditions (Ikeda, 1996). To further simplify the discussion, we consider a piezoelectric material of the 4-mm point group (e.g. the tetragonal PZT; Ikeda, 1996; Uchino, 1996). A general discussion on the applicability of these conditions is included at the end of Section 6.

3. The electromechanical coupling factor for plane-stress conditions

In this section, we assume that plane-stress conditions apply (i.e. there is no stress in \( e_1 \) and \( e_2 \)). In this case, the \( T-E \) form of the governing equations is

\[
S_3 = s_{33}^E T_3 + d_{33} E_3
\]

\[
D_3 = d_{33} T_3 + e_{33}^T E_3
\]  

(3)

For the structure in Figure 1 and plane-stress conditions, the relevant coefficients ratio \( \kappa_{33}^2 \) is

\[
\kappa_{33}^2 = \frac{d_{33}^2}{s_{33}^E e_{33}^T}
\]  

(4)

In the following two sections, we consider closed cycles in which the system is loaded mechanically, and the converted electric energy is evaluated (Wolf, 2000). The top and bottom electrodes can be initially disconnected or initially shorted. These electric conditions affect the mechanical stiffness of the system and hence affect the coupling factor. Therefore, we will analyze the two different cases separately.

3.1. Mechanical loading with initially shorted electrodes

Figure 2 describes a loading cycle for initially shorted electrodes, under mechanical loading (ANSI/IEEE Std 176-1987, 1988; Mattiat, 2013; Wolf, 2000). From the initial unloaded state 1, the system is quasi-statically subjected to a uniform strain \( S_3 = S_0 \), while the electrodes are shorted (Figure 2, path 1–2). Because the electrodes are shorted, the electric field remains zero, \( E_3 = 0 \), and an electric flux develops (charge flows between the electrodes).

At state 2, the stress and electric field (derived from equation (3)) are

\[
S_3 = S_0, \quad T_3 = \frac{1}{s_{33}^E} S_0, \quad D_3 = \frac{d_{33}^2}{s_{33}^E} S_0, \quad E_3 = 0
\]  

(5)
At state 2, there is charge on the electrodes, but there is no electric energy in the structure because the electrostatic field is zero. The only way electric energy can be obtained is by disconnecting the two electrodes (Figure 2, stage 2') and slowly releasing the stress in the system (Figure 2, path 2'–3). Since the electrodes are now disconnected, the electric field can develop while the amplitude of charge distribution in the electrodes is locked at $D_3 = S_0d_{33}/\varepsilon_0^{\varepsilon}$.

In path 2'–3, electric energy develops since the charges are now in an electrostatic field, while stress and hence the mechanical energy are reduced to zero. By disconnecting the electrodes, we made the system stiffer (the disconnection constrains the degree of freedom of charge migration from one electrode to the other), and hence the release of all the stress does not release all the strain. The difference between the supplied mechanical energy and the mechanical energy that is released (the shaded area in Figure 2) is the electric energy that remains in the system.

The values of the state variables at stage 3 are

$$S_3 = \kappa_{33}^2 S_0, \quad T_3 = 0, \quad D_3 = \frac{d_{33}}{\varepsilon_0^{\varepsilon}} S_0, \quad E_3 = \frac{\kappa_{33}^2}{d_{33}} S_0$$

where $\kappa_{33}^2$ is defined in equation (4). To complete the cycle, the electric energy in the structure may, for example, be dumped on a resistor that will consume the converted electric energy (Figure 2, path 3'–4).

The mechanical energy converted by the system is given by

$$U_{\text{converted}} = \frac{1}{2} D_3 E_3 = \frac{1}{2} \frac{\kappa_{33}^2}{\varepsilon_0^{\varepsilon}} S_0^2$$

The supplied electric energy is given by

$$U_{\text{supplied}} = \frac{1}{2} S_0 T_{3(_{\text{state2)}}} = \frac{1}{2} \frac{1}{\varepsilon_0^{\varepsilon}} S_0^2$$

It follows that the coupling factor is

$$k_{33}^2 = \frac{U_{\text{converted}}}{U_{\text{supplied}}} = \kappa_{33}^2$$

This result seems to imply that the coupling factor $k_{33}^2$ is identical to the non-dimensional mathematical coefficients ratio $\kappa_{33}^2$, but we will soon show that in general this is not true.

### 3.2. Mechanical loading with initially disconnected electrodes

Figure 3 describes a loading cycle for initially disconnected electrodes, under mechanical loading (Brand et al., 2015; Wolf, 2000). From the initial unloaded state 1, the system is quasi-statically subjected to a uniform strain $S_3 = S_0$, while the electrodes are disconnected.

Because the electrodes are disconnected, the electric displacement remains zero, $D_3 = 0$ (i.e. no charge flows between the electrodes), and an electric field develops. At state 2, the stress and electric field (derived from equation (3)) are

$$S_3 = S_0, \quad T_3 = \frac{1}{1 - \kappa_{33}^2} \frac{1}{\varepsilon_0^{\varepsilon}} S_0, \quad D_3 = 0,$$

$$E_3 = \frac{\kappa_{33}^2}{1 - \kappa_{33}^2} \frac{1}{\varepsilon_0^{\varepsilon}} S_0$$

The stress in the system is higher than the value obtained by the linear Hook law $T_3 = S_0/d_{33}$, since the disconnection between the electrodes increases the stiffness of the structure.

We may now connect the two electrodes through a resistor (that will consume the converted electrical energy; Figure 3, path 2–2'), while holding the strain $S_3 = S_0$, so that no mechanical work is done in this cycle path (Figure 3, path 2'–3). Along this path, charge flows between the electrodes until there is no voltage difference between them (i.e. the electric field vanishes). Half the product of the electric displacement and the electric field is the converted electric energy, represented by the shaded area in Figure 3. The extraction of electric energy reduces the total mechanical energy in the system, because although the strain $S_3$ is fixed, the stress $T_3$ decreases in amplitude.
It is important to emphasize that the field $E_3$ in path $2'–3$ is negative, whereas the flux $D_3$ is positive. It follows that the converted electric energy is negative. The physical meaning of this negative energy is that the system can absorb energy from the environment. By analogy to the gravitational energy of water, we may extract energy from water that is at a higher elevation, or extract energy from a vacancy for water, which is created at a lower elevation. In this section, the negative field is like a vacancy for charge that may flow into the system.

At state 3, the state variables are

$$S_3 = S_0, \quad T_3 = \frac{1}{k_{33}} S_0, \quad D_3 = \frac{d_{33}}{k_{33}} S_0, \quad E_3 = 0 \quad (11)$$

To complete the cycle, the strain is released while the electrodes are shorted, releasing the remaining mechanical energy (Figure 3, path 3–4).

The converted mechanical energy is given by

$$U_{\text{converted}} = \frac{1}{2} |D_3 E_3| = \frac{1}{2} k_{33}^2 \frac{1}{k_{33}} S_0^2 \quad (12)$$

The supplied electric energy is given by

$$U_{\text{supplied}} = \frac{1}{2} S_0 T_3(\text{state} 2) = \frac{1}{2} \frac{1}{k_{33}} \frac{1}{k_{33}} S_0^2 \quad (13)$$

where the absolute value is used because the field and flux are opposite in sign (Figure 3, path $2'–3$). It follows that the coupling factor is

$$k_{33}^2 = \frac{U_{\text{converted}}}{U_{\text{supplied}}} = k_{33}^2 \quad (14)$$

This result, once again, seems to imply that the coupling factor $k_{33}^2$ is identical to the non-dimensional mathematical coefficients ratio $k_{33}^2$, but we will soon show that in general this is not true.

### 3.3. Electric loading

In the two previous sections, the piezoelectric layer was used to convert part of the mechanical energy into electric energy. However, the piezoelectric layer can convert electric energy into mechanical energy as well. The layer can be subjected to a flux (analogous to the strain in the previous examples). The response of the system can then be considered for boundary conditions of either no axial strain (analogous to open electrodes in the previous examples) or no axial stress (analogous to shorted electrodes in the previous examples). For plane-stress conditions, for either boundary conditions on axial strain or axial stress, the coupling factor $k_{33}^2$ is equal to the coefficients ratio $k_{33}^2$. This similarity between $k_{33}^2$ and $k_{33}^2$ was shown for the mechanical loading cycles in Sections 3.1 and 3.2.

### 4. The electromechanical coupling factor for plane-strain conditions

We next consider the system described in Figure 1, when plane-strain conditions apply ($S_1 = S_2 = 0$), and therefore use the $S–E$ form of the constitutive equations

$$T_3 = C_{33}^E S_3 - e_{33} E_3$$

$$D_3 = e_{33} S_3 + e_{33} E_3 \quad (15)$$

Since the boundary conditions of the problem have changed, it may be expected that the coupling factor will change as well. For plane-strain, the relevant non-dimensional ratio is given by

$$k_{33}^2 = \frac{e_{33}^2}{C_{33}^E S_0} \quad (16)$$

where the over-bar is used to distinguish it from the mathematical ratio $k_{33}^2$ that was defined for plane-stress in equation (4).

The different stages of the initially shorted electrodes cycle, and of the initially disconnected electrodes cycle, are similar to what was done for plane-stress conditions, but with parameters appropriate of the $S–E$ form (equation (15)).

#### 4.1. Mechanical loading with initially shorted electrodes

The mechanical load cycle for initially shorted electrodes is the same as in Figure 2. The values of the different variables in each stage are presented in Table 1.

| Stage | $S_3$ | $T_3$ | $D_3$ | $E_3$ |
|-------|-------|-------|-------|-------|
| 1, 4  | 0     | 0     | 0     | 0     |
| 2     | $S_0$ | $C_{33}^F S_0$ | $e_{33} S_0$ | 0     |
| 3     | $\frac{S_0}{1 + k_{33}^2}$ | $0$ | $e_{33} S_0$ | $\frac{1}{1 + k_{33}^2} S_0$ |

With the different variables in each state, we can compute the converted and supplied energies. The converted energy, marked by the shaded area in Figure 2, is

$$U_{\text{converted}} = \frac{1}{2} D_3 E_3 = \frac{1}{2} \frac{k_{33}^2}{1 + k_{33}^2} C_{33}^E S_0^2 \quad (17)$$

and the supplied energy is given by

$$U_{\text{supplied}} = \frac{1}{2} S_0 T_3(\text{state} 2) = \frac{1}{2} e_{33}^2 S_0^2 \quad (18)$$

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**Table 1.** The values of the different variables at different stages of the load cycle (Figure 2), when the electrodes are initially shorted.
Table 2. The values of the different variables at different stages of the load cycle (Figure 3), when the electrodes are initially disconnected.

| Stage | $S_3$ | $T_3$ | $D_3$ | $E_3$ |
|-------|-------|-------|-------|-------|
| 1, 4  | 0     | 0     | 0     | 0     |
| 2     | $S_0$ | $C_{33}^E (1 + \kappa_{33}^2) S_0$ | 0     | $-\frac{C_{32} S_0}{S_3}$ |
| 3     | $S_0$ | $C_{33} S_0$ | $e_{33} S_0$ | 0     |

The coupling factor is therefore

$$k_{33}^2 = \frac{U_{\text{converted}}}{U_{\text{supplied}}} = \frac{\kappa_{33}^2}{1 + \kappa_{33}^2}$$

(19)

In contrast to the case of plane-stress (Section 3.1), here the coupling factor $k_{33}^2$ is not equal to the non-dimensional coefficient ratio $\kappa_{33}^2$.

If we had considered the ratio between the converted electric energy and the mechanical energy released in stage 3–4 (instead of the total supplied energy), then we would have obtained

$$\frac{U_{\text{converted}}}{U_{\text{mech\_released}}} = k_{33}^2$$

(20)

Although this result is appealing, the energy ratio on the left-hand side is not compatible with definition (1). This demonstrates part of the confusion between $k_{33}^2$ and $\kappa_{33}^2$ (or $k_{33}^2$ and $\kappa_{33}^2$ in this case).

4.4. Interim conclusion 1

We have shown that the two definitions of the coupling factor are not identical in the general case. For plane-stress conditions, the coupling factor $k_{33}^2$ and the coefficients ratio $\kappa_{33}^2$ are identical, but for plane-strain conditions, the value of $k_{33}^2$ is different than that of $\kappa_{33}^2$. In addition, we have shown that for plane-strain conditions, there is a different energy ratio (not $k_{33}^2$) that is equal to $\kappa_{33}^2$, which adds confusion to the definition of $k_{33}^2$.

4.3. Electric loading

In a similar manner, we can evaluate the coupling factor under electric loading, for either axial strain constraining or axial stress constraining. For both evaluations, the coupling factor will be identical to equations (19) and (23), which confirms that the coupling factor $k_{33}^2$ is not equal to $\kappa_{33}^2$.

5. How much energy can really be converted in a piezoelectric structure?

In the previous sections, we evaluated the transduction of mechanical energy to electric energy, for various loading cycles and boundary conditions. But, have we really considered the maximal energy that can be converted in a quasi-static cycle? We next examine this point for both plane-stress and plane-strain conditions.

5.1. Plane-stress conditions

Figure 4 overlays Figures 2 and 3, and we now consider a combined cycle, under mechanical loading. Up to state 3, the cycle is identical to the initially disconnected electrodes cycle. It turns out that point 3 in the disconnected electrodes cycle is identical to point 2 in the shorted electrodes cycle, so that the combined cycle is simply the concatenation of the two. Accordingly, in state 3, the switch that was closed to produce the segment 2’–3 is reopened so that when the mechanical stress is released in segment 3’–4, the flux $D_3$ remains fixed. Hence, the electromechanical coupling factor $k_{33}^2$ of the combined cycle has to be larger than $\kappa_{33}^2$.

The ratio between the sum of the converted energies (equations (7) and (12)) and the supplied energy (equation (13)) is given by

$$\frac{U_{\text{converted\_disconnected}} + U_{\text{converted\_shorted}}}{U_{\text{supplied}}} = 2\kappa_{33}^2 - \kappa_{33}^4$$

(25)
And indeed, since \( 0 < k_{33}^2 < 1 \), it follows that \( k_{33}^2 > k_{33}^2 \). The same \( k_{33}^2 \) will be obtained in a combined loading cycle in which the system is driven by electric flux, and some of the supplied energy is converted to the mechanical domain.

5.2. Plane-strain conditions

In a similar manner, the ratio between the converted energies (equations (17) and (21)) and the supplied energy (equation (22)) is given by

\[
\frac{E_{\text{converted, disconnected}} + E_{\text{converted, shorted}}}{E_{\text{supplied}}} = \frac{k_{33}^2 (2 + k_{33}^2)}{(1 + k_{33}^2)^2}
\]

(26)

Notice that, again, this value of the effective coupling factor for the combined cycle is larger than the coupling factor of the initially shorted electrodes cycle (or the initially disconnected electrodes cycle) under plane-strain conditions.

5.3. Interim conclusion 2

It is shown that the piezoelectric coupling factor \( k_{33}^2 \) can be enlarged, using a “smart” switching of the circuit connected to the piezoelectric structure. For both plane-stress and plane-strain conditions, we can use a combined cycle to convert (store) more mechanical energy than in the initially shorted cycle or in the initially disconnected cycle.

6. Discussion

Figure 5 presents a comparison between the coupling factor, \( k_{33}^2 \), and the non-dimensional mathematical coefficients ratio. The plot on the left is for plane-stress conditions (\( k_{33}^2 \)), and the plot on the right is for plane-strain conditions (\( k_{33}^2 \)). In each of these plots, the red dashed line relates to shorted or disconnected electrodes cycles, and the blue solid curve relates to the combined cycle. For simplicity, we will refer only to the initially shorted electrodes cycle, since the results for initially disconnected electrodes cycles are the same.

In the plane-stress problem (Figure 5, left), there is an identity between \( k_{33}^2 \) and \( k_{33}^2 \) for the shorted cycle, as was shown in Section 3. In contrast, for the plane-strain problem (Figure 5, right), we see that the coupling factor of the shorted cycle is smaller than \( k_{33}^2 \) in the entire domain.

For both plane-stress and plane-strain, \( k_{33}^2 \), for the combined cycle is always larger than \( k_{33}^2 \) of the shorted cycle. This means that the combined cycle enables to convert more energy than is commonly considered and clearly more than is suggested by \( k_{33}^2 \) or \( k_{33}^2 \).

In the plane-strain case, for values of \( k_{33}^2 < 0.618 \), the coupling factor \( k_{33}^2 \) is greater than \( k_{33}^2 \).
When comparing the combined cycles of the two problems, the coupling factor $k_{33}^2$ for the plane-stress case is larger than the coupling factor $k_{33}^2$ for the plane-strain case, for any given non-dimensional ratio ($\kappa_{33}^2$ or $\kappa_{33}$).

However, when comparing the coupling factor $k_{33}^2$ of the plane-stress and the plane-strain problems, we made no distinction between the non-dimensional ratios $\kappa_{33}^2$ and $\kappa_{33}^2$. Although the functional forms of all the previous equations are correct, it is worthwhile to emphasize that in general, $\kappa_{33}^2$ and $\kappa_{33}^2$ have distinctively different values. For example, in PZT-5A, $\kappa_{33}^2 = 0.494$, whereas $\kappa_{33}^2 = 0.307$ (Gautschi, 2002; Yang, 2006).

If the two non-dimensional ratios $\kappa_{33}^2$ and $\kappa_{33}^2$ were identical, then the plots in Figure 5 would suggest that a plane-stress condition is preferable to a plane-strain condition, in that it enables a higher energy ratio $k_{33}^2$.

There are two insights to be gained here:

1. Since we have shown that for PZT-5A, $k_{33}^2 > k_{33}^2$, it follows that a plane-stress condition is even more preferable to a plane-strain condition (compare the two plots in Figure 5).

2. For PZT-5A, and a given value of $S_3$, the supplied energy for plane-stress is proportional to $1/\kappa_{33}^2 = 0.053 \times 10^{12} \text{[Pa]}$ (i.e. $U_{\text{mech}} \propto 1/(\kappa_{33}^2)$) whereas the supplied energy for plane-strain is proportional to $C_{13}^E = 0.111 \times 10^{12} \text{[Pa]}$ (i.e. $U_{\text{mech}} \propto C_{13}^E S_3^2$). So this difference in supplied energy may work in favor of the plane-strain conditions.

In short, for each material, the superiority of plane-stress or plane-strain must be analyzed with care.

![Figure 6. The ratio between the coupling factor $k_{33}^2$ of the combined cycle and the coupling factor $k_{33}^2$ of the disconnected (or shorted) cycle in respect to the non-dimensional ratio $\kappa_{33}^2$ or $\kappa_{33}^2$. The coupling factor ratio for the plane-stress problem is marked with a dashed line, and for the plane-strain problem is marked with a dotted line.](image)

![Figure 7. A unimorph constructed from a thin piezoelectric layer (top layer) that is bonded to a thick elastic substrate (lower layer). When the structure is bent, the strains in $e_1$ and $e_2$ in the piezoelectric layer are not uniform, and are determined by the response of the structure as a whole.](image)
common in literature, was shown to be misleading. For plane-stress conditions, the identity between $k_{33}^2$ and $k_{33}^2$ holds. However, when the plane-strain conditions apply, the value of $k_{33}^2$ is smaller than $k_{33}^2$.

In any case, if we consider the combination of the two cycles of disconnected electrodes and shorted electrodes, then the transformed energy is larger than in either one of these cycles, and therefore, the coupling factor of the combined cycle is larger.

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