

Fundamentals of Piezoelectricity

Introductory Course on Multiphysics Modelling

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1 Introduction

1.1 The piezoelectric effects

Observed phenomenon

Piezoelectricity is the ability of some materials (notably crystals and certain ceramics) to generate an **electric charge** in response to applied **mechanical stress**. If the material is not short-circuited, the applied charge induces a **voltage** across the material.

Reversibility. The piezoelectric effect is reversible, that is, all piezoelectric materials exhibit in fact two phenomena:

1. **the direct piezoelectric effect** – the production of electricity when stress is applied,

- 2. the converse piezoelectric effect** – the production of stress and/or strain when an electric field is applied. (For example, lead zirconate titanate crystals will exhibit a maximum shape change of about 0.1% of the original dimension.)

Some historical facts and etymology

- The (direct) piezoelectric phenomenon was discovered in 1880 by the brothers Pierre and Jacques Curie during experiments on quartz.
- The existence of the reverse process was predicted by Lippmann in 1881 and then immediately confirmed by the Curies.
- The word *piezoelectricity* means “*electricity by pressure*” and is derived from the Greek *piezein*, which means to squeeze or press.

1.2 Simple molecular model of piezoelectric effect

Figure 1 presents a simple molecular model which – together with the discussion below – explains the direct piezoelectric effect.

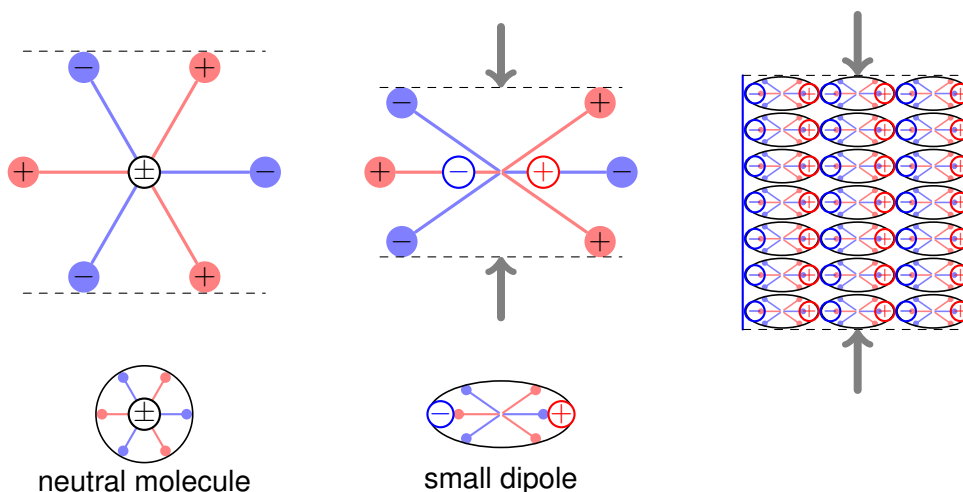


FIGURE 1: Simple molecular model for explaining the piezoelectric effect: an unperturbed molecule (*left*), the molecule subjected to an external force (*middle*), a polarizing effect on the material surfaces (*right*).

Before subjecting the material to some external stress (see Figure 1(*left*)):

- the centres of the negative and positive charges of each molecule coincide,
- the external effects of the charges are reciprocally cancelled,
- as a result, an electrically neutral molecule appears.

After exerting some pressure on the material (see Figure 1(*middle*)):

- the internal structure is deformed,

- that causes the separation of the positive and negative centres of the molecules,
- as a result, little dipoles are generated.

Eventually (see Figure 1(right)):

- the facing poles inside the material are mutually cancelled,
- a distribution of a linked charge appears in the material's surfaces and the material is polarized,
- the polarization generates an electric field and can be used to transform the mechanical energy of the material's deformation into electrical energy.

2 Equations of piezoelectricity

2.1 Piezoelectricity viewed as electro-mechanical coupling

Piezoelectricity is an electro-mechanical phenomenon which couples the elastic behaviour of a material to its behaviour as a dielectric, and all this is done through the piezoelectric effects (see Figure 2). Therefore, a mathematical model of piezoelectricity would consist of:

- (M) **mechanical equations** describing elastodynamics (or, in a particular case: elastostatics) of a linearly elastic material,
- (E) **electrical equations** describing electrostatic behaviour of a dielectric material.

Scalar, vector, and tensor quantities

In Table 1, all mathematical quantities used by the piezoelectric model are grouped together (mostly in pairs, relating a mechanical quantity to an electrical counterpart). Apart from the quantities relevant for elastodynamics (M) and electrostatics (E), the only additional one is the third-order tensor of piezoelectric material constants.

TABLE 1: Scalar, vector, and tensor quantities for piezoelectric equations

(M) – mechanical behaviour (E) – electrical behaviour ($i, j, k, l = 1, 2, 3$)

| | |
|--|--|
| (M) $u_i - \left[\frac{\text{m}}{\text{m}} \right]$ the mechanical displacements | (M) $f_i - \left[\frac{\text{N}}{\text{m}^3} \right]$ the mechanical body forces |
| (E) $\varphi - \left[\text{V} = \frac{\text{J}}{\text{C}} \right]$ the electric field potential | (E) $q - \left[\frac{\text{C}}{\text{m}^3} \right]$ the electric body charge |
| (M) $S_{ij} - \left[\frac{\text{m}}{\text{m}} \right]$ the strain tensor | (M) $\rho - \left[\frac{\text{kg}}{\text{m}^3} \right]$ the mass density |
| (E) $E_i - \left[\frac{\text{V}}{\text{m}} = \frac{\text{N}}{\text{C}} \right]$ the electric field vector | (M) $c_{ijkl} - \left[\frac{\text{N}}{\text{m}^2} \right]$ the elastic constants |
| (M) $T_{ij} - \left[\frac{\text{N}}{\text{m}^2} \right]$ the stress tensor | $e_{kij} - \left[\frac{\text{C}}{\text{m}^2} \right]$ the piezoelectric constants |
| (E) $D_i - \left[\frac{\text{C}}{\text{m}^2} \right]$ the electric displacements | (E) $\epsilon_{ij} - \left[\frac{\text{F}}{\text{m}} = \frac{\text{C}}{\text{Vm}} \right]$ the dielectric constants |

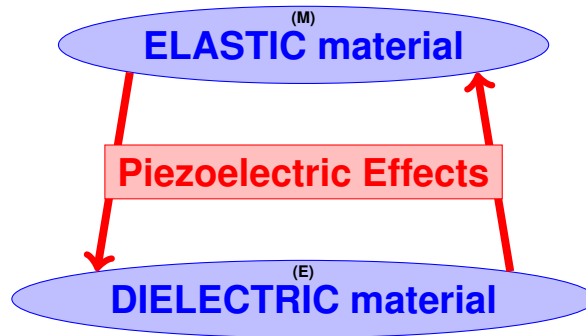


FIGURE 2: Piezoelectric effects couple the mechanical problem (M) of elastic material and the electrical problem (E) of dielectric into a multi-physics problem

2.2 Field equations of linear piezoelectricity

The field equations for the piezoelectric model are given below. They are governing equations for the mechanical (M) and electrical (E) sub-problems, namely: elastodynamics and electrostatics), coupled solely inside the constitutive relations.

Although the mechanical problem is modelled as fully dynamic (i.e., inertial forces are involved), its electrical counterpart is *quasi-static*, namely:

- it is assumed that the electric field changes in time sufficiently slowly, so that no significant magnetic field is induced;
- therefore, electrodynamic effects are *not* involved and purely electrostatic equations are used instead.

Remark: A slow change in time from the perspective of a quasi-static (piezo-)electric problem means, for example, time-harmonic variations up to tens of kilohertz, which is, in fact, rather fast from the mechanical “point of view”.

All field equations of piezoelectricity are presented here in the index notation and also in the “vector (bold-symbol) notation” – for the elasto-dynamic (electrically quasi-static) case. The fully static case is obtained by simply assuming that all fields do not depend on time. Then, the equations of motion (1) presented below are reduced to the static case by simply noting that the mechanical accelerations are zero, namely, $\ddot{u}_i \equiv 0$. The electrostatic equation (2) remains virtually the same.

(M) Equations of motion (*Elastodynamics*)

$$T_{ij|j} + f_i = \rho \ddot{u}_i \quad \text{or} \quad \nabla \cdot \mathbf{T} + \mathbf{f} = \rho \ddot{\mathbf{u}} \quad (1)$$

(E) Gauss' law (*Electrostatics*)

$$D_{i|i} - q = 0 \quad \text{or} \quad \nabla \cdot \mathbf{D} - q = 0 \quad (2)$$

The kinematic relations (3) define the strain tensor as a symmetric part of the gradient

of mechanical displacements, whereas the Maxwell's law (4) states that the electric vector field is the (negative) gradient of electric potential.

(M) Kinematic relations

$$S_{ij} = \frac{1}{2}(u_{i|j} + u_{j|i}) \quad \text{or} \quad \mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T) \quad (3)$$

(E) Maxwell's law

$$E_i = -\varphi_{|i} \quad \text{or} \quad \mathbf{E} = -\nabla \varphi \quad (4)$$

The **electro-mechanical coupling** appears *only* in the constitutive relations where the coupling terms involve the third-order tensor of piezoelectric coupling coefficients e_{kij} :

Constitutive equations – with piezoelectric coupling

$$T_{ij} = c_{ijkl} S_{kl} - e_{kij} E_k \quad \text{or} \quad \mathbf{T} = \mathbf{c} : \mathbf{S} - \mathbf{e}^T \cdot \mathbf{E} \quad (5)$$

$$D_k = e_{kij} S_{ij} + \epsilon_{ki} E_i \quad \text{or} \quad \mathbf{D} = \mathbf{e} : \mathbf{S} - \boldsymbol{\epsilon} \cdot \mathbf{E} \quad (6)$$

2.3 Boundary conditions

Boundary conditions in this electro-mechanical problem of piezoelectricity are “**uncoupled**”, in that way that the standard mechanical conditions are applied separately from the electrical conditions, and this also entails that the partition of boundary into disjunctive parts, dedicated to various *essential* and *natural* boundary conditions, can be done completely independently for mechanical and electrical sub-problems.

Boundary conditions (“uncoupled”)

| | (essential) | | (natural) | |
|------------------|---------------------------|----|--------------------------|-----|
| (M) mechanical : | $u_i = \hat{u}_i$ | or | $T_{ij} n_j = \hat{F}_i$ | (7) |
| (E) electrical : | $\varphi = \hat{\varphi}$ | or | $D_i n_i = -\hat{Q}$ | (8) |

$\hat{u}_i, \hat{\varphi}$ – the specified mechanical displacements [m] and electric potential [V]

\hat{F}_i, \hat{Q} – the specified surface forces $\left[\frac{\text{N}}{\text{m}^2}\right]$ and surface charge $\left[\frac{\text{C}}{\text{m}^2}\right]$

n_i – the outward unit normal vector components

2.4 Final set of partial differential equations

The kinematic relations (3) and Maxwell's law (4) were used for the constitutive equations, which were then used for the equations of motion (1) and Gauss' law (2), so that the only dependent variables left are the mechanical displacements u_i and electric potential φ – the primary dependent variables. The final set of piezoelectric equations is given below. It forms an Initial Boundary-Value Problem (IBVP) for the primary unknown fields, together with the boundary conditions (7) and (8), and the initial conditions (at time $t = 0$): $u_i(\mathbf{x}, t = 0) = u_i^0(\mathbf{x})$, $\dot{u}_i(\mathbf{x}, t = 0) = v_i^0(\mathbf{x})$ ($i = 1, 2, 3$), where u_i^0 and v_i^0 are the initial values for the fields of displacement and velocity.

Piezoelectric equations in primary dependent variables

Coupled field equations for mechanical displacement (\mathbf{u}) and electric potential (φ) in a piezoelectric medium are as follows:

$$-\rho \ddot{\mathbf{u}} + \nabla \cdot [\mathbf{c} : (\nabla \mathbf{u})] + \nabla \cdot [\mathbf{e} \cdot (\nabla \varphi)] + \mathbf{f} = \mathbf{0}, \quad (9)$$

$$\nabla \cdot [\mathbf{e} : (\nabla \mathbf{u})] - \nabla \cdot [\boldsymbol{\epsilon} \cdot (\nabla \varphi)] - q = 0; \quad (10)$$

or, in index notation and assuming constant material properties:

$$-\rho \ddot{u}_i + c_{ijkl} u_{k|l|j} + e_{kij} \varphi_{|kj} + f_i = 0 \quad [3 \text{ eqs. (in 3D)}], \quad (11)$$

$$e_{kij} u_{i|kj} - \epsilon_{kj} \varphi_{|kj} - q = 0 \quad [1 \text{ eq.}]. \quad (12)$$

In a general three-dimensional case, this system contains **4 partial differential equations** in **4 unknown fields** (4 DOFs in FE model), namely, three mechanical displacements and an electric potential:

$$u_i = ? \quad (i = 1, 2, 3), \quad \varphi = ?$$

3 Forms of constitutive law

3.1 Four forms of constitutive relations

There are **4 mathematically-equivalent forms of piezoelectric constitutive relations**, each one involves one of 4 different third-order tensors of piezoelectric coupling coefficients – see Table 2 and equations below.

1. Stress-Charge form:

$$\begin{aligned} \mathbf{T} &= \mathbf{c}_{E=0} : \mathbf{S} - \mathbf{e}^\top \cdot \mathbf{E}, \\ \mathbf{D} &= \mathbf{e} : \mathbf{S} + \boldsymbol{\epsilon}_{S=0} \cdot \mathbf{E}. \end{aligned} \quad (13)$$

TABLE 2: Forms of piezoelectric constitutive relations, related piezoelectric tensors, and the naming convention

| | Stress $\left[\frac{\text{N}}{\text{m}^2}\right]$ | Strain $\left[\frac{\text{m}}{\text{m}}\right]$ | |
|---|--|--|-------------|
| “Charge” $\left[\frac{\text{C}}{\text{m}^2}\right]$ | $T, D \xleftarrow[c_{E=0}, \epsilon_{S=0}]{e} (S, E)$ | $S, D \xleftarrow[s_{E=0}, \epsilon_{T=0}]{d} (T, E)$ | (“voltage”) |
| “Voltage” $\left[\frac{\text{V}}{\text{m}}\right]$ | $T, E \xleftarrow[c_{D=0}, \epsilon_{S=0}^{-1}]{q} (S, D)$ | $S, E \xleftarrow[s_{D=0}, \epsilon_{T=0}^{-1}]{g} (T, D)$ | (“charge”) |
| | (strain) | (stress) | |

2. *Stress-Voltage form:*

$$\begin{aligned} T &= c_{D=0} : S - \mathbf{q}^\top \cdot D, \\ E &= -\mathbf{q} : S + \epsilon_{S=0}^{-1} \cdot D. \end{aligned} \quad (14)$$

3. *Strain-Charge form:*

$$\begin{aligned} S &= s_{E=0} : T + \mathbf{d}^\top \cdot E, \\ D &= \mathbf{d} : T + \epsilon_{T=0} \cdot E. \end{aligned} \quad (15)$$

4. *Strain-Voltage form:*

$$\begin{aligned} S &= s_{D=0} : T + \mathbf{g}^\top \cdot D, \\ E &= -\mathbf{g} : T + \epsilon_{T=0}^{-1} \cdot D. \end{aligned} \quad (16)$$

Here, the following **tensors of constitutive coefficients** appear:

■ **fourth-order** tensors of **elastic** material constants:

stiffness $c \left[\frac{\text{N}}{\text{m}^2}\right]$, and *compliance* $s = c^{-1} \left[\frac{\text{m}^2}{\text{N}}\right]$, obtained in the absence of electric field ($E=0$) or charge ($D=0$);

■ **second-order** tensors of **dielectric** material constants:

electric permittivity $\epsilon \left[\frac{\text{F}}{\text{m}}\right]$, and its inverse $\epsilon^{-1} \left[\frac{\text{m}}{\text{F}}\right]$, obtained in the absence of mechanical strain ($S=0$) or stress ($T=0$);

■ **third-order** tensors of **piezoelectric** coupling coefficients:

$\mathbf{e} \left[\frac{\text{C}}{\text{m}^2}\right]$ – the piezoelectric coefficients for **Stress-Charge** form,

$\mathbf{q} \left[\frac{\text{m}^2}{\text{C}}\right]$ – the piezoelectric coefficients for **Stress-Voltage** form,

$\mathbf{d} \left[\frac{\text{C}}{\text{N}}\right]$ – the piezoelectric coefficients for **Strain-Charge** form,

$\mathbf{g} \left[\frac{\text{N}}{\text{C}}\right]$ – the piezoelectric coefficients for **Strain-Voltage** form.

3.2 Transformations for converting constitutive data

1. *Strain-Charge* \rightleftharpoons *Stress-Charge*:

$$c_{E=0} = s_{E=0}^{-1}, \quad e = d : s_{E=0}^{-1}, \quad \epsilon_{S=0} = \epsilon_{T=0} - d \cdot s_{E=0}^{-1} \cdot d^\top. \quad (17)$$

2. Strain-Charge \rightleftharpoons Strain-Voltage:

$$\mathbf{s}_{D=0} = \mathbf{s}_{E=0} - \mathbf{d}^\top \cdot \boldsymbol{\epsilon}_{T=0}^{-1} \cdot \mathbf{d}, \quad \mathbf{g} = \boldsymbol{\epsilon}_{T=0}^{-1} \cdot \mathbf{d}. \quad (18)$$

3. Strain-Charge \rightleftharpoons Stress-Voltage: ...

4. Stress-Charge \rightleftharpoons Stress-Voltage:

$$\mathbf{c}_{D=0} = \mathbf{c}_{E=0} - \mathbf{e}^\top \cdot \boldsymbol{\epsilon}_{S=0}^{-1} \cdot \mathbf{e}, \quad \mathbf{q} = \boldsymbol{\epsilon}_{S=0}^{-1} \cdot \mathbf{e}. \quad (19)$$

5. Stress-Charge \rightleftharpoons Strain-Voltage: ...

6. Strain-Voltage \rightleftharpoons Stress-Voltage:

$$\mathbf{c}_{D=0} = \mathbf{s}_{D=0}^{-1}, \quad \mathbf{q} = \mathbf{g} : \mathbf{s}_{D=0}^{-1}, \quad \boldsymbol{\epsilon}_{S=0}^{-1} = \boldsymbol{\epsilon}_{T=0}^{-1} + \mathbf{g} \cdot \mathbf{s}_{D=0}^{-1} \cdot \mathbf{g}^\top. \quad (20)$$

3.3 Piezoelectric relations in matrix notation

Rule of change of subscripts (Kelvin-Voigt notation)

$$11 \rightarrow 1, \quad 22 \rightarrow 2, \quad 33 \rightarrow 3, \quad 23 \rightarrow 4, \quad 13 \rightarrow 5, \quad 12 \rightarrow 6.$$

Using this rule the following *matrix notation* for relevant quantities is adopted:

$$\begin{aligned} T_{ij} &\rightarrow [T_\alpha]_{(6 \times 1)}, & S_{ij} &\rightarrow [S_\alpha]_{(6 \times 1)}, & E_i &\rightarrow [E_i]_{(3 \times 1)}, & D_i &\rightarrow [D_i]_{(3 \times 1)}, \\ c_{ijkl} &\rightarrow [c_{\alpha\beta}]_{(6 \times 6)}, & s_{ijkl} &\rightarrow [s_{\alpha\beta}]_{(6 \times 6)}, & \epsilon_{ij} &\rightarrow [\epsilon_{ij}]_{(3 \times 3)}, & \epsilon_{ij}^{-1} &\rightarrow [\epsilon_{ij}^{-1}]_{(3 \times 3)}, \\ e_{kij} &\rightarrow [e_{k\alpha}]_{(3 \times 6)}, & d_{kij} &\rightarrow [d_{k\alpha}]_{(3 \times 6)}, & q_{kij} &\rightarrow [q_{k\alpha}]_{(3 \times 6)}, & g_{kij} &\rightarrow [g_{k\alpha}]_{(3 \times 6)}. \end{aligned}$$

Here: $i, j, k, l = 1, 2, 3$, and $\alpha, \beta = 1, \dots, 6$. Exceptionally: $S_4 = 2S_{23}$, $S_5 = 2S_{13}$, $S_6 = 2S_{12}$.

Now, the constitutive relations can be written in the matrix notation as shown below for two cases.

■ Strain-Charge form:

$$\mathbf{S}_{(6 \times 1)} = \mathbf{s}_{(6 \times 6)} \mathbf{T}_{(6 \times 1)} + \mathbf{d}_{(6 \times 3)}^\top \mathbf{E}_{(3 \times 1)}, \quad (21)$$

$$\mathbf{D}_{(3 \times 1)} = \mathbf{d}_{(3 \times 6)} \mathbf{T}_{(6 \times 1)} + \boldsymbol{\epsilon}_{(3 \times 3)} \mathbf{E}_{(3 \times 1)}. \quad (22)$$

■ Stress-Charge form:

$$\mathbf{T}_{(6 \times 1)} = \mathbf{c}_{(6 \times 6)} \mathbf{S}_{(6 \times 1)} - \mathbf{e}_{(6 \times 3)}^\top \mathbf{E}_{(3 \times 1)}, \quad (23)$$

$$\mathbf{D}_{(3 \times 1)} = \mathbf{e}_{(3 \times 6)} \mathbf{S}_{(6 \times 1)} + \boldsymbol{\epsilon}_{(3 \times 3)} \mathbf{E}_{(3 \times 1)}. \quad (24)$$

For **orthotropic** piezoelectric materials there are $9 + 5 + 3 = 17$ material constants, and

the matrices of material constants read:

$$\mathbf{c}_{(6 \times 6)} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{22} & c_{23} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & \text{sym.} & & c_{44} & 0 & 0 \\ & & & & c_{55} & 0 \\ & & & & & c_{66} \end{bmatrix}, \quad (25)$$

$$\mathbf{e}_{(3 \times 6)} = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{24} & 0 & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{\epsilon}_{(3 \times 3)} = \begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}. \quad (26)$$

Many piezoelectric materials (e.g., PZT ceramics) can be treated as **transversally isotropic**. Then, there are only 10 material constants, since $4 + 2 + 1 = 7$ of the orthotropic constants depend on the others:

$$\begin{aligned} c_{22} &= c_{11}, & c_{23} &= c_{13}, & c_{55} &= c_{44}, & c_{66} &= \frac{c_{11} - c_{12}}{2}, \\ e_{24} &= e_{15}, & e_{32} &= e_{31}, & \epsilon_{22} &= \epsilon_{11}. \end{aligned} \quad (27)$$

4 Thermoelastic analogy

Thermal analogy approach

It is a simple but useful approximation of the converse piezoelectric effect based on the resemblance between the thermoelastic and converse piezoelectric constitutive equations.

The **stress vs. strain and voltage relation** (i.e., the first from the *Stress-Charge* form of piezoelectric constitutive equations), namely:

$$T_{ij} = c_{ijkl} S_{kl} - e_{mij} E_m = c_{ijkl} (S_{kl} - d_{mkl} E_m) \quad (\text{with } d_{mkl} = e_{mij} c_{ijkl}^{-1}) \quad (28)$$

resembles the Hooke's constitutive relation with initial strain S_{kl}^0 **or initial temperature** θ^0

$$T_{ij} = c_{ijkl} (S_{kl} - S_{kl}^0) = c_{ijkl} (S_{kl} - \alpha_{kl} \theta^0). \quad (29)$$

Thus, this **thermoelastic law** (or, simply, initial strains) can be used to **approximate** the converse **piezoelectric problem**. In this case the thermal expansion coefficients (or initial strains) are determined as

$$\alpha_{kl} = \frac{1}{\theta^0} S_{kl}^0 \quad \text{where} \quad S_{kl}^0 = d_{mkl} E_m = -d_{mkl} \varphi_{|m}. \quad (30)$$