Fundamentals of Piezoelectricity

Introductory Course on Multiphysics Modelling

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Outline

1. **Introduction**
   - The piezoelectric effects
   - Simple molecular model of piezoelectric effect

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Introduction: the piezoelectric effects

Observed phenomenon

Piezoelectricity is the ability of some materials 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.

Introduction: the piezoelectric effects

Observed phenomenon

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***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.

Introduction: the piezoelectric effects

Observed phenomenon

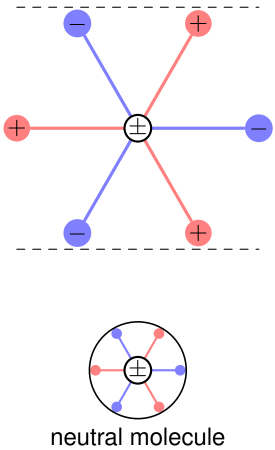
Piezoelectricity is the ability of some materials to generate an **electric charge** in response to applied **mechanical stress**. If the material is not short-circuited, the applied charge induces a **voltage** across the material.

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.

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.

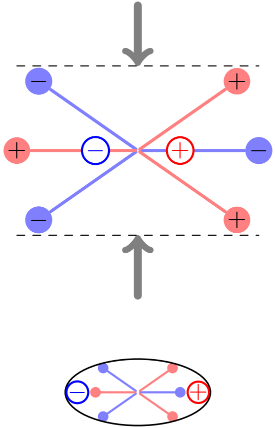
Introduction: a simple molecular model



Before subjecting the material to some external stress:

- 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.

Introduction: a simple molecular model

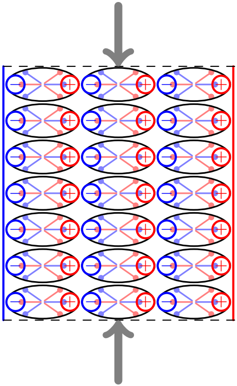


small dipole

After exerting some pressure on the material:

- 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.

Introduction: a simple molecular model



Eventually:

- 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.

Outline

Equations of piezoelectricity

Piezoelectricity viewed as electro-mechanical coupling

Scalar, vector, and tensor quantities

(M) – mechanical behaviour (E) – electrical behaviour

$(i, j, k, l = 1, 2, 3)$

(M) u_i – $[\mathrm{m}]$ the mechanical displacements

(E) φ – $\left[\mathrm{V} = \frac{\mathrm{J}}{\mathrm{C}}\right]$ the electric field potential

(M) S_{ij} – $\left[\frac{\mathrm{m}}{\mathrm{m}}\right]$ the strain tensor

(E) E_i – $\left[\frac{\mathrm{V}}{\mathrm{m}} = \frac{\mathrm{N}}{\mathrm{C}}\right]$ the electric field vector

(M) T_{ij} – $\left[\frac{\mathrm{N}}{\mathrm{m}^2}\right]$ the stress tensor

(E) D_i – $\left[\frac{\mathrm{C}}{\mathrm{m}^2}\right]$ the electric displacements

(M) f_i – $\left[\frac{\mathrm{N}}{\mathrm{m}^3}\right]$ the mechanical body forces

(E) q – $\left[\frac{\mathrm{C}}{\mathrm{m}^3}\right]$ the electric body charge

(M) ϱ – $\left[\frac{\mathrm{kg}}{\mathrm{m}^3}\right]$ the mass density

(M) c_{ijkl} – $\left[\frac{\mathrm{N}}{\mathrm{m}^2}\right]$ the elastic constants

(E) ϵ_{ij} – $\left[\frac{\mathrm{F}}{\mathrm{m}} = \frac{\mathrm{C}}{\mathrm{V\,m}}\right]$ the dielectric constants

(M)
ELASTIC material

+

(E)
DIELECTRIC material

Equations of piezoelectricity

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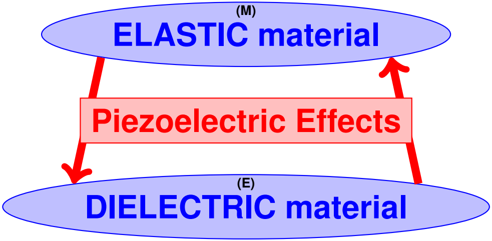

Equations of piezoelectricity

Field equations of linear piezoelectricity

Scalar, vector, and tensor quantities

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(M) Equations of motion
(*Elastodynamics*)

$$T_{ij|j} + f_i = \varrho\,\ddot{u}_i$$

(E) Gauss' law
(*Electrostatics*)

$$D_{i|i} - q = 0$$

Equations of piezoelectricity

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$$T_{ij|j} + f_i = \varrho\,\ddot{u}_i$$

(M) Kinematic relations

$$S_{ij} = \frac{1}{2}\left(u_{i|j} + u_{j|i}\right)$$

(E) Gauss' law (*Electrostatics*)

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(E) Maxwell's law

$$E_i = -\varphi_{|i}$$

Equations of piezoelectricity

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Constitutive equations – with Piezoelectric Effects

$$T_{ij} = c_{ijkl}\, S_{kl} - e_{kij}\, E_k$$

$$D_k = e_{kij}\, S_{ij} + \epsilon_{ki}\, E_i$$

ELECTROMECHANICAL COUPLING !

Equations of piezoelectricity

Boundary conditions

Scalar, vector, and tensor quantities

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Boundary conditions ("uncoupled")

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

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

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

n_i – the outward unit normal vector components

Equations of piezoelectricity

Final set of partial differential equations

Piezoelectric equations in primary dependent variables

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

$$-\varrho\,\ddot{\boldsymbol{u}} + \nabla\cdot\big[\boldsymbol{c} : (\nabla\boldsymbol{u})\big] + \nabla\cdot\big[\boldsymbol{e}\cdot(\nabla\varphi)\big] + \boldsymbol{f} = \boldsymbol{0}\,,$$

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

or, in index notation and assuming constant material properties:

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

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

Equations of piezoelectricity

Final set of partial differential equations

Piezoelectric equations in primary dependent variables

Coupled field equations:

$$-\varrho\,\ddot{\boldsymbol{u}} + \nabla\cdot\big[\boldsymbol{c} : (\nabla\boldsymbol{u})\big] + \nabla\cdot\big[\boldsymbol{e}\cdot(\nabla\varphi)\big] + \boldsymbol{f} = \boldsymbol{0}\,,$$

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

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:

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

Outline

Four forms of constitutive relations

	Stress $\left[\frac{\mathrm{N}}{\mathrm{m}^2}\right]$	*Strain* $\left[\frac{\mathrm{m}}{\mathrm{m}}\right]$	
"Charge" $\left[\frac{\mathrm{C}}{\mathrm{m}^2}\right]$	$\boldsymbol{T}, \boldsymbol{D} \xleftarrow[\boldsymbol{c}_{E=0},\ \boldsymbol{\epsilon}_{S=0}]{\boldsymbol{e}} (\boldsymbol{S}, \boldsymbol{E})$	$\boldsymbol{S}, \boldsymbol{D} \xleftarrow[\boldsymbol{s}_{E=0},\ \boldsymbol{\epsilon}_{T=0}]{\boldsymbol{d}} (\boldsymbol{T}, \boldsymbol{E})$	("voltage")
"Voltage" $\left[\frac{\mathrm{V}}{\mathrm{m}}\right]$	$\boldsymbol{T}, \boldsymbol{E} \xleftarrow[\boldsymbol{c}_{D=0},\ \boldsymbol{\epsilon}^{-1}_{S=0}]{\boldsymbol{q}} (\boldsymbol{S}, \boldsymbol{D})$	$\boldsymbol{S}, \boldsymbol{E} \xleftarrow[\boldsymbol{s}_{D=0},\ \boldsymbol{\epsilon}^{-1}_{T=0}]{\boldsymbol{g}} (\boldsymbol{T}, \boldsymbol{D})$	("charge")
	(strain)	(stress)	

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1. *Stress-Charge form*:

$$\boldsymbol{T} = \boldsymbol{c}_{E=0} : \boldsymbol{S} - \boldsymbol{e}^{\mathsf{T}} \cdot \boldsymbol{E} \,,$$

$$\boldsymbol{D} = \boldsymbol{e} : \boldsymbol{S} + \boldsymbol{\epsilon}_{S=0} \cdot \boldsymbol{E} \,.$$

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2. *Stress-Voltage form*:

$$\boldsymbol{T} = \boldsymbol{c}_{D=0} : \boldsymbol{S} - \boldsymbol{q}^{\mathsf{T}} \cdot \boldsymbol{D}\,,$$

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Four forms of constitutive relations

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3. *Strain-Charge form*:

$$\boldsymbol{S} = \boldsymbol{s}_{E=0} : \boldsymbol{T} + \boldsymbol{d}^{\mathsf{T}} \cdot \boldsymbol{E}\,,$$

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Four forms of constitutive relations

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4. *Strain-Voltage form*:

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Four forms of constitutive relations

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"Voltage" $\left[\frac{\mathrm{V}}{\mathrm{m}}\right]$	$\boldsymbol{T},\ \boldsymbol{E} \xleftarrow[\boldsymbol{c}_{\boldsymbol{D}=\mathbf{0}},\ \boldsymbol{\epsilon}^{-1}_{\boldsymbol{S}=\mathbf{0}}]{\boldsymbol{q}} (\boldsymbol{S},\ \boldsymbol{D})$	$\boldsymbol{S},\ \boldsymbol{E} \xleftarrow[\boldsymbol{s}_{\boldsymbol{D}=\mathbf{0}},\ \boldsymbol{\epsilon}^{-1}_{\boldsymbol{T}=\mathbf{0}}]{\boldsymbol{g}} (\boldsymbol{T},\ \boldsymbol{D})$	("charge")
	(strain)	(stress)	

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

- **fourth-order** tensors of **elastic** material constants: *stiffness* $\boldsymbol{c}$ $\left[\frac{\mathrm{N}}{\mathrm{m}^2}\right]$, and *compliance* $\boldsymbol{s} = \boldsymbol{c}^{-1}$ $\left[\frac{\mathrm{m}^2}{\mathrm{N}}\right]$, obtained in the absence of electric field ($_{\boldsymbol{E}=\mathbf{0}}$) or charge ($_{\boldsymbol{D}=\mathbf{0}}$);

Four forms of constitutive relations

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	(strain)	(stress)	

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

- **fourth-order** tensors of **elastic** material constants: *stiffness* $\boldsymbol{c}$ $\left[\frac{\mathrm{N}}{\mathrm{m}^2}\right]$, and *compliance* $\boldsymbol{s} = \boldsymbol{c}^{-1}$ $\left[\frac{\mathrm{m}^2}{\mathrm{N}}\right]$, obtained in the absence of electric field ($_{E=0}$) or charge ($_{D=0}$);
- **second-order** tensors of **dielectric** material constants: *electric permittivity* $\boldsymbol{\epsilon}$ $\left[\frac{\mathrm{F}}{\mathrm{m}}\right]$, and its inverse $\boldsymbol{\epsilon}^{-1}$ $\left[\frac{\mathrm{m}}{\mathrm{F}}\right]$, obtained in the absence of mechanical strain ($_{S=0}$) or stress ($_{T=0}$);

Four forms of constitutive relations

	Stress $\left[\frac{\mathrm{N}}{\mathrm{m}^2}\right]$	*Strain* $\left[\frac{\mathrm{m}}{\mathrm{m}}\right]$	
“Charge” $\left[\frac{\mathrm{C}}{\mathrm{m}^2}\right]$	$\boldsymbol{T},\,\boldsymbol{D} \xleftarrow[\boldsymbol{c}_{E=0},\ \boldsymbol{\epsilon}_{S=0}]{\boldsymbol{e}} (\boldsymbol{S},\,\boldsymbol{E})$	$\boldsymbol{S},\,\boldsymbol{D} \xleftarrow[\boldsymbol{s}_{E=0},\ \boldsymbol{\epsilon}_{T=0}]{\boldsymbol{d}} (\boldsymbol{T},\,\boldsymbol{E})$	(“voltage”)
“Voltage” $\left[\frac{\mathrm{V}}{\mathrm{m}}\right]$	$\boldsymbol{T},\,\boldsymbol{E} \xleftarrow[\boldsymbol{c}_{D=0},\ \boldsymbol{\epsilon}^{-1}_{S=0}]{\boldsymbol{q}} (\boldsymbol{S},\,\boldsymbol{D})$	$\boldsymbol{S},\,\boldsymbol{E} \xleftarrow[\boldsymbol{s}_{D=0},\ \boldsymbol{\epsilon}^{-1}_{T=0}]{\boldsymbol{g}} (\boldsymbol{T},\,\boldsymbol{D})$	(“charge”)
	(strain)	(stress)	

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

- **third-order** tensors of **piezoelectric** coupling coefficients:
  - $\boldsymbol{e}$ $\left[\frac{\mathrm{C}}{\mathrm{m}^2}\right]$ – the piezoelectric coefficients for ***Stress-Charge*** form,
  - $\boldsymbol{q}$ $\left[\frac{\mathrm{m}^2}{\mathrm{C}}\right]$ – the piezoelectric coefficients for ***Stress-Voltage*** form,
  - $\boldsymbol{d}$ $\left[\frac{\mathrm{C}}{\mathrm{N}}\right]$ – the piezoelectric coefficients for ***Strain-Charge*** form,
  - $\boldsymbol{g}$ $\left[\frac{\mathrm{N}}{\mathrm{C}}\right]$ – the piezoelectric coefficients for ***Strain-Voltage*** form.

Transformations for converting constitutive data

1. *Strain-Charge* $\rightleftarrows$ *Stress-Charge*:

$$\boldsymbol{c}_{E=0} = \boldsymbol{s}_{E=0}^{-1}\,, \qquad \boldsymbol{e} = \boldsymbol{d} : \boldsymbol{s}_{E=0}^{-1}\,, \qquad \boldsymbol{\epsilon}_{S=0} = \boldsymbol{\epsilon}_{T=0} - \boldsymbol{d} \cdot \boldsymbol{s}_{E=0}^{-1} \cdot \boldsymbol{d}^{\mathsf{T}}\,.$$

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2. *Strain-Charge* $\rightleftarrows$ *Strain-Voltage*:

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Piezoelectric relations in matrix notation

Rule of change of subscripts (Kelvin-Voigt notation)

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

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

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- *Strain-Charge* form:

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Matrix notation of constitutive relations

For **orthotropic** piezoelectric materials there are $9+5+3=17$ material constants, and the matrices of material constants read:

$$\mathbf{c}_{(6\times6)} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{22} & c_{23} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & \text{sym.} & & & c_{55} & 0 \\ & & & & & c_{66} \end{bmatrix},$$

$$\mathbf{e}_{(3\times6)} = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{24} & 0 & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & 0 \end{bmatrix}, \qquad \boldsymbol{\epsilon}_{(3\times3)} = \begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}.$$

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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:

$$c_{22} = c_{11}\,, \quad c_{23} = c_{13}\,, \quad c_{55} = c_{44}\,, \quad c_{66} = \frac{c_{11}-c_{12}}{2}\,,$$

$$e_{24} = e_{15}\,, \quad e_{32} = e_{31}\,, \qquad \epsilon_{22} = \epsilon_{11}\,.$$

Outline

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Thermal analogy approach

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

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

$$T_{ij} = c_{ijkl}\big(S_{kl} - S^0_{kl}\big) = c_{ijkl}\big(S_{kl} - \alpha_{kl}\,\theta^0\big)\,.$$

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$$T_{ij} = c_{ijkl}\big(S_{kl} - S^0_{kl}\big) = c_{ijkl}\big(S_{kl} - \alpha_{kl}\,\theta^0\big)\,.$$

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

$$\alpha_{kl} = \frac{1}{\theta^0} S^0_{kl} \quad \text{where} \quad S^0_{kl} = d_{mkl}\,E_m = -d_{mkl}\,\varphi_{|m}\,.$$