

Hysteresis in Piezoelectric Ceramics

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Introduction

Many piezoelectric materials are ferroelectric. Ferroelectric materials exhibit nonlinear polarization behavior such as hysteresis and saturation at large applied electric fields. In addition, the polarization and mechanical deformations in such materials can be strongly coupled due to the electrostriction effect. This model uses Ferroelectroelasticity interface to analyze a simple actuator made of PZT piezoelectric ceramic material, which is subjected to applied electric field and mechanical load.

Model Definition

The direct electrostrictive effect for a material of arbitrary symmetry can be represented as the following additive contribution to the strain:

$$\varepsilon_{\rm em} = \mathbf{Q} : (\mathbf{P} \otimes \mathbf{P})$$

which is quadratic in polarization **P**. Due to the symmetry, the fourth order tensor **Q** can be effectively represented by a 6-by-6 coupling matrix. For piezoelectric ceramics, the matrix can be characterized by three independent components: Q_{11} , Q_{12} , and Q_{44} .

For ferroelectroelastic materials, the polarization vector is nonlinear function of the electric field and possible mechanical stress in the material. The Jiles–Atherton model is available in COMSOL Multiphysics for modeling ferroelectric hysteresis. It assumes that the total polarization can be represented as a sum of reversible and irreversible parts. The polarization change is computed from the following incremental equation:

$$d\mathbf{P} = c_r d\mathbf{P}_{an} + (\mathbf{I} - c_r) d\mathbf{P}_{irr}$$

where the reversibility is characterized by the parameter c_r , and the anhysteretic polarization is found from a relation:

$$\mathbf{P}_{an} = P_{s}L(|\mathbf{E}_{eff}|) \frac{\mathbf{E}_{eff}}{|\mathbf{E}_{eff}|}$$

where P_s is the saturation polarization. The polarization shape is characterized by the Langevin function

$$L = \operatorname{coth}\left(\frac{|\mathbf{E}_{eff}|}{a}\right) - \frac{a}{|\mathbf{E}_{eff}|}$$

where a is a material parameter called the domain wall density.

The effective electric field is given by

$$\mathbf{E}_{\text{eff}} = \mathbf{E} + \alpha \mathbf{P} + 2(\boldsymbol{\sigma}_{\text{m}} : \mathbf{Q})\mathbf{P}$$
(1)

where **E** is the applied electric field, α is a material parameter called the inter-domain coupling, and the mechanics stress is computed assuming mechanically linear material as

$$\sigma_{\rm m}$$
 = C : ($\epsilon - \epsilon_{\rm em}$)

where C is the fourth order elasticity tensor. The last term in Equation 1 represents the inverse electrostrictive effect.

Finally, the change of the irreversible polarization is computed from the following incremental relation:

$$d\mathbf{P}_{irr} = \max(\zeta \cdot d\mathbf{E}_{eff}, 0) \frac{\zeta}{|\zeta|}$$
$$\zeta = k_p^{-1} (\mathbf{P}_{an} - \mathbf{P}_{irr})$$

where the pinning loss is characterized by the parameter k_{p} .

The ferroelectroelastic actuator in this model example is a rectangular plate with dimensions of 1.5 in-by-0.25 in-by-0.015 in, which is composed of PZT-5H piezoelectric ceramic material. The following polarization parameter values have been estimated in Ref. 1 based on experimental data:

MATERIAL PROPERTY	VALUE	DESCRIPTION
Ps	0.425 C/m ²	Saturation polarization
a	6.410 ⁵ V/m	Domain wall density
α	4.2·10 ⁶ m/F	Inter-domain coupling
c _r	0.2	Polarization reversibility
k _p	I∙10 ⁶ V/m	Pinning loss

TABLE I: MATERIAL PROPERTIES OF PZT-5H.

The mechanical properties for PZT-5H are available in the Material Library of COMSOL.

The coupling coefficients for PZT ceramics can vary with the material composition and temperature. The reference values used in this example are give in the table below (Ref. 2):

MATERIAL PROPERTY	VALUE
Q_{11}	3.579·10 ⁻² m ⁴ /C ²
Q_{12}	-5.33510 ⁻³ m ⁴ /C ²
Q_{44}	1.923·10 ⁻² m ⁴ /C ²

TABLE 2: ELECTROSTRICTIVE COUPLING COEFFICIENTS.

The upper surface of the actuator is grounded, while the lower one is subjected to an electric potential that can cyclically vary in small increments between $-V_{max}$ and $+V_{max}$.

The actuator can be subjected to a compressive stress by applying boundary loads of various magnitude.

Because of the symmetry, it is sufficient to model one quarter of the actual geometry.



Figure 1: Model geometry.

Because of the large aspect ratio of the actuator and the unidirectional nature of the electrical and mechanical loading, a course mesh can be used for the discretization.





Results and Discussion

Three full cycles have been computed for each value of V_{max} . The variation of polarization and electrostrictive strain is studied at the point in the middle of the actuator. The first cycle includes the initial transient, Figure 3 and Figure 4. The hysteresis loops become fully established after two full cycles, Figure 5 and Figure 6.

Finally, Figure 7 and Figure 8 show the effect of the applied compressive stress.



Figure 3: Polarization hysteresis loop including the initial transient for the maximum applied voltage of 600 V.



Figure 4: Electrostrictive strain hysteresis loop including the initial transient for the maximum applied voltage of 600 V.



Figure 5: Polarization hysteresis loops fully established after two initial cycles for different values of the maximum applied voltage.



Figure 6: Electrostrictive strain hysteresis loops fully established after two initial cycles for different values of the maximum applied voltage.



Figure 7: Fully established polarization hysteresis loops for different values of the mechanical load and maximum applied voltage of 1200 V.



Figure 8: Fully established strain hysteresis loops for different values of the mechanical load and maximum applied voltage of 1200 V.

In this example, you study the hysteresis with respect to the incremental variation of the applied electric potential using a stationary parametric study. The same hysteresis model can be also used for time dependent studies.

References

1. R.C. Smith and Z. Ounaies. "A Domain Wall Model for Hysteresis in Piezoelectric Materials," *J. Int. Mat. Sys. Struct.*, vol. 11, no. 1, pp. 62–79, 2000.

2. B. Völker, P. Marton, C. Elsässer, and M. Kamlah, "Multiscale modeling for ferroelectric materials: a transition from the atomic level to phase-field modeling," *Continuum Mech. Thermodyn.*, vol. 23, pp. 435–451, 2011.

Application Library path: Structural_Mechanics_Module/ Piezoelectric_Effects/piezoelectric_hysteresis

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 间 3D.
- 2 In the Select Physics tree, select Structural Mechanics>Electromagnetics-Structure Interaction>Ferroelectroelasticity.
- 3 Click Add.
- 4 Click 🔿 Study.
- 5 In the Select Study tree, select General Studies>Stationary.
- 6 Click 🗹 Done.

GLOBAL DEFINITIONS

Parameters 1

Define parameters for the geometry, material properties, and applied voltage and mechanical load.

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
t	0[s]	0 s	Time parameter
W	1.5[in]	0.0381 m	Actiator width
D	0.25[in]	0.00635 m	Actuator depth
Н	0.015[in]	3.81E-4 m	Actuator height
alpha	4.2e6[m/F]	4.2E6 m/F	Inter-domain coupling
а	6.4e5[V/m]	6.4E5 V/m	Domain wall density
С	0.2	0.2	Polarization reversibility
k	1e6[V/m]	IE6 V/m	Pinning loss
Ps	0.425[C/ m^2]	0.425 C/ m ²	Saturation polarization
Q11	3.579e- 2[m^4/C^2]	0.03579 m^4/C ²	Electrostriction coupling parameter
Q12	-5.335e- 3[m^4/C^2]	-0.005335 m^4/C ²	Electrostriction coupling parameter
Q44	1.923e- 2[m^4/C^2]	0.01923 m^4/C²	Electrostriction coupling parameter
Vmax	1200[V]	1200 V	Maximum applied voltage
F0	O[MPa]	0 Pa	Applied mechanical load

DEFINITIONS

Variables I

- I In the Model Builder window, under Component I (compl) right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, locate the Variables section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
V0	Vmax*sin(2*pi*t[1/s])	V	Applied voltage

This variation of the potential with respect to the parameter at one of the actuator boundaries will cause the electric field within the material to gradually change between -Vmax and Vmax.

GEOMETRY I

Block I (blkI)

I In the **Geometry** toolbar, click **[]** Block.

Because of the symmetry, it is sufficient to model one quarter of the actuator.

- 2 In the Settings window for Block, locate the Size and Shape section.
- **3** In the **Width** text field, type W/2.
- 4 In the **Depth** text field, type D/2.
- 5 In the **Height** text field, type H/2.
- 6 Click 🟢 Build All Objects.

SOLID MECHANICS (SOLID)

Linear Elastic Material I

You will prescribe the material stiffness using the data available in the material library for PZT-5H, which is represented by the whole elasticity matrix.

- I In the Model Builder window, under Component I (comp1)>Solid Mechanics (solid) click Linear Elastic Material I.
- **2** In the **Settings** window for **Linear Elastic Material**, locate the **Linear Elastic Material** section.
- 3 From the Solid model list, choose Anisotropic.
- 4 From the Material data ordering list, choose Voigt (11, 22, 33, 23, 13, 12).

ELECTROSTATICS (ES)

Charge Conservation, Ferroelectric 1

I In the Model Builder window, under Component I (compl)>Electrostatics (es) click Charge Conservation, Ferroelectric I.

- 2 In the Settings window for Charge Conservation, Ferroelectric, locate the Ferroelectric Material Properties section.
- 3 Select the Hysteresis Jiles-Atherton model check box.

MATERIALS

In the Home toolbar, click 📑 Windows and choose Add Material from Library.

ADD MATERIAL

- I Go to the Add Material window.
- 2 In the tree, select Built-in>Lead Zirconate Titanate (PZT-5H).

3 Click **a** Add to Component I (compl).

MATERIALS

Lead Zirconate Titanate (PZT-5H) (mat1)

Define the remaining ferroelectric properties for the material using the parameters.

- I In the Model Builder window, under Component I (compl)>Materials click Lead Zirconate Titanate (PZT-5H) (matl).
- 2 In the Settings window for Material, locate the Material Contents section.
- **3** In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Saturation polarization	Psat	Ps	C/m²	Ferroelectric
Inter-domain coupling	alphaJAe_iso ; alphaJAeii = alphaJAe_iso, alphaJAeij = 0	alpha	m/F	Ferroelectric
Domain wall density	aJAe_iso ; aJAeii = aJAe_iso, aJAeij = 0	a	V/m	Ferroelectric
Pinning loss	kJAe_iso ; kJAeii = kJAe_iso, kJAeij = 0	k	V/m	Ferroelectric
Polarization reversibility	cJAe_iso ; cJAeii = cJAe_iso, cJAeij = 0	С	I	Ferroelectric

SOLID MECHANICS (SOLID)

In the Model Builder window, under Component I (compl) click Solid Mechanics (solid).

Symmetry I

- I In the Physics toolbar, click 📄 Boundaries and choose Symmetry.
- **2** Select Boundaries 1–3 only.

Boundary Load I

- I In the Physics toolbar, click 🔚 Boundaries and choose Boundary Load.
- **2** Select Boundary 4 only.
- 3 In the Settings window for Boundary Load, locate the Force section.
- **4** Specify the \mathbf{F}_{A} vector as



ELECTROSTATICS (ES)

In the Model Builder window, under Component I (compl) click Electrostatics (es).

Ground I

- I In the Physics toolbar, click 🔚 Boundaries and choose Ground.
- **2** Select Boundary 4 only.

Electric Potential I

- I In the Physics toolbar, click 🔚 Boundaries and choose Electric Potential.
- 2 Select Boundary 3 only.

Because of the symmetry, the voltage at the horizontal symmetry plane equals to a half of that applied at the bottom surface.

- 3 In the Settings window for Electric Potential, locate the Electric Potential section.
- **4** In the V_0 text field, type V0/2.

MULTIPHYSICS

Electrostriction I (efe I)

You study the electrostriction in the material using a fully coupled model.

I In the Model Builder window, under Component I (compl)>Multiphysics click Electrostriction I (efel).

- 2 In the Settings window for Electrostriction, locate the Coupling Type section.
- **3** From the list, choose **Fully coupled**.

Because of certain symmetry in the material microstructure, you need three parameters to characterize the electrostrictive coupling.

- 4 Locate the Electrostriction section. From the Solid model list, choose Cubic crystal.
- **5** In the Q_{11} text field, type Q11.
- 6 In the Q_{12} text field, type Q12.
- 7 In the Q_{44} text field, type Q44.

MESH I

Mapped I

- I In the Mesh toolbar, click \bigwedge Boundary and choose Mapped.
- **2** Select Boundary 4 only.

Size

- I In the Model Builder window, click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 From the **Predefined** list, choose **Coarse**.

Swept I

In the Mesh toolbar, click As Swept.

Distribution I

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Distribution section.
- 3 In the Number of elements text field, type 2.
- 4 Click 📗 Build All.

STUDY I

Step 1: Stationary

In the first study, no mechanical load is assumed, so that the entire excitation is via the applied electric field.

- I In the Model Builder window, under Study I click Step I: Stationary.
- 2 In the Settings window for Stationary, click to expand the Study Extensions section.
- **3** Select the **Auxiliary sweep** check box.

4 Click + Add.

You compute three full cycles for the applied electric potential for each given maximum value.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
t (Time parameter)	range(0,0.005,3)	S

Parametric Sweep

- I In the Study toolbar, click **Parametric Sweep**.
- 2 In the Settings window for Parametric Sweep, locate the Study Settings section.
- 3 Click + Add.
- **4** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vmax (Maximum applied	600 1000 1600	V
voltage)		

5 In the **Study** toolbar, click **= Compute**.

RESULTS

Polarization

- I In the Home toolbar, click 📠 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Polarization in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study I/ Parametric Solutions I (sol2).
- 4 Locate the Grid section. Select the Manual spacing check box.
- **5** In the **y** spacing text field, type **0.1**.
- 6 Locate the Legend section. From the Position list, choose Lower right.

Point Graph 1

- I Right-click Polarization and choose Point Graph.
- **2** Select Point 1 only.
- 3 In the Settings window for Point Graph, locate the y-Axis Data section.
- 4 In the **Expression** text field, type es.PZ.
- 5 Locate the x-Axis Data section. From the Parameter list, choose Expression.

- 6 In the Expression text field, type es.EZ.
- 7 From the Unit list, choose MV/m.
- 8 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Point** check box.
- 9 Select the Show legends check box.
- **IO** In the **Polarization** toolbar, click **IO Plot**.

Electrostriction

- I In the Model Builder window, right-click Polarization and choose Duplicate.
- 2 In the Settings window for ID Plot Group, type Electrostriction in the Label text field.
- 3 Locate the Grid section. In the y spacing text field, type 0.001.

Point Graph 1

- I In the Model Builder window, expand the Electrostriction node, then click Point Graph I.
- 2 In the Settings window for Point Graph, locate the y-Axis Data section.
- 3 In the **Expression** text field, type efe1.emZZ.
- **4** In the **Electrostriction** toolbar, click **I Plot**.

ROOT

In the Home toolbar, click 📑 Windows and choose Add Study.

ADD STUDY

I Go to the Add Study window.

Add one more stationary study to analyze the mechanical load effect.

- 2 Find the Studies subsection. In the Select Study tree, select General Studies>Stationary.
- 3 Click + Add Study.

STUDY 2

Step 1: Stationary

- I In the Model Builder window, under Study 2 click Step I: Stationary.
- 2 In the Settings window for Stationary, locate the Study Extensions section.
- **3** Select the **Auxiliary sweep** check box.
- 4 Click + Add.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
t (Time parameter)	range(0,0.005,3)	S

Parametric Sweep

- I In the Study toolbar, click **Parametric Sweep**.
- 2 In the Settings window for Parametric Sweep, locate the Study Settings section.
- 3 Click + Add.
- **4** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
F0 (Applied mechanical load)	0 -25 -50	MPa

5 In the **Study** toolbar, click **= Compute**.

RESULTS

Polarization 1

- I In the Model Builder window, right-click Polarization and choose Duplicate.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Dataset list, choose Study 2/Parametric Solutions 2 (sol7).
- 4 In the Polarization I toolbar, click **I** Plot.

Strain

- I In the Model Builder window, right-click Electrostriction and choose Duplicate.
- 2 In the Settings window for ID Plot Group, type Strain in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 2/ Parametric Solutions 2 (sol7).
- **4** In the **Strain** toolbar, click **I** Plot.

Point Graph 1

- I In the Model Builder window, expand the Strain node, then click Point Graph I.
- 2 In the Settings window for Point Graph, locate the y-Axis Data section.
- 3 In the **Expression** text field, type solid.eZZ.

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