Created in COMSOL Multiphysics 6.1

Hysteresis in Ferroelectric Material

Introduction

Ferroelectric materials exhibit nonlinear polarization behavior such as hysteresis and saturation at large applied electric fields. Many piezoelectric materials are ferroelectric. This model analyzes a simple actuator made of a PZT piezoelectric ceramic material, which is subjected to an applied electric field.

Model Definition

In its ferroelectric phase, the material exhibits spontaneous polarization, so that it is constituted of domains with nonzero polarization even at zero applied field. The application of an electric field can rearrange the domains, resulting in a net polarization in the material. At very large electric fields, the polarization saturates, as all ferroelectric domains in the material are aligned along the direction of the applied field. Domain wall interactions can also lead to a significant hysteresis in the polarization.

The Jiles–Atherton hysteresis model for ferroelectric materials is available in COMSOL Multiphysics. It assumes that the total polarization can be represented as a sum of reversible and irreversible parts. The polarization change is computed from the incremental equation

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

where the reversibility is characterized by the parameter $\mathrm{c_r}$, and the anhysteretic polarization is found from the relation

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

where P_{s} is the saturation polarization. The effective electric field is given by

$$\mathbf{E}_{\mathrm{eff}} = \mathbf{E} + \alpha\mathbf{P} \qquad (1)$$

where α is a material parameter called the inter-domain coupling. The polarization shape is characterized by the Langevin function

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

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

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

$$d\mathbf{P}_{\mathrm{irr}} = \max(\zeta \cdot d\mathbf{E}_{\mathrm{eff}}, 0)\frac{\zeta}{|\zeta|}$$

$$\zeta = \mathrm{k}_{\mathrm{p}}^{-1}(\mathbf{P}_{\mathrm{an}} - \mathbf{P}_{\mathrm{irr}})$$

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

The ferroelectric actuator in this model is a simple disk with the radius of 0.5 in and thickness of 0.01 in, which is composed of PZT-5A piezoelectric ceramic material. The following parameter values have been estimated in Ref. 1 based on experimental data:

TABLE 1: MATERIAL PROPERTIES OF PZT-5A.

MATERIAL PROPERTY	VALUE	DESCRIPTION
P_s	0.49 C/m^2	Saturation polarization
a	$4.4 \cdot 10^5$ V/m	Domain wall density
α	$3.6 \cdot 10^6$ m/F	Inter-domain coupling
c_r	0.18	Polarization reversibility
k_{p}	$1.9 \cdot 10^6$ V/m	Pinning loss

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 $-V_{\mathrm{max}}$ and $+V_{\mathrm{max}}$.

The actuator is surrounded by air. Because of the symmetry, it is sufficient to model only the upper half of the setup.

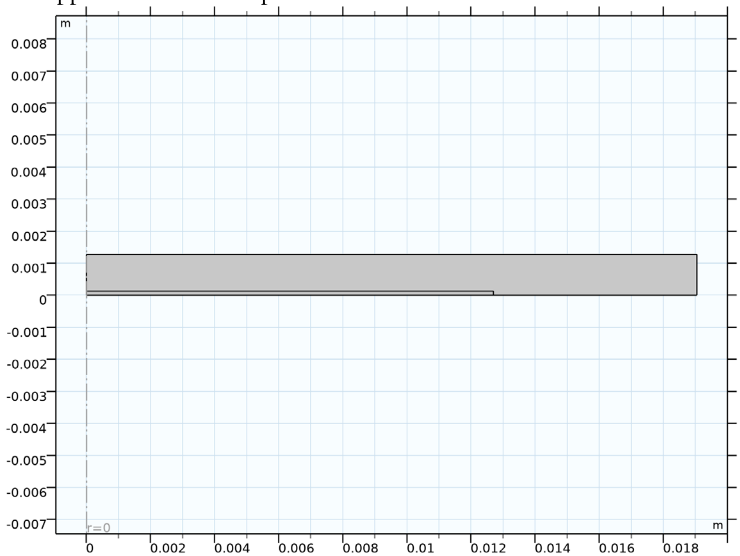

Figure 1: Model geometry. The smaller domain represents the upper half of the ferroelectric actuator. The larger domain is used for modeling the surrounding air.

Because of the actuator aspect ratio, a relatively coarse mesh can be used everywhere except in the regions near the disk edge.

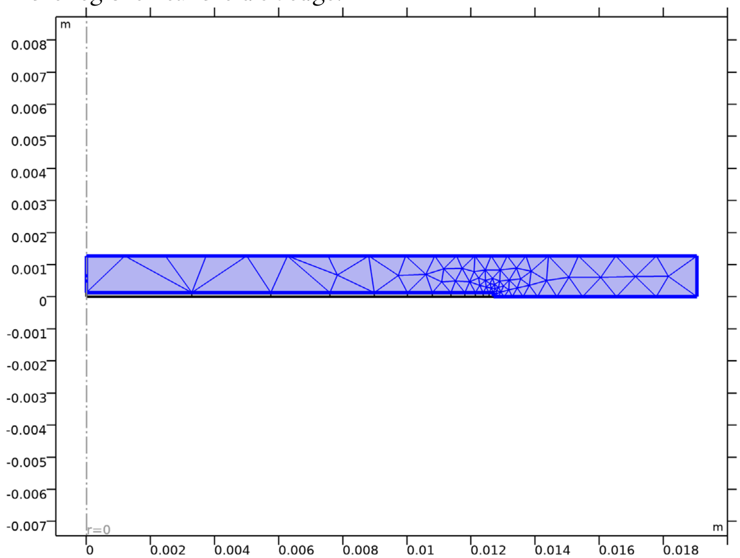

Figure 2: Model mesh.

Results and Discussion

The typical distribution of the electric potential is show in Figure 3.

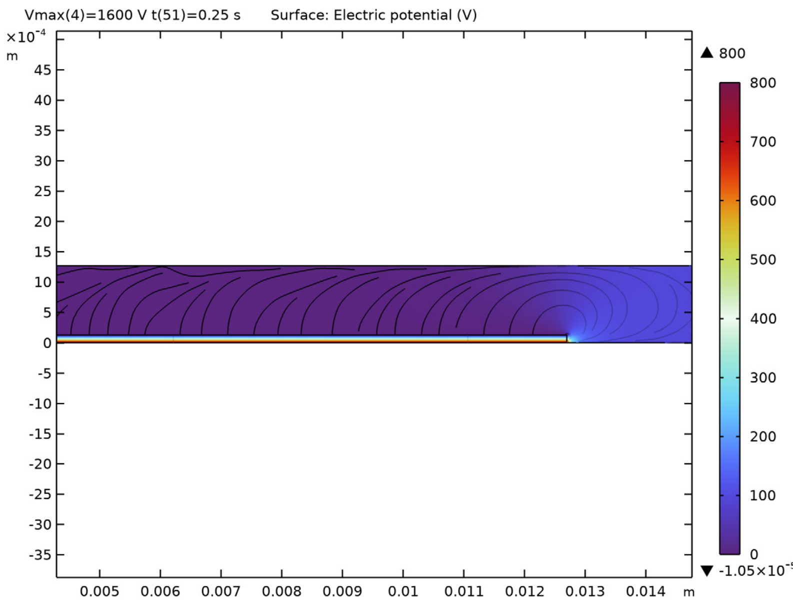

Figure 3: Electric potential field.

Four full cycles have been computed for each value of V_{max}. The polarization variation is studied at the point in the middle of the actuator.

The first cycle includes the initial transient; see Figure 4. The hysteresis loops become fully established after three full cycles; see Figure 5. The results agree well with those presented in Ref. 1.

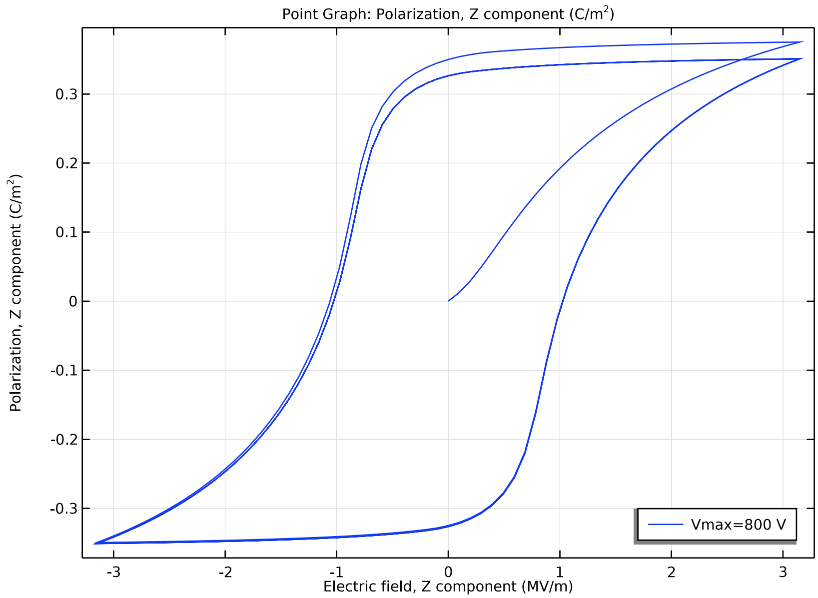

Figure 4: Hysteresis loop including the initial transient for the maximum applied voltage of 800 V.

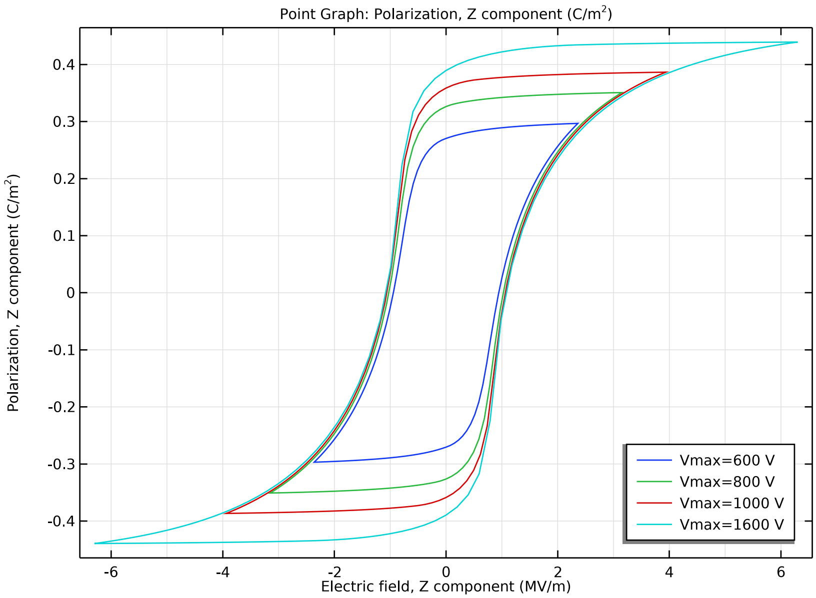

Figure 5: Hysteresis loops fully established after three cycles for different values of the maximum applied voltage.

Notes About the COMSOL Implementation

The Ferroelectric dielectric model option becomes available in any Charge Conservation feature under Electrostatics interface as soon as the material type for that feature is set to Solid.

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.

Reference

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.

Application Library path: `ACDC_Module/Devices,_Capacitive/ferroelectric_hysteresis`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **AC/DC>Electric Fields and Currents>Electrostatics (es)**.

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.

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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
H0	0.01[in]	2.54E-4 m	Actuator thickness
R0	0.5[in]	0.0127 m	Actuator radius
Vmax	1600[V]	1600 V	Maximum applied voltage
alpha	3.6e6[m/F]	3.6E6 m/F	Interdomain coupling
a	4.4e5[V/m]	4.4E5 V/m	Domain wall density
c	0.18	0.18	Polarization reversibility

Name	Expression	Value	Description
k	1.9e6[V/m]	1.9E6 V/m	Pinning loss
Ps	0.49[C/m^2]	0.49 C/m²	Saturation polarization

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** 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 change at the frequency of 1 Hz.

GEOMETRY 1

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type R0.

Because of the symmetry, it is sufficient to model only the upper half of the actuator.

4 In the **Height** text field, type H0/2.

Rectangle 2 (r2)

1 Right-click **Rectangle 1 (r1)** and choose **Duplicate**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type 1.5*R0.

4 In the **Height** text field, type 5*H0.

5 Click **Build All Objects**.

ELECTROSTATICS (ES)

The default Charge Conservation feature will be used for modeling the air domain. Add one more such feature to model the ferroelectric material.

Charge Conservation: PZT5A

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electrostatics (es)** and choose **Charge Conservation**.

You need to set the feature material type to solid to be able to select a ferroelectric type of the constitutive model.

2 In the **Settings** window for **Charge Conservation**, type `Charge Conservation: PZT5A` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **Material Type** section. From the **Material type** list, choose **Solid**.

5 Locate the **Constitutive Relation D-E** section. From the **Dielectric model** list, choose **Ferroelectric**.

6 Locate the **Ferroelectric Material Properties** section. Select the **Hysteresis Jiles–Atherton model** check box.

Ground 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Ground**.

2 Select Boundary 4 only.

Electric Potential 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Potential**.

Because of the symmetry, you set the potential at the symmetry boundary to a half of that applied to the whole actuator.

2 Select Boundary 2 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the V_0 text field, type `V0/2`.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Built-in>Air**.

4 Right-click and choose **Add to Component 1 (comp1)**.

5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Air (mat1)

Select Domain 2 only.

PZT5A

1 In the **Model Builder** window, right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, type `PZT5A` in the **Label** text field.

3 Select Domain 1 only.

Define the ferroelectric properties for the material using the parameters.

4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Saturation polarization	Psat	`Ps`	C/m^2	Ferroelectric
Interdomain 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	`c`	1	Ferroelectric

MESH 1

Mapped 1

1 In the **Mesh** toolbar, click **Mapped**.

2 In the **Settings** window for **Mapped**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 1 only.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.
2 In the **Settings** window for **Distribution**, locate the **Distribution** section.
3 In the **Number of elements** text field, type `1`.
4 Select Boundaries 1 and 6 only.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.
2 Select Boundaries 2 and 4 only.
3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
4 From the **Distribution type** list, choose **Predefined**.
5 In the **Number of elements** text field, type `12`.
6 In the **Element ratio** text field, type `24`.
7 From the **Growth rate** list, choose **Exponential**.
8 Click **Build All**.

Free Triangular 1

1 In the **Mesh** toolbar, click **Free Triangular**.
2 In the **Settings** window for **Free Triangular**, click **Build All**.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: 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**.

Compute four 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(0,0.005,4)`	s

Parametric Sweep

1 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 voltage)	600 800 1000 1600	V

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

RESULTS

Electric Potential (es)

1 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

2 From the **Parameter value (t (s))** list, choose **0.25**.

3 In the **Electric Potential (es)** toolbar, click **Plot**.

Polarization

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

Plot the axial polarization variation with respect to the applied electric field at the center of the actuator.

2 In the **Settings** window for **1D Plot Group**, type `Polarization` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (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

1 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. Select the **Show legends** check box.

9 Find the **Include** subsection. Clear the **Point** check box.

10 In the **Polarization** toolbar, click **Plot**.