Model created in COMSOL Multiphysics 6.4

Pyroelectric Detector

Introduction

The pyroelectric phenomenon, when absorbed energy causes a change in temperature and polarization within a pyroelectric material, is the basis of operation of some laser energy meters. The change in polarization manifests itself as a pyroelectric current, which can be measured by an ammeter circuit. Laser energy meters based on the pyroelectric phenomenon are used to calibrate of laser sources.

This 2D axisymmetric model demonstrates the operation of a pyroelectric detector based on a lithium niobate ($LiNbO_3$) crystal sandwiched between two electrodes with connection to an external circuit. To represent the absorbed laser energy, an energy flux that varies with position and time is applied to the top surface of the disk. This model uses (i) the **Piezoelectricity and Pyroelectricity** multiphysics interface and (ii) the **Electrical Circuit** interface. A time-dependent study solves for temperature evolution in the disk and the pyroelectric current generated.

Model Definition

A 25 μm-thick $LiNbO_3$ crystal in the shape of a disk with a diameter of 3 mm is bonded to an electrically conductive base by a 40 μm thick ring-shaped silver (Ag) pad. Most material properties of the $LiNbO_3$ and Ag domains are defined by material models from the material library and some properties need to be added manually. The pyroelectric coefficient of $LiNbO_3$ was specified as $-83\ \mu C/(m^2 \cdot K)$. The top and bottom surfaces of the crystal are coated with a thin metal layer, forming the top and bottom electrodes. The model geometry is fully parameterized to allow for easy changes in the device structure for future optimization.

This model uses the **Piezoelectricity and Pyroelectricity** multiphysics interface, which automatically sets up the **Electrostatics**, **Solid Mechanics**, and **Heat Transfer** interfaces together with **Pyroelectricity**, **Piezoelectricity**, and **Thermal Expansion** couplings. In the **Electrostatics** interface, a **Charge Conservation, Piezoelectric** material model is assigned to the $LiNbO_3$ domain. In the **Solid Mechanics** interface, a **Fixed Constraint** is applied to the base of the Ag pad. In the **Heat Transfer** interface, an **Heat Flux** applied to the top surface of the disk represents the laser energy while a constant temperature of 293.15 K is assigned to the base of the Ag pad. These assignments can be seen in Figure 1.

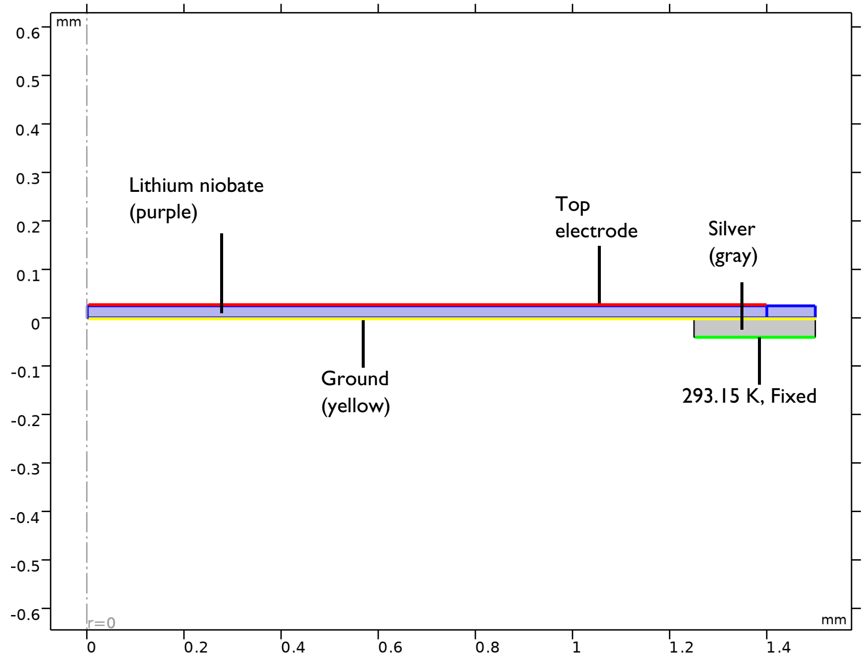

Figure 1: A cross section of the 2D axi-symmetric model showing the material models and boundary conditions used. The disk is lithium niobate (purple) and the pad is silver (gray). The bottom surface of the disk is grounded (yellow) while the top electrode (red) is connected to an external circuit. A fixed constraint and T = 293.15 K is applied to the bottom of the silver pad.

To calculate output power, the device is connected to an external circuit using the **Electrical Circuit** interface. The terminals of the $LiNbO_3$ disk is connected in parallel to the capacitor C1 with a capacitance value of C_{ext} = 100 pF. The disk is also connected to the load R1 with resistance value of $R_{ext} = 0.1, 5\cdot10^6, 5\cdot10^7$, or 10^9 Ω. The electric power is calculated as the product of the voltage and current across R1. The circuit components are parameterized to allow for easy changes in the device structure for future optimization.

The model solves a multiphysics problem involving **Pyroelectricity**, **Piezoelectricity**, and **Thermal Expansion** couplings using a time-dependent study. In the first study, the model includes all couplings and is referred to as the full model. In the second study, the **Piezoelectricity** and **Thermal Expansion** couplings are disabled, and the model is referred to as pyroelectricity-only.

Results and Discussion

A plot of temperature and current through R1versus time is shown in Figure 2 with the temperature measured at the center of the disk.

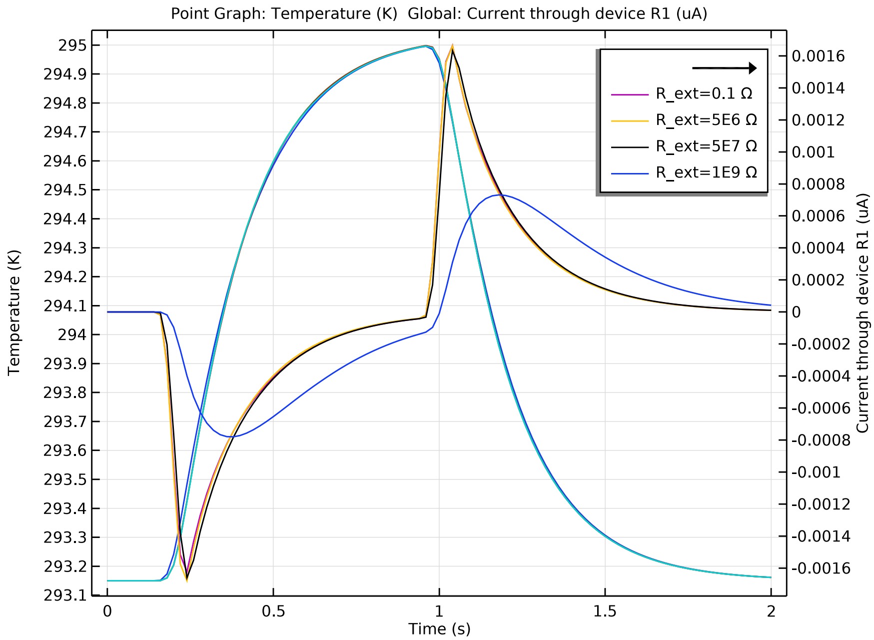

Figure 2: Temperature and current through R1 versus time at the center of the disk.

Figure 3 shows a plot of voltage versus time with the voltage measurements taken across the load R1.

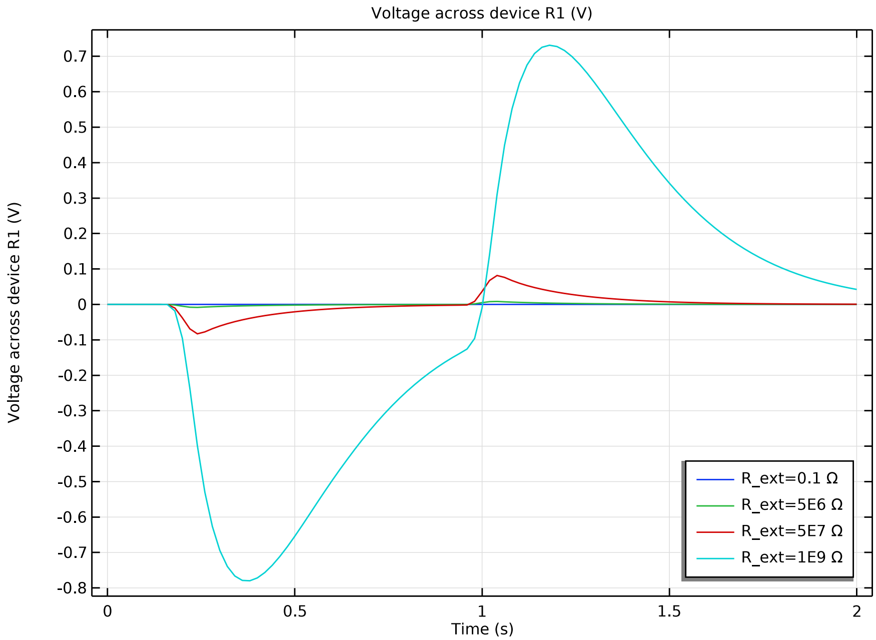

Figure 3: Voltage versus time. Voltage measurements taken across the load R1.

Figure 4 shows a plot of electric power versus time, with the electric power measurements taken through the load R1.

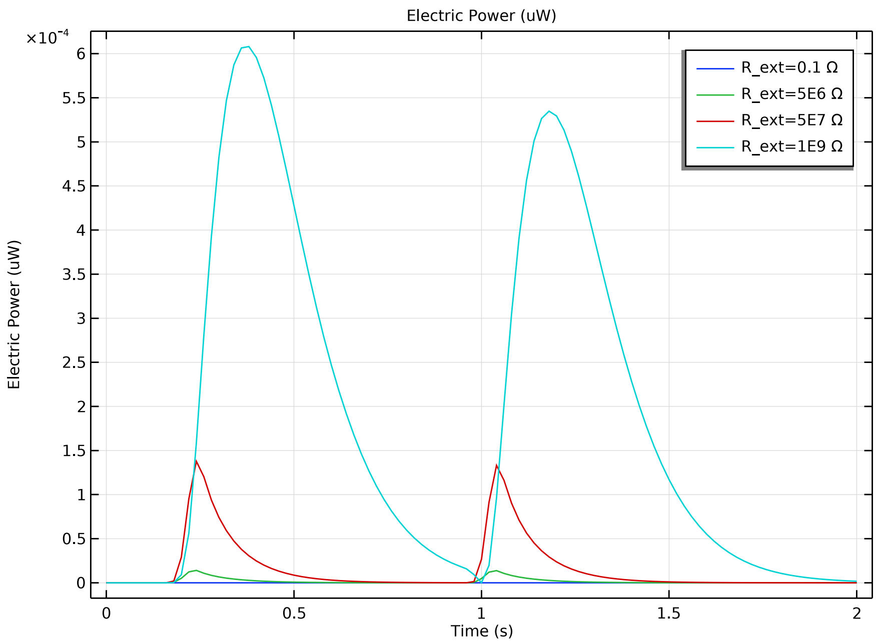

Figure 4: Electric power versus time. Electric power measurements taken through the load R1.

Figure 5 shows a comparison of the electric power between the full model and the pyroelectricity-only model. The electric power for the full model is about 8% less than for the pyroelectricity-only model.

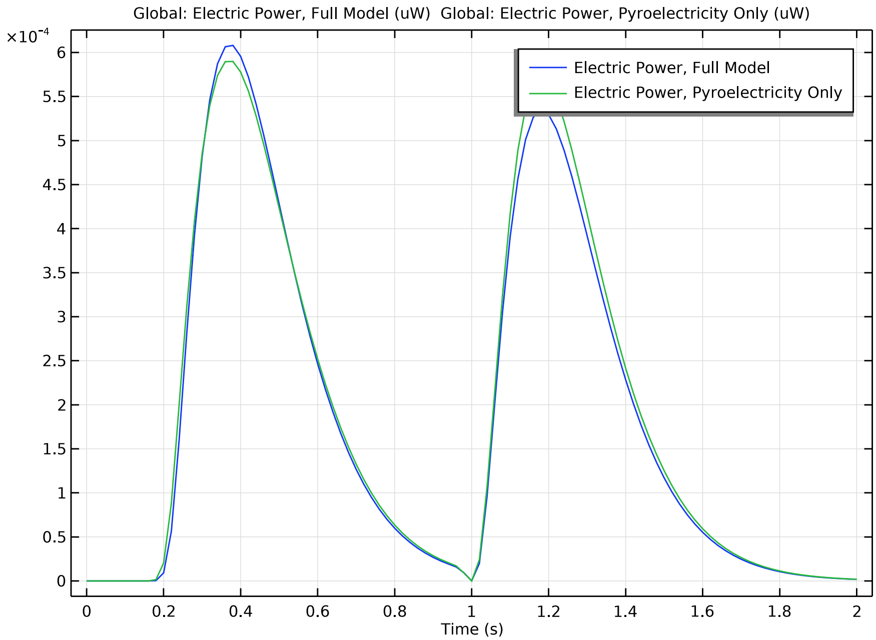

Figure 5: Comparison of electric power between full model and pyroelectricity-only model.

Application Library path: `MEMS_Module/Sensors/pyroelectric_detector`

Modeling Instructions

Start by creating a new 2D axi-symmetric model with the **Piezoelectricity and Pyroelectricity** multiphysics interface and the **Electrical Circuit** interface.

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** > **Electromagnetics and Mechanics** > **Piezoelectricity** > **Piezoelectricity and Pyroelectricity**.
3 Click **Add**.
4 In the **Select Physics** tree, select **AC/DC** > **Electrical Circuit (cir)**.
5 Click **Add**.
6 Click **Study**.
7 In the **Select Study** tree, select **General Studies** > **Time Dependent**.
8 Click **Done**.

Define and enter the values for the following global parameters.

GLOBAL DEFINITIONS

Parameters 1

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
r_el	1.4[mm]	0.0014 m	Radius of top electrode
r_s	0.25[mm]	2.5E-4 m	Width of standoff
r_d	1.5[mm]	0.0015 m	Radius of crystal
t_d	0.025[mm]	2.5E-5 m	Thickness of crystal
t_s	0.040[mm]	4E-5 m	Thickness of standoff
w_b	2[mm]	0.002 m	Width of laser beam
Qmax	500[W/m^2]	500 W/m²	Maximum laser power density
pulse	1[s]	1 s	Duration of laser pulse
C_ext	100[pF]	1E-10 F	Capacitance of C1
R_ext	1000[ohm]	1000 Ω	Resistance of R1

Define a rectangular function and an analytical function describing the shape of laser pulse.

DEFINITIONS

Rectangle 1 (rect1)

1 In the **Definitions** toolbar, click f(X) **More Functions** and choose **Rectangle**.
2 In the **Settings** window for **Rectangle**, locate the **Parameters** section.
3 In the **Lower limit** text field, type `0.2`.
4 In the **Upper limit** text field, type `1`.

Analytic 1 (an1)

1 In the **Definitions** toolbar, click f(X) **Analytic**.
2 In the **Settings** window for **Analytic**, locate the **Definition** section.
3 In the **Expression** text field, type `exp(-((r^2)/(2*(10000)^2)))`.
4 In the **Arguments** text field, type `r`.
5 Locate the **Units** section. In the table, enter the following settings:

Argument	Unit
r	um

Define the expression for the energy flux representing laser pulse using the functions previously defined.

Variables 1

1 In the **Model Builder** window, 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
Flux	Qmax*an1(r)*rect1(t/pulse)	W/m²	Power density distribution

GEOMETRY 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
2 In the **Settings** window for **Geometry**, locate the **Units** section.
3 From the **Length unit** list, choose **mm**.

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 `r_d`.

4 In the **Height** text field, type `t_d`.

Rectangle 2 (r2)

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 `r_s`.

4 In the **Height** text field, type `t_s`.

5 Locate the **Position** section. In the **r** text field, type `r_d-0.3`.

6 In the **z** text field, type `-t_p`.

7 In the **r** text field, type `r_d-r_s`.

8 In the **z** text field, type `-t_s`.

Rectangle 3 (r3)

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 `r_el`.

4 In the **Height** text field, type `t_d`.

5 Click **Build Selected**.

MULTIPHYSICS

Pyroelectricity 1 (pye1)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Multiphysics** click **Pyroelectricity 1 (pye1)**.

2 Select Domains 1 and 3 only.

Add the lithium niobate model from the library.

ADD MATERIAL

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

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

3 In the tree, select **Piezoelectric** > **Lithium Niobate**.

4 Click the **Add to Component** button in the window toolbar.

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

MATERIALS

Lithium Niobate (mat1)

Next, enter missing properties for lithium niobate.

1 In the **Settings** window for **Material**, locate the **Material Contents** section.

2 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	4.2	W/(m·K)	Basic
Heat capacity at constant pressure	Cp	628	J/(kg·K)	Basic
Coefficient of thermal expansion	{alpha11, alpha22, alpha33} ; alphaij = 0	{6.5e-6, 6.5e-6, 14.8e-6}	1/K	Basic
Total pyroelectric coefficient	{pET1,pET2, pET3}	{0,0,-8.3e-5}	$C/(m^2\cdot K)$	Pyroelectric

Set up the boundary conditions for the **Electrostatics** interface.

ELECTROSTATICS (ES)

Charge Conservation, Piezoelectric 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Electrostatics (es)** click **Charge Conservation, Piezoelectric 1**.

2 Select Domains 1 and 3 only.

Charge Conservation in Solids 1

1 In the **Physics** toolbar, click **Domains** and choose **Charge Conservation in Solids**.

2 Select Domain 2 only.

Ground 1

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

2 Select Boundaries 2, 6, and 8 only.

Boundary Terminal 1

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

2 In the **Settings** window for **Boundary Terminal**, locate the **Boundary Selection** section.

3 Click Paste Selection.

4 In the **Paste Selection** dialog, type 3 in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Boundary Terminal**, locate the **Terminal** section.

7 From the **Terminal type** list, choose **Circuit**.

SOLID MECHANICS (SOLID)

Piezoelectric Material 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Solid Mechanics (solid)** click **Piezoelectric Material 1**.

2 Select Domains 1 and 3 only.

Set up the boundary conditions for the **Solid Mechanics** interface.

Fixed Constraint 1

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

2 Select Boundary 5 only.

Set up the boundary conditions for the **Heat Transfer** interface.

HEAT TRANSFER IN SOLIDS (HT)

In the **Model Builder** window, under **Component 1 (comp1)** click **Heat Transfer in Solids (ht)**.

Heat Flux 1

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

2 In the **Settings** window for **Heat Flux**, locate the **Material Type** section.

3 From the **Material type** list, choose **Solid**.

4 Locate the **Heat Flux** section. In the q_0 text field, type `Flux`.

5 Select Boundaries 3 and 9 only.

Temperature 1

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

2 Select Boundary 5 only.

Add the **Electrical Circuit** interface, define the capacitor C_ext and the load R_ext and how they are connected to the detector terminals.

ELECTRICAL CIRCUIT (CIR)

In the **Model Builder** window, under **Component 1 (comp1)** click **Electrical Circuit (cir)**.

Resistor 1 (R1)

1 In the **Electrical Circuit** toolbar, click **Resistor**.
2 In the **Settings** window for **Resistor**, locate the **Node Connections** section.
3 In the table, enter the following settings:

Label	Node names
n	0

4 Locate the **Device Parameters** section. In the R text field, type `R_ext`.

Capacitor 1 (C1)

1 In the **Electrical Circuit** toolbar, click **Capacitor**.
2 In the **Settings** window for **Capacitor**, locate the **Node Connections** section.
3 In the table, enter the following settings:

Label	Node names
p	1
n	0

4 Locate the **Device Parameters** section. In the C text field, type `C_ext`.

External I-Terminal 1 (termI1)

1 In the **Electrical Circuit** toolbar, click **External I-Terminal**.
2 In the **Settings** window for **External I-Terminal**, locate the **Node Connections** section.
3 In the **Node name** text field, type `1`.
4 Locate the **External Terminal** section. From the V list, choose **Terminal voltage (es/term1)**.

Add material model for silver.

ADD MATERIAL

1 In the **Materials** toolbar, click **Add Material** to open the **Add Material** window.
2 Go to the **Add Material** window.
3 In the tree, select **MEMS** > **Metals** > **Ag - Silver**.
4 Click the **Add to Component** button in the window toolbar.
5 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Ag - Silver (mat2)

Next, enter missing properties for silver.

1 Select Domain 2 only.

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
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	1	1	Basic

4 Click the **Zoom Extents** button in the **Graphics** toolbar.

MESH 1

Free Triangular 1

In the **Mesh** toolbar, click **Free Triangular**.

Size 1

1 Right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely fine**.

4 Click **Build Selected**.

Add a time-dependent study using the full model to analyze effect of thermal expansion, piezoelectricity and pyroelectricity.

STUDY 1

Time Dependent, Full Model

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

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,0.02,2)`.

4 In the **Label** text field, type `Time Dependent, Full Model`.

5 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

6 Click + **Add**.

7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
R_ext (Resistance of R1)	`0.1 5e6 5e7 1e9`	Ω

8 In the **Model Builder** window, click **Study 1**.

9 In the **Settings** window for **Study**, locate the **Study Settings** section.

10 Clear the **Generate default plots** checkbox.

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

Add a time-dependent study using the pyroelectricity-only model to analyze effect of pyroelectricity.

ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies** > **Time Dependent**.

4 Click the **Add Study** button in the window toolbar.

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

STUDY 2

Time Dependent - Pyroelectricity Only

1 In the **Settings** window for **Time Dependent**, type `Time Dependent - Pyroelectricity Only` in the **Label** text field.

2 Locate the **Study Settings** section. In the **Output times** text field, type `range(0,0.02,2)`.

3 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Solid Mechanics (solid)**.

4 In the **Solve for** column of the table, under **Component 1 (comp1)** > **Multiphysics**, clear the checkboxes for **Piezoelectricity 1 (pze1)** and **Thermal Expansion 1 (te1)**.

5 Locate the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

6 Click + **Add**.

7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
R_ext (Resistance of R1)	`0.1 5e6 5e7 1e9`	Ω

8 In the **Model Builder** window, click **Study 2**.

9 In the **Settings** window for **Study**, locate the **Study Settings** section.

10 Clear the **Generate default plots** checkbox.

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

Plot temperature and current density versus time, taking measurement at the center of the disk.

RESULTS

Temperature and Current Density, Full Model

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Temperature and Current Density, Full Model` in the **Label** text field.

3 Locate the **Plot Settings** section. Select the **Two y-axes** checkbox.

Temperature

1 Right-click **Temperature and Current Density, Full Model** and choose **Point Graph**.

2 Click the **Zoom Extents** button in the **Graphics** toolbar.

3 Select Point 2 only.

4 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

5 In the **Expression** text field, type `T`.

6 Select the **Description** checkbox.

7 In the **Temperature and Current Density, Full Model** toolbar, click **Plot**.

8 In the **Label** text field, type `Temperature`.

Circuit Current

1 In the **Model Builder** window, right-click **Temperature and Current Density, Full Model** and choose **Global**.

2 In the **Settings** window for **Global**, type `Circuit Current` in the **Label** text field.

3 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
cir.R1.i	uA	Current through device R1

5 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

6 In the **Temperature and Current Density, Full Model** toolbar, click **Plot**.

Temperature and Current Density, Full Model

1 In the **Model Builder** window, click **Temperature and Current Density, Full Model**.

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

3 In the table, select the **Plot on secondary y-axis** checkbox for **Circuit Current**.

4 In the **Temperature and Current Density, Full Model** toolbar, click **Plot**.

Plot voltage versus time, taking measurement across the load R_ext.

Voltage, Full Model

1 In the **Results** toolbar, click **1D Plot Group**.

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

3 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Voltage, Full Model** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Electrical Circuit** > **Devices** > **R1** > **cir.R1.v - Voltage across device R1 - V**.

3 Locate the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

4 In the **Voltage, Full Model** toolbar, click **Plot**.

Plot electric power versus time, taking measurement across the load R_ext.

Electric Power, Full Model

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Electric Power, Full Model` in the **Label** text field.

Global 1

1 Right-click **Electric Power, Full Model** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
realdot(cir.R1.i,cir.R1.v)	uW	Electric Power

4 Locate the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

5 In the **Electric Power, Full Model** toolbar, click **Plot**.

Plot electric power versus time for R_ext = 1e9 ohms for the full model and the pyroelectricity-only model.

Full Model vs. Pyroelectricity Only

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Full Model vs. Pyroelectricity Only` in the **Label** text field.

Electric Power, Full Model

1 Right-click **Full Model vs. Pyroelectricity Only** and choose **Global**.

2 In the **Settings** window for **Global**, type `Electric Power, Full Model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

4 From the **Parameter selection (R_ext)** list, choose **From list**.

5 In the **Parameter values (R_ext (Ω))** list box, select **1E9**.

6 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
realdot(cir.R1.i,cir.R1.v)	uW	Electric Power, Full Model

7 Locate the **Legends** section. Find the **Include** subsection. Clear the **Solution** checkbox.

Electric Power, Pyroelectricity Only

1 Right-click **Electric Power, Full Model** and choose **Duplicate**.

2 In the **Settings** window for **Global**, type `Electric Power, Pyroelectricity Only` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`realdot(cir.R1.i,cir.R1.v)`	`uW`	`Electric Power, Pyroelectricity Only`

5 In the **Full Model vs. Pyroelectricity Only** toolbar, click **Plot**.