9. ADVANCED MODELING: THERMOELECTRICITY

Thermoelectric and Thermomagnetic Phenomena

Heat flux:

$$\mathbf{q} = \underbrace{V\mathbf{J}}_{\text{Joule}} \underbrace{-k\nabla T}_{\text{Fourier}} + \underbrace{P\mathbf{J}}_{\text{Peltier}} + \underbrace{NT\mathbf{B}\times\mathbf{J}}_{\text{Ettingshausen}} + \underbrace{kM\mathbf{B}\times\nabla T}_{\text{Righi-Leduc}}$$

Electrical filed intensity:

$$-\nabla V = \underbrace{\rho\mathbf{J}}_{\text{Ohm}} + \underbrace{S\nabla T}_{\text{Seebeck}} + \underbrace{R\mathbf{B}\times\mathbf{J}}_{\text{Hall}} + \underbrace{N\mathbf{B}\times\nabla T}_{\text{Nernst}}$$

Application areas:

- aerospace industry
- semiconductor industry
- electronics
- renewable energy sources
- bioengineering

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Thermoelectric Effect

- Thermoelectric effect: Direct conversion of temperature difference to electric voltage
  or
  Direct conversion of electric voltage to temperature difference

- Historically, thermoelectric effect is known under three different names, reflecting its discovery in experiments by Seebeck, Peltier, and Thomson

- Seebeck effect: conversion of temperature differences into electricity

- Peltier effect: conversion of electricity to temperature differences

- Thomson effect: heat production by product of current density and temperature gradients

  - Joule heating is an irreversible phenomena

  - Thermoelectric effect is in principle reversible

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Thermodynamics of Thermoelectric Effect

Thomson relations:

$$P = ST$$

$$\mu = T\frac{dS}{dT}$$

P : Peltier coefficient, $[V]$

S : Seebeck coefficient, $[V/K]$

μ : Thomson coefficient, $[V/K]$

T : temperature, $[K]$

Heat flux: $\mathbf{q} = -k\nabla T + P\mathbf{J}$

Electric current density: $\mathbf{J} = -\sigma\nabla V - \sigma S\nabla T$

Thermoelectricity Conservation Laws

Energy balance:

$$\rho C \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = Q \qquad \mathbf{q} = -k\nabla T + P\mathbf{J}$$

Current balance (continuity):

$$\nabla \cdot \mathbf{J} = 0 \qquad \mathbf{J} = -\sigma \nabla V - \sigma S \nabla T$$

These terms are not implemented in Comsol interfaces

Electric potential: $\mathbf{E} = -\nabla V$

Joule heating: $Q = \mathbf{J} \cdot \mathbf{E}$

Weak contribution features can be used to account for missing terms

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Energy Balance Weak Formulation

- Multiply energy balance equation by test function T_{test} and integrate over computational domain Ω:

$$\int_{\Omega} \rho C \frac{\partial T}{\partial t} T_{test} d\Omega + \int_{\Omega} (\nabla \cdot \mathbf{q}) T_{test} d\Omega = \int_{\Omega} Q T_{test} d\Omega$$

- Use vector identity $\nabla \cdot (T_{test}\mathbf{q}) = \mathbf{q} \cdot \nabla T_{test} + T_{test} \nabla \cdot \mathbf{q}$ to write equation as:

$$\int_{\Omega} \rho C \frac{\partial T}{\partial t} T_{test} d\Omega + \int_{\Omega} \nabla \cdot (T_{test}\mathbf{q}) d\Omega - \int_{\Omega} \mathbf{q} \cdot \nabla T_{test} d\Omega = \int_{\Omega} Q T_{test} d\Omega$$

- Use Gauss theorem $\int_{\Omega} \nabla \cdot (T_{test}\mathbf{q}) d\Omega = \int_{\partial\Omega} T_{test} \mathbf{q} \cdot \mathbf{n} \partial\Omega$:

$$0 = \int_{\Omega} \left[-\rho C \frac{\partial T}{\partial t} T_{test} + \mathbf{q} \cdot \nabla T_{test} + Q T_{test} \right] d\Omega - \int_{\partial\Omega} (\mathbf{q} \cdot \mathbf{n}) T_{test} \partial\Omega$$

Comsol convection is to collect all terms on the right side

Energy Balance Weak Formulation (cont'd)

- Use energy flux $\mathbf{q} = -k\nabla T + P\mathbf{J}$:

$$0 = \int_{\Omega} \Big[\underbrace{-\rho C_p \frac{\partial T}{\partial t} T_{test}}_{\text{dweak}} + \underbrace{(-k\nabla T)\cdot \nabla T_{test}}_{\text{weak thermal}} + \underbrace{(P\mathbf{J})\cdot \nabla T_{test}}_{\text{weak Peltier}} + \underbrace{Q T_{test}}_{\text{weak source}} \Big] d\Omega - \int_{\partial\Omega} \underbrace{(\mathbf{q}\cdot\mathbf{n}) T_{test}}_{\text{Neumann BC}} \partial\Omega$$

- The only term not implemented in Comsol is Peltier weak contribution:

$$weak_P = (P\mathbf{J})\cdot \nabla T_{test} = PJ_x \frac{\partial T_{test}}{\partial x} + PJ_y \frac{\partial T_{test}}{\partial y} + PJ_z \frac{\partial T_{test}}{\partial z} =$$

$$= P * ec.Jx * test(Tx) + P * ec.Jy * test(Ty) + P * ec.Jz * test(Tz)$$

✓ Comsol notation for test function: $T_{test} = test(T)$

✓ Comsol notation for partial derivatives: $\frac{\partial T}{\partial x} = Tx,\ \frac{\partial T}{\partial y} = Ty,\ \frac{\partial T}{\partial z} = Tz$

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Current Balance Weak Formulation

- Multiply current balance equation by test function V_{test} and integrate over computational domain Ω:

$$\int_{\Omega} (\nabla \cdot \mathbf{J}) V_{test} d\Omega = 0$$

- Use vector identity and Gauss theorem to write equation as:

$$0 = \int_{\Omega} [\mathbf{J} \cdot \nabla V_{test}] d\Omega - \int_{\partial\Omega} (\mathbf{J} \cdot \mathbf{n}) V_{test} \partial\Omega$$

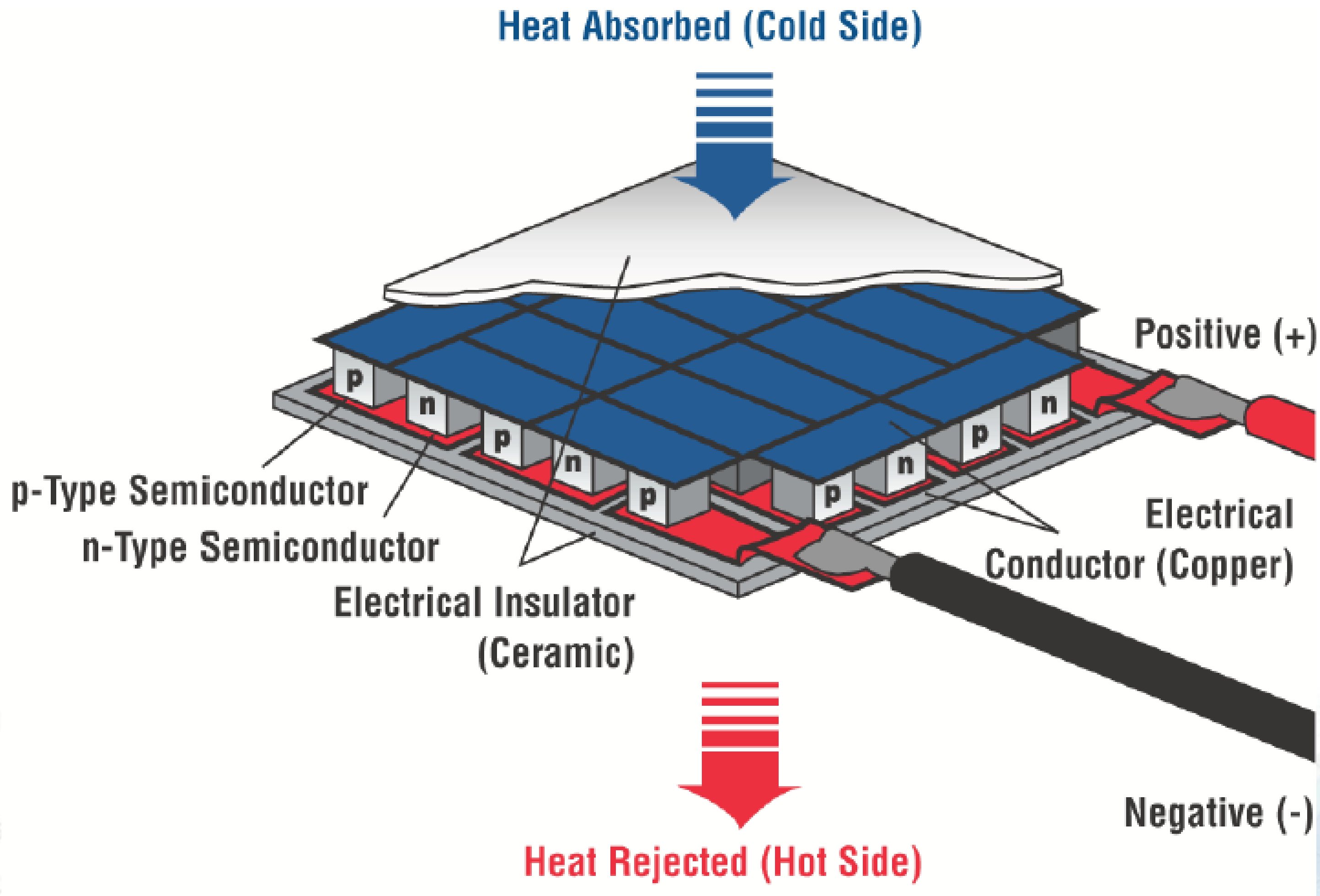
- Use current density $\mathbf{J} = -\sigma \nabla V - S\sigma \nabla T$:

$$0 = \int_{\Omega} \Big[\underbrace{(-\sigma \nabla V) \cdot \nabla V_{test}}_{\text{weak ec}} - \underbrace{(\sigma S \nabla T) \cdot \nabla V_{test}}_{\text{weak Seebeck}} \Big] d\Omega - \int_{\partial\Omega} \underbrace{(\mathbf{J} \cdot \mathbf{n}) V_{test}}_{\text{Neumann BC}} \partial\Omega$$

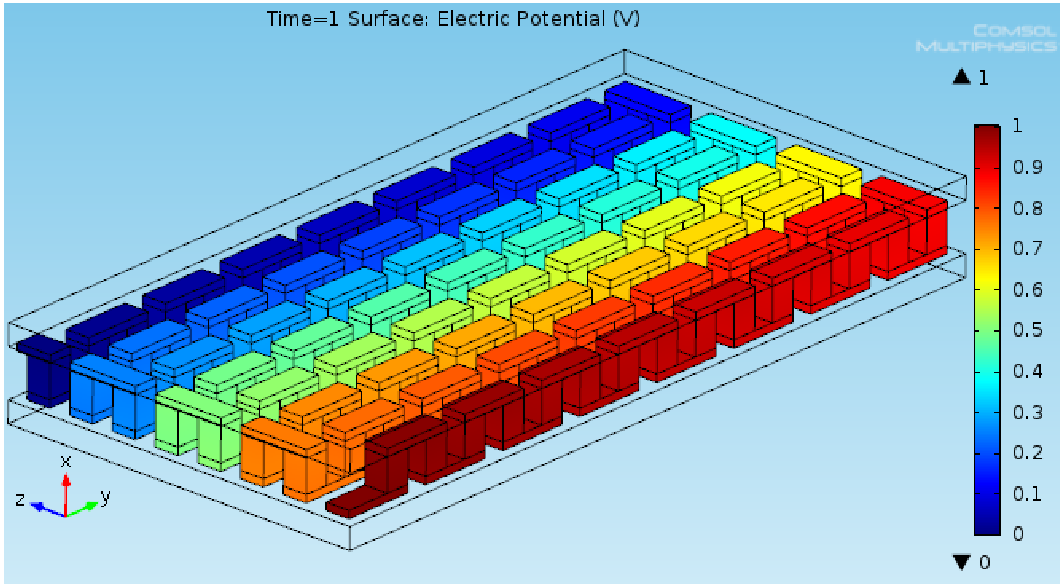
- The only term not implemented in Comsol is Seebeck weak contribution:

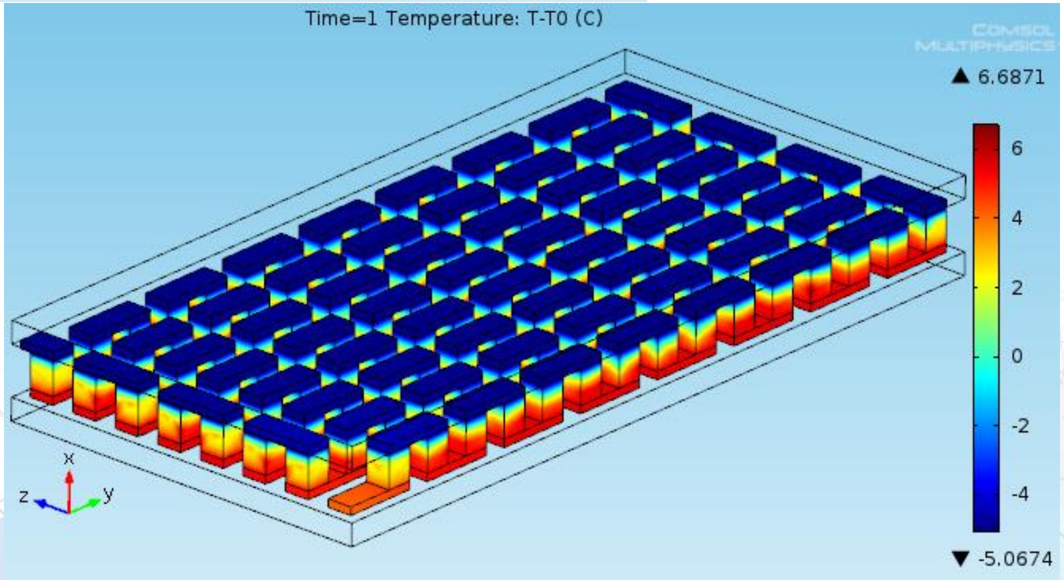
$$weak_S = -(\sigma S \nabla T) \cdot \nabla V_{test}$$

Thermoelectric Cell (TEC)



Thermoelectric Cell: Model Example

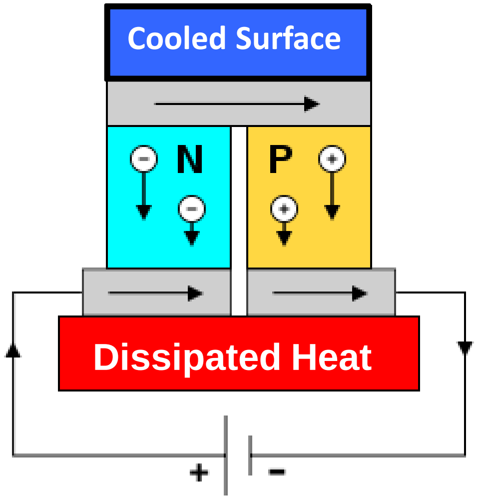




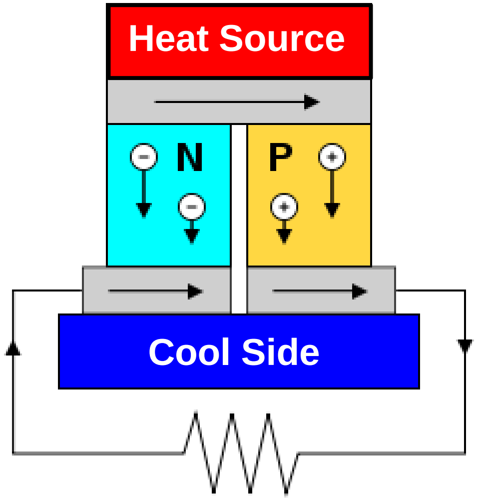
Thermoelectric Circuit

- A thermoelectric circuit composed of materials of different Seebeck coefficient: **p-doped** and **n-doped** semiconductors

Peltier effect



Seebeck effect



- ❑ The Seebeck circuit configured as a **thermoelectric cooler**
- ❑ The Seebeck circuit configured as a **thermoelectric generator**

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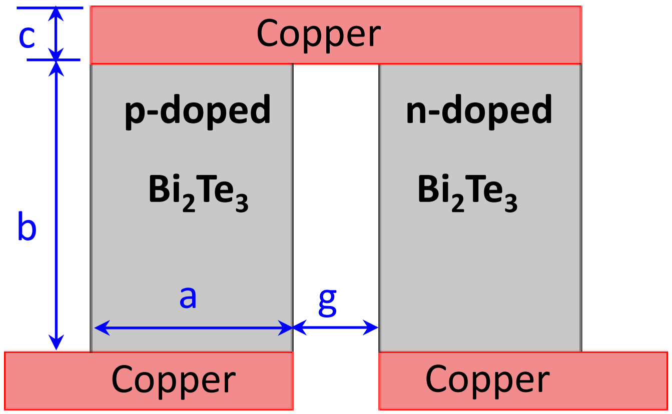
Jean Charles Athanase Peltier
(1785-1845)

PELTIER EFFECT IMPLEMENTATION

Peltier Effect Example Model



a=0.7mm
c=1mm
b=0.2mm
g=0.3mm

Bismuth Telluride properties:

Seebeck Coefficient, [V/K]	p: $S = 200 \cdot 10^{-6}$ n: $S = -200 \cdot 10^{-6}$
Electric conductivity, [S/m]	$\sigma = 1.1 \cdot 10^{5}$
Thermal conductivity, [W/m/K]	$k = 1.6$
Heat capacity, [J/kg/K]	$C = 154.4$
Density, [kg/m^3]	$\rho = 7740$

Model objectives:

- Implement Peltier effect as a weak contribution to energy balance
- Apply appropriate boundary conditions to demonstrate conversion of electricity to temperature differences

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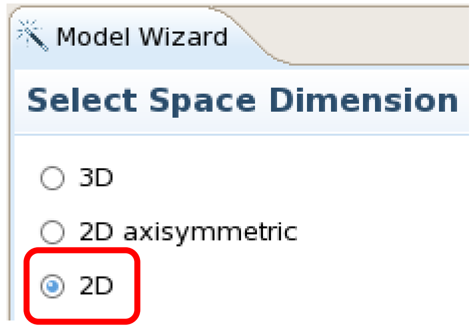
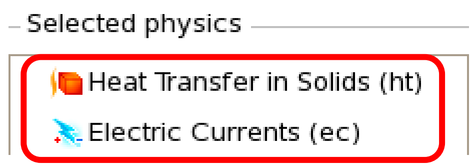
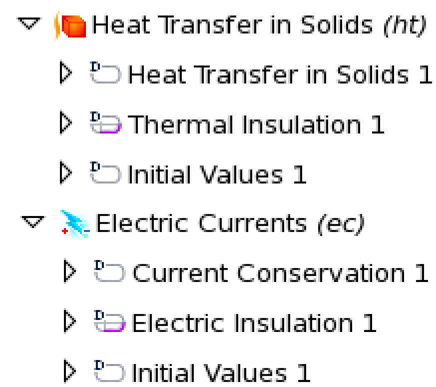
Peltier Effect: Model Wizard

1) Space dimension:

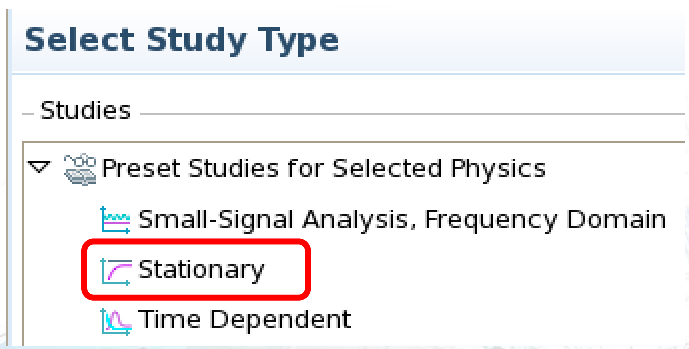


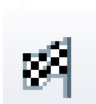
2) Physics selection:





1) Study type:





Peltier Effect: Global Parameters & Geometry

1 Define Global Parameters:

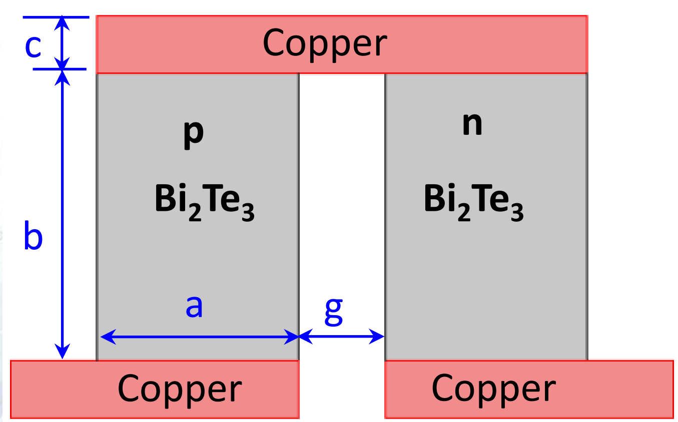
- Peltier_effect.mph *(root)*
  - Global Definitions
    - Parameters

Parameters

Name	Expression	Description
a	0.7[mm]	pellet width
b	1[mm]	pellet height
c	0.2[mm]	electrode thickness
g	0.3[mm]	gap between pellets
S_Bi2Te3	200e-6[V/K]	Seebeck coefficient
sig_Bi2Te3	1.1e5[S/m]	electric conductivity
k_Bi2Te3	1.6[W/(m*K)]	thermal conductivity
Cp_Bi2Te3	154.4[J/(kg*K)]	specific heat capacity
rho_Bi2Te3	7740[kg/m^3]	density
V0	1[V]	applied voltage
T0	20[degC]	reference temperature

2 Build geometry:

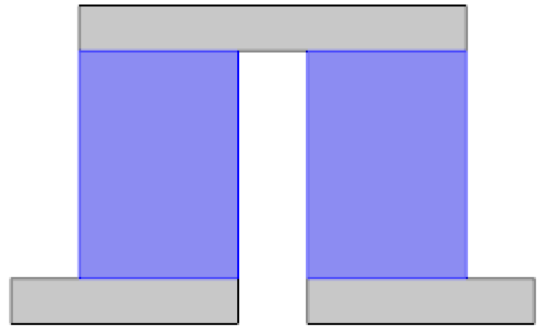
- Geometry 1
  - Rectangle 1:P-pellet *(r1)*
  - Copy 1:N-pellet *(copy1)*
  - Rectangle 2:Top Electrode *(r2)*
  - Rectangle 3:Bottom Left Electrode *(r3)*
  - Copy 2:Bottom Right Electrode *(copy2)*
  - Form Union *(fin)*



Materials

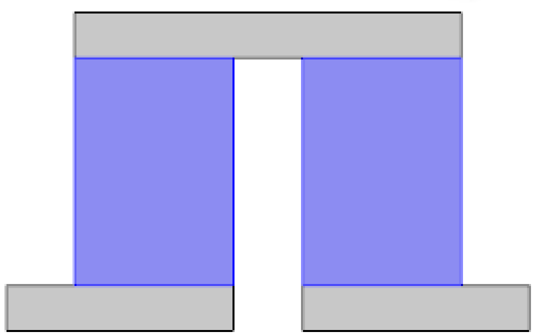
1 Define copper material:

- Materials
  - Copper *(mat1)*



2 Define bismuth telluride material:

- Materials
  - Copper *(mat1)*
  - Material 2:Bismuth Telluride *(mat2)*



Material Contents

	Property	Name	Value
✓	Thermal conductivity	k	k_Bi2Te3
✓	Density	rho	rho_Bi2Te3
✓	Heat capacity at constant	Cp	Cp_Bi2Te3
✓	Electrical conductivity	sigma	sig_Bi2Te3
✓	Relative permittivity	epsilonr	1

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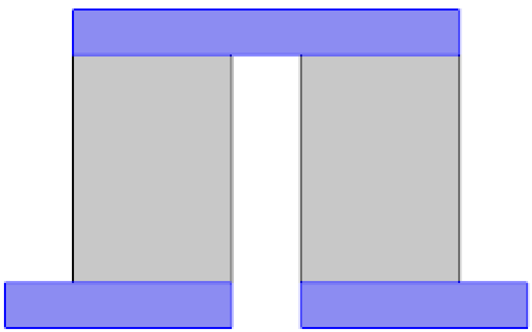
Materials (cont'd)

- Define Seebeck and Peltier coefficients as domain variables "**S**" and "**P**" to make it available for **Weak Contribution** node

3 **Copper** domain variables **S** and **P**

Definitions

a= Variables 1: S, P (copper)



Geometric Entity Selection

Geometric entity level: Domain

Selection: Manual

1
3
4

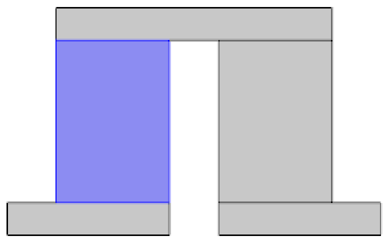
Variables

Name	Expression	Unit	Description
S	0		Seebeck coefficient
P	0		Peltier coefficient

Materials (cont'd)

4 **p-doped** domain variables **S** and **P**

- Definitions
  - a= Variables 1: S, P (copper)
  - a= Variables 2: S, P (p-dopped)



Geometric Entity Selection

Geometric entity level: Domain

Selection: Manual

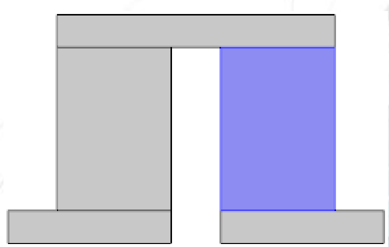
2

Variables

Name	Expression	Unit	Description
S	S_Bi2Te3	V/K	Seebeck coefficient
P	S_Bi2Te3*T	V	Peltier coefficient

5 **n-doped** domain variables **S** and **P**

- Definitions
  - a= Variables 1: S, P (copper)
  - a= Variables 2: S, P (p-dopped)
  - a= Variables 3: S, P (n-doped)



Geometric Entity Selection

Geometric entity level: Domain

Selection: Manual

5

Variables

Name	Expression	Unit	Description
S	-S_Bi2Te3	V/K	Seebeck coefficient
P	-S_Bi2Te3*T	V	Peltier coefficient

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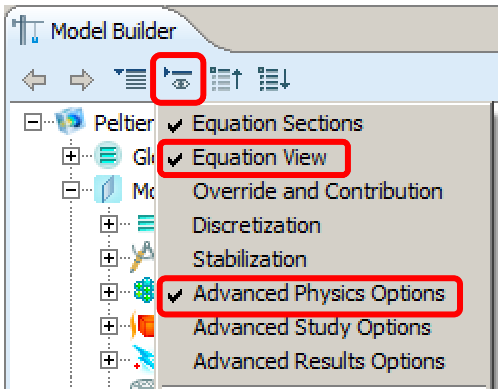
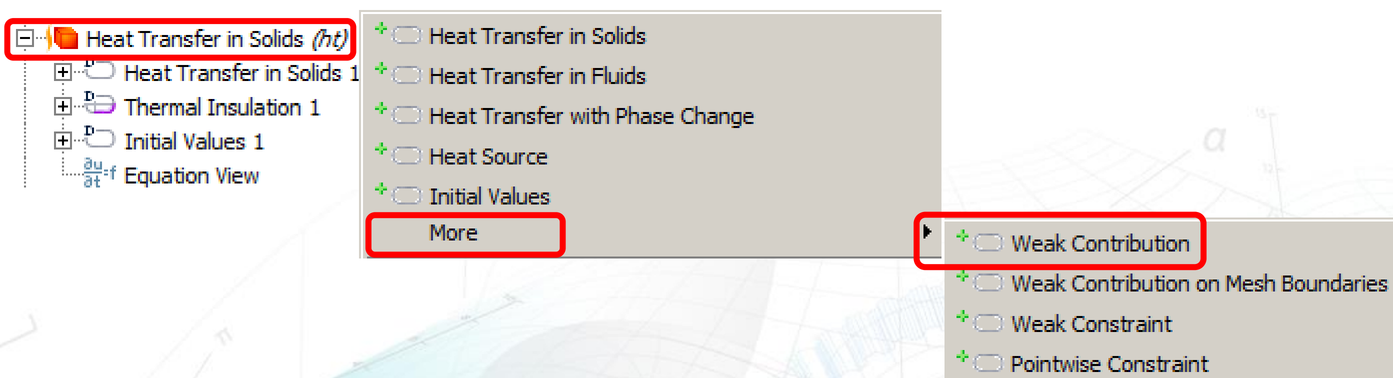
Peltier Weak Contribution

1 In the **Model Builder**, click **Show** button and then select **Equation View** and **Advanced Physics Option** to display these options under physics interface nodes

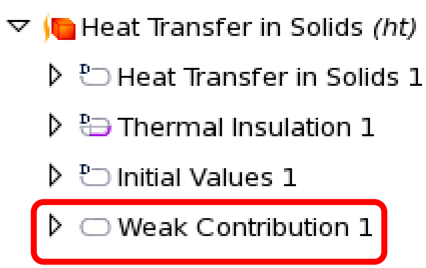


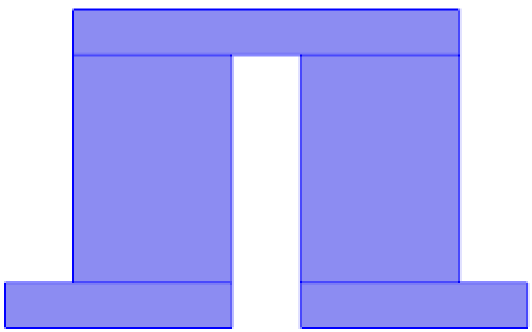
2 Add **Weak Contribution** domain node under **Heat transfer in Solids (ht)** interface

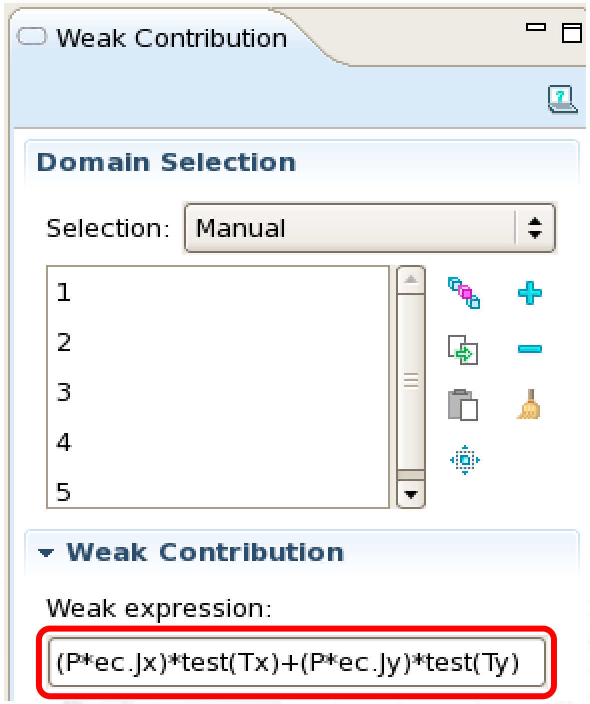


Peltier Weak Contribution (cont'd)

3 Select all domains and enter Peltier effect weak contribution in the **Weak expression** edit window







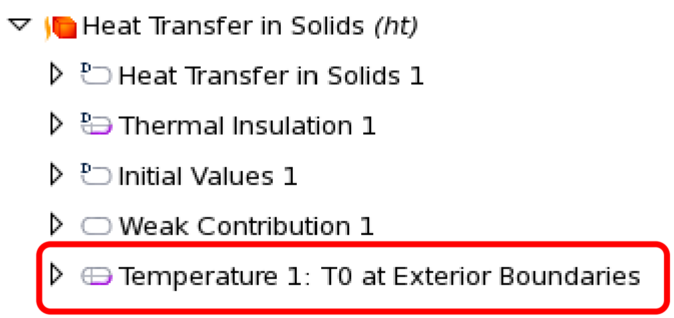
Check **Equation View** under **Heat Transfer in Solids 1** node to see the implementation of the rest weak terms in the energy balance equation

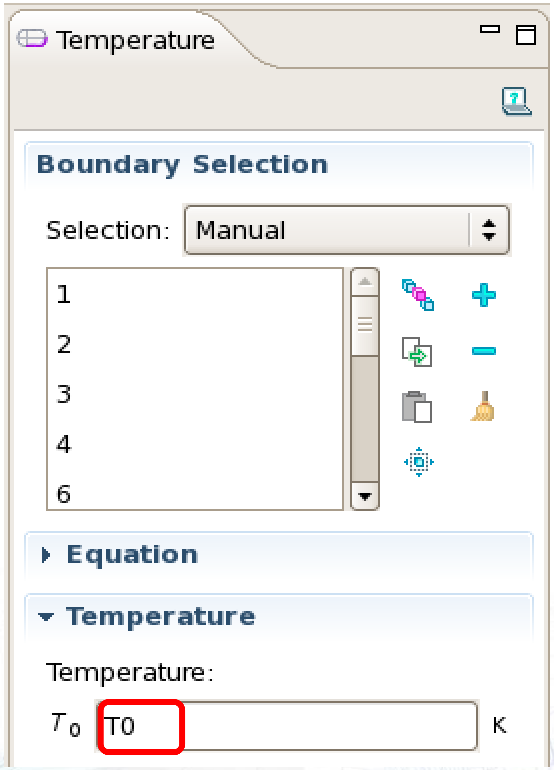
$$weak_P = (P\mathbf{J})\cdot\nabla T_{test} = PJ_x \frac{\partial T_{test}}{\partial x} + PJ_y \frac{\partial T_{test}}{\partial y} =$$

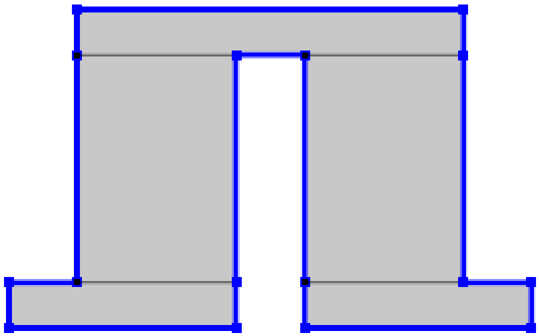
$$= P*ec.Jx*test(Tx) + P*ec.Jy*test(Ty)$$

Peltier Effect: Thermal BC

- Apply fixed temperature T0 at all exterior boundaries

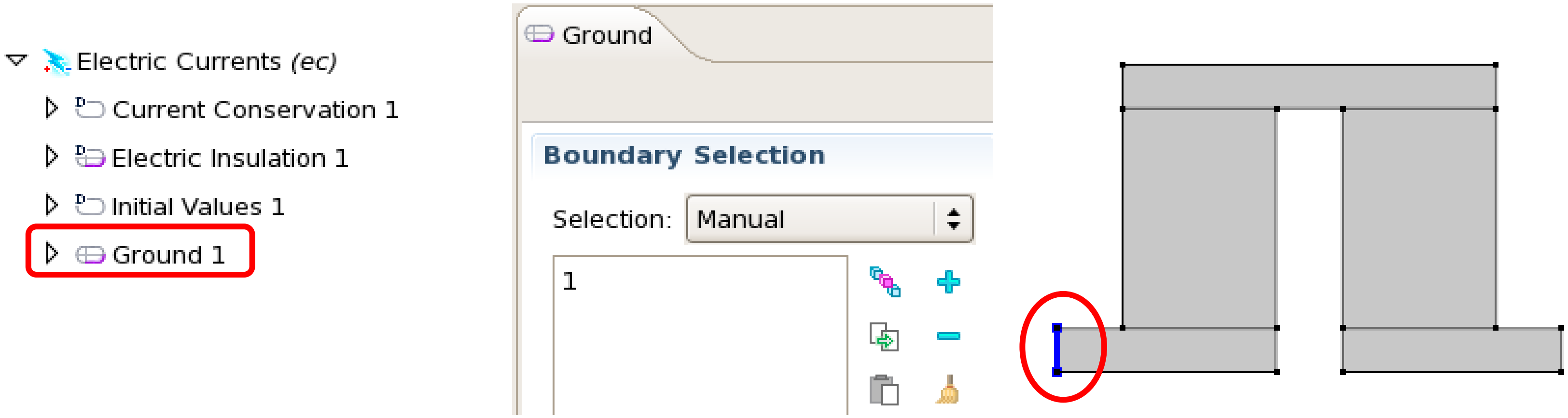




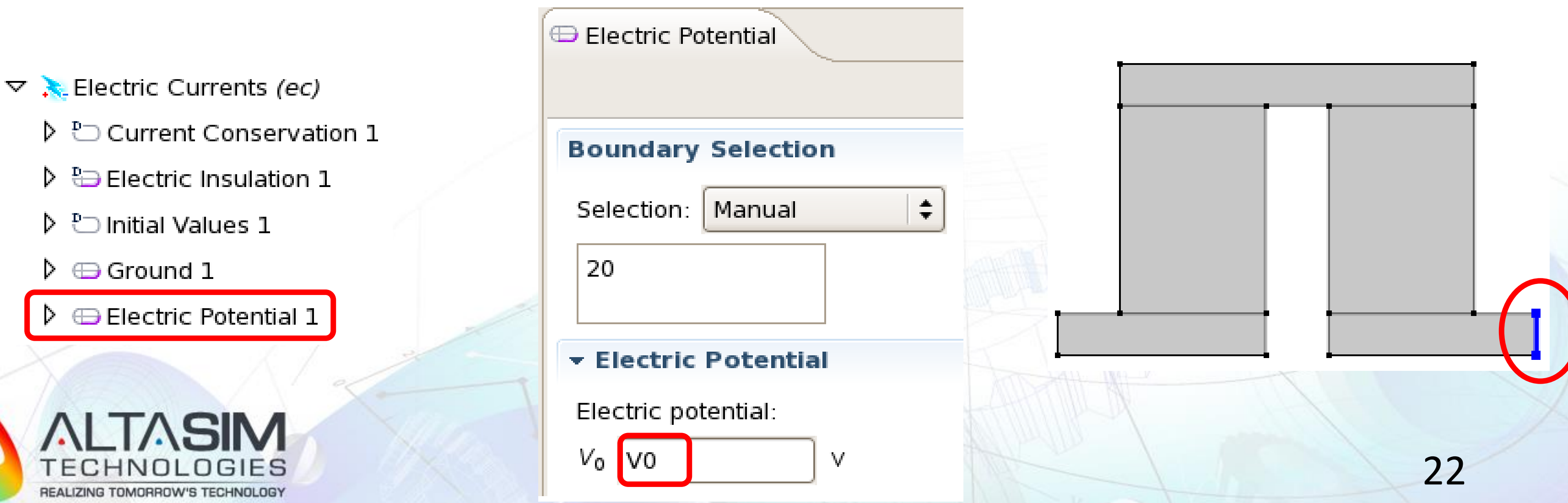


Peltier Effect: Electrical BC

1 Apply ground potential at the left boundary of bottom electrode



2 Apply fixed electrical potential V0 at the right boundary of bottom electrode



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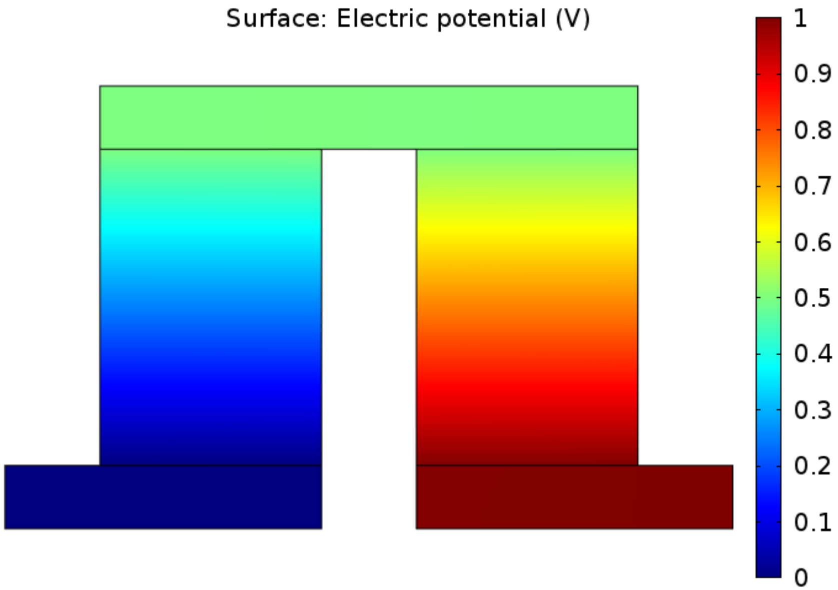
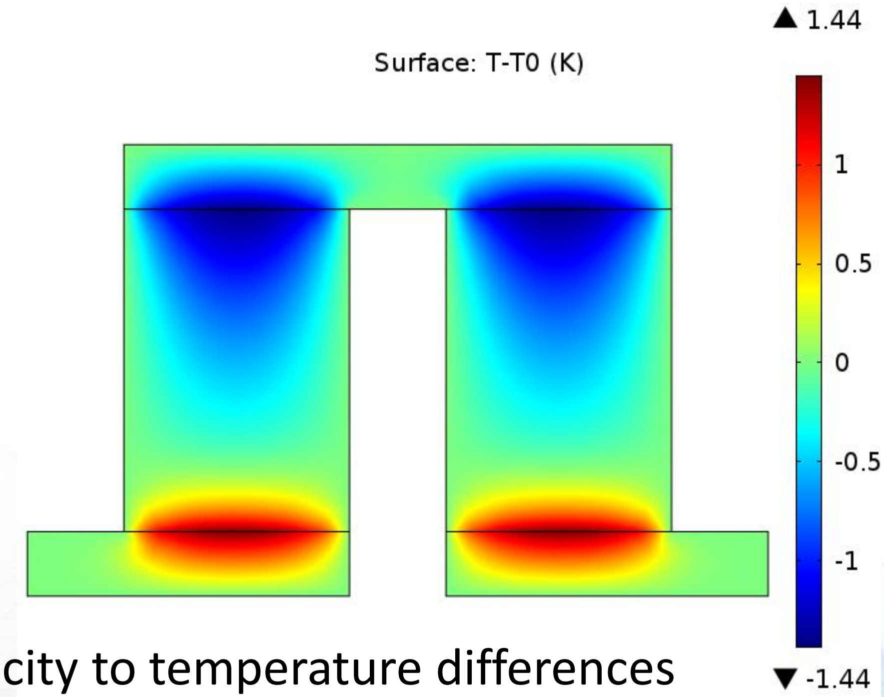
Peltier Effect: Results





- Peltier effect: conversion of electricity to temperature differences

• Save model as “Peltier_effect.mph”

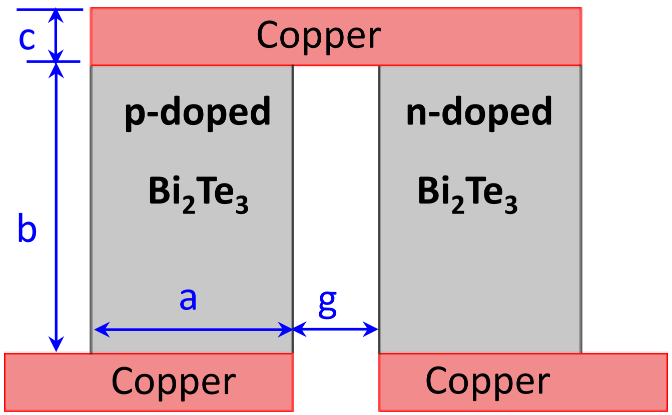

Thomas Johann Seebeck
(1770-1831)

SEEBECK EFFECT IMPLEMENTATION

Seebeck Effect Example Model

Model objectives:

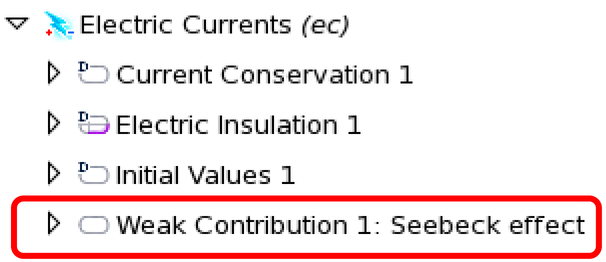
- Implement Seebeck effect as a weak contribution to current balance
- Apply appropriate boundary conditions to demonstrate conversion of temperature differences into electricity

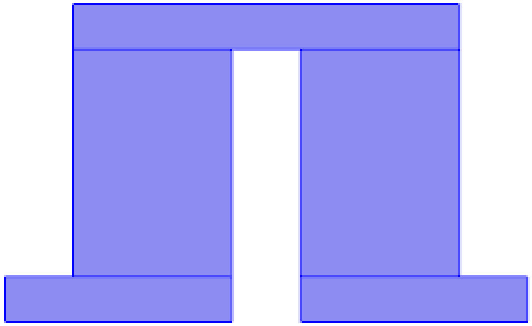


- Open previously created model "Peltier_effect.mph"
- This model will be modified to add Seebeck effect
- Remove previously imposed thermal and electrical boundary conditions
- Save the model as "Seebeck_effect.mph"

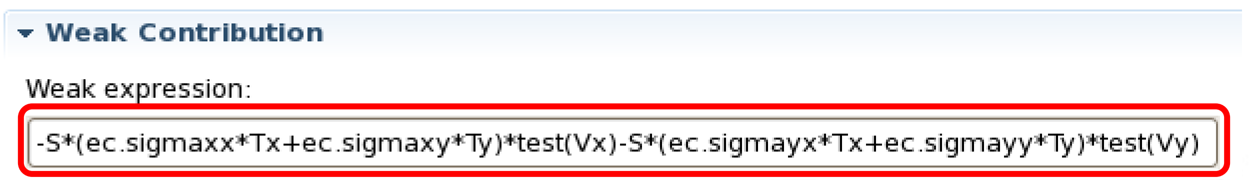
Seebeck Weak Contribution

1 Add **Weak Contribution** domain node under **Electric Currents (ec)** interface and select all domains





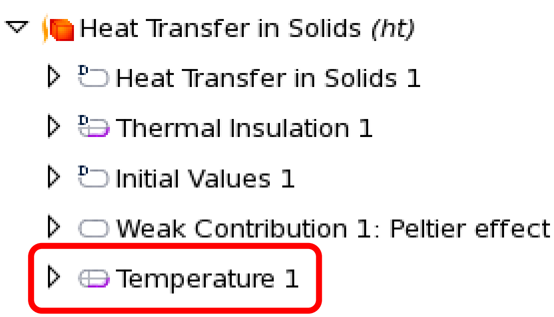
2 Enter Seebeck effect weak contribution in the **Weak expression** edit window

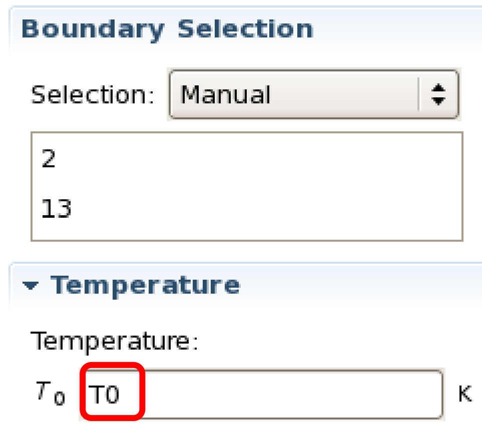


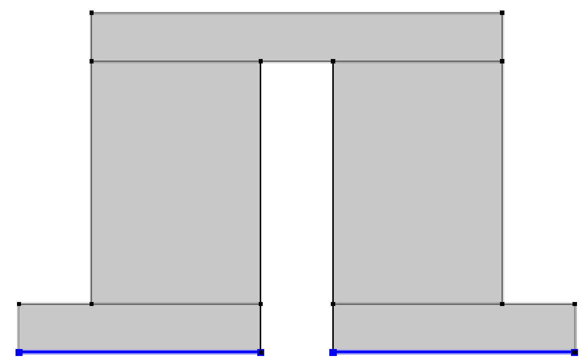
$$
\begin{aligned}
weak_S &= -\left(\sigma \cdot S \nabla T\right) \cdot \nabla V_{test} \\
&= -S\left(\sigma_{xx}\frac{\partial T}{\partial x} + \sigma_{xy}\frac{\partial T}{\partial y}\right)\frac{\partial V_{test}}{\partial x} - S\left(\sigma_{yx}\frac{\partial T}{\partial x} + \sigma_{yy}\frac{\partial T}{\partial y}\right)\frac{\partial V_{test}}{\partial y}
\end{aligned}
$$

Seebeck Effect: Thermal BC

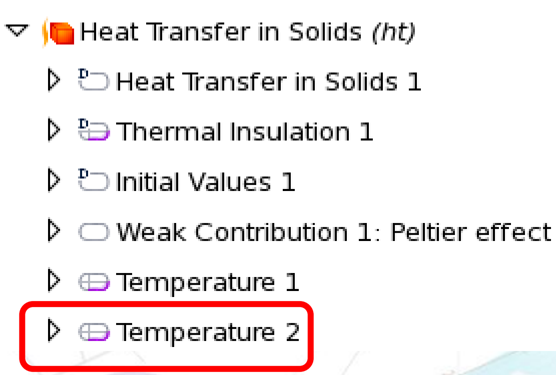
1 Apply fixed temperature T0 at bottom electrodes

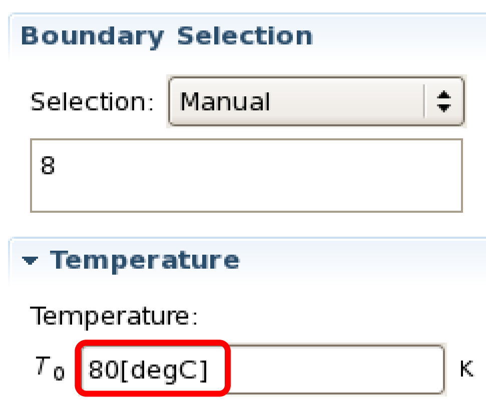


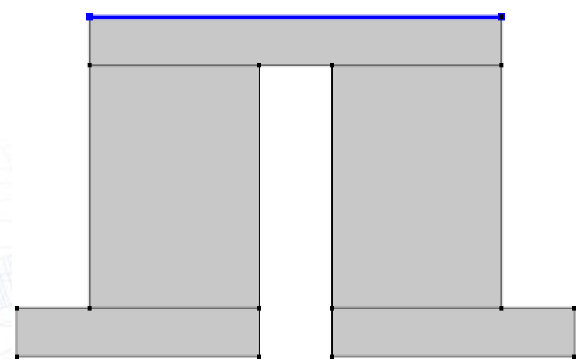




2 Apply fixed temperature 80°C at top electrode







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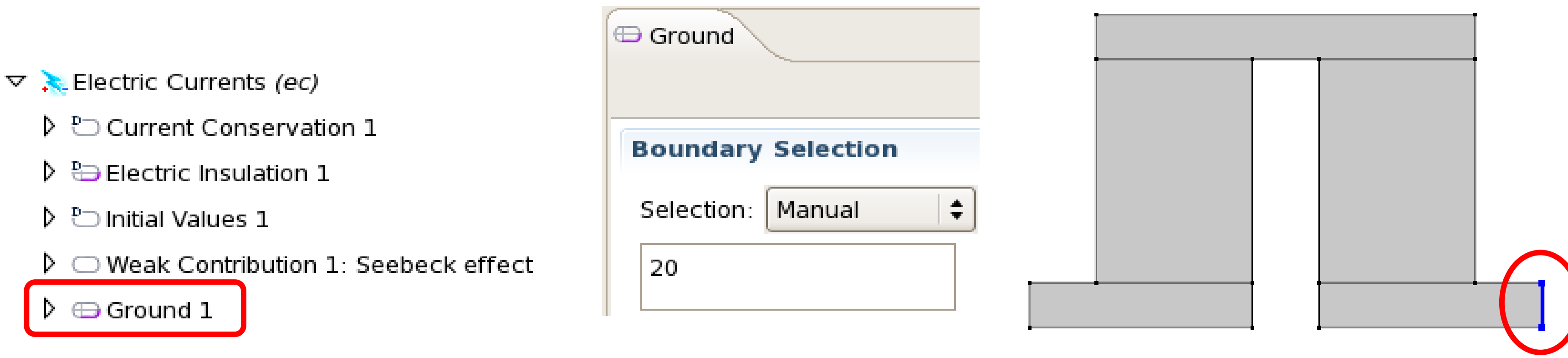
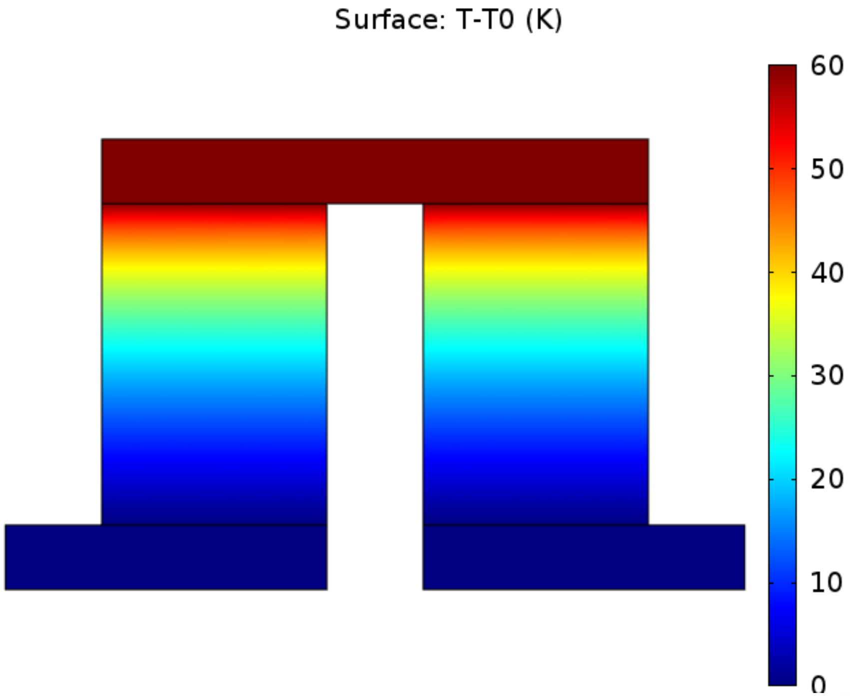
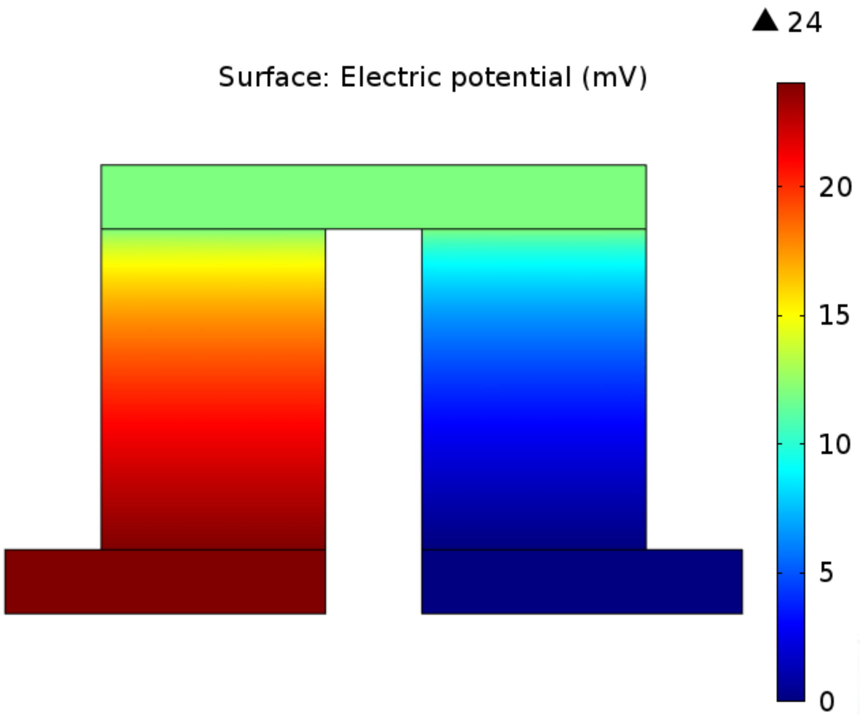
Seebeck Effect: Electrical BC

- Apply ground reference potential at the right boundary of bottom electrode



Seebeck Effect: Results





- Seebeck effect: conversion of temperature differences into electricity