Multiphysics Analysis of Thermoelectric Phenomena

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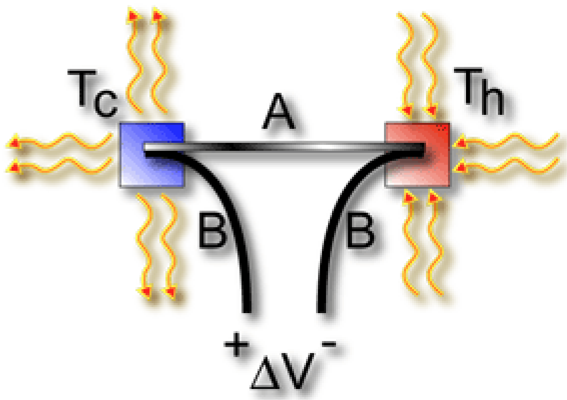
Thermoelectric materials

- **Behavior described by effects:**
  - Seebeck
  - Peltier
  - Thomson
- **Effects linked:**
  - Seebeck is result of Peltier and Thomson

Thermoelectric materials

- **Seebeck effect:**
  - **Voltage due to temperature difference**
  - **Example: Thermocouples, energy conversion**



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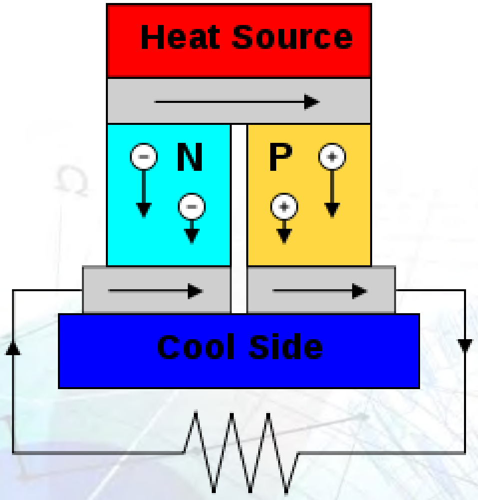
Thermoelectric materials

- **Peltier effect:**
  - Temperature at junction of two materials due to flow of current
  - Direction of current flow determines heating/cooling
  - Examples: Solid state heating/cooling

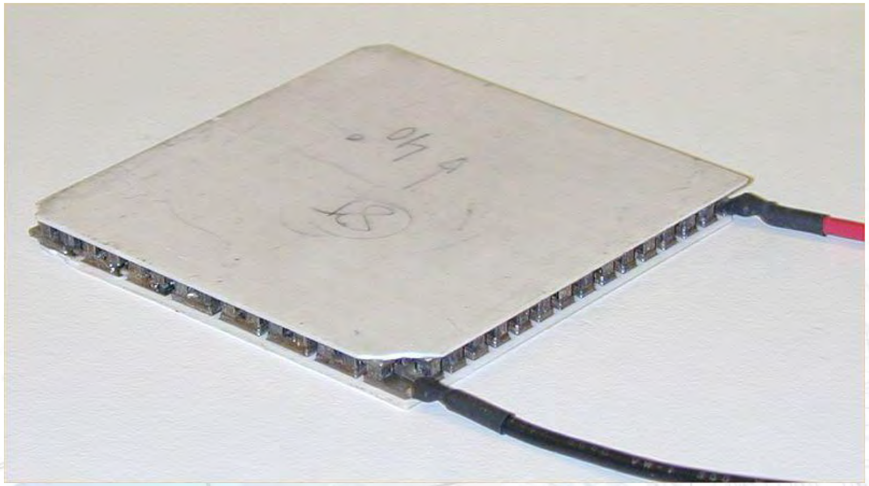


Thermoelectric materials

- **Thomson effect:**
  - **Current flow in a temperature gradient**
  - **Power absorbed or rejected**
  - **Heat is proportional to electric current and temperature**
  - **Seebeck is result of Peltier and Thomson effects**
    - Thomson's second relationship: P = -S . T(K)

Thermoelectric devices

- **Arrays of Peltier cells**
- **Typically Bismuth Telluride**
- **Doped “n” or “p” type semiconductors**
- **Solid state heaters/coolers, thermocouples**



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Governing equations

- **Electric current balance:** $-\nabla \cdot \left(\sigma . \nabla V\right) = 0$
- **Heat energy balance:** $\begin{cases} \rho C_p \dfrac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = Q \\ \mathbf{q} = -k \nabla T + \underline{\underline{P}}\mathbf{J} \end{cases}$
- **Thomson's second relationship:** $P = -ST$
- **Q_{tot} = $Q_{heat\ pump}$ + $Q_{resistive}$ + $Q_{conductive}$**

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Implementation in COMSOL

- **FE methodology**
- **Weak form implementation**
  - **Implment in heat transfer module**
  - **Convert energy balance to weak form**
  - **Multiply each side of energy balance equation by test function**
  - **Integrate over the computational domain**

$$\int_{\Omega} \rho C_p \frac{\partial T}{\partial t} T_{test} d\Omega + \int_{\Omega} \left(\nabla\right) T_{test} d\Omega = \int_{\Omega} Q T_{test} d\Omega$$

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Weak form implementation

- **Apply vector identity:**

$$\nabla \cdot \left(T_{test}\mathbf{q}\right) = \mathbf{q} \cdot \nabla T_{test} + T_{test} \nabla \cdot \mathbf{q}$$

- **Equation becomes:**

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

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Weak form implementation

- **Apply Gauss' theorem:**

$$\int_{\Omega} \nabla\left(T_{test} \cdot \mathbf{q}\right) = \int_{\partial\Omega} T_{test}\mathbf{q} \cdot \mathbf{n}\partial\Omega$$

- **Revised equation:**

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

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Weak form implementation

- **Energy flux:**

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

- **Revised equation:**

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

- **Weak Peltier contribution:**

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

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

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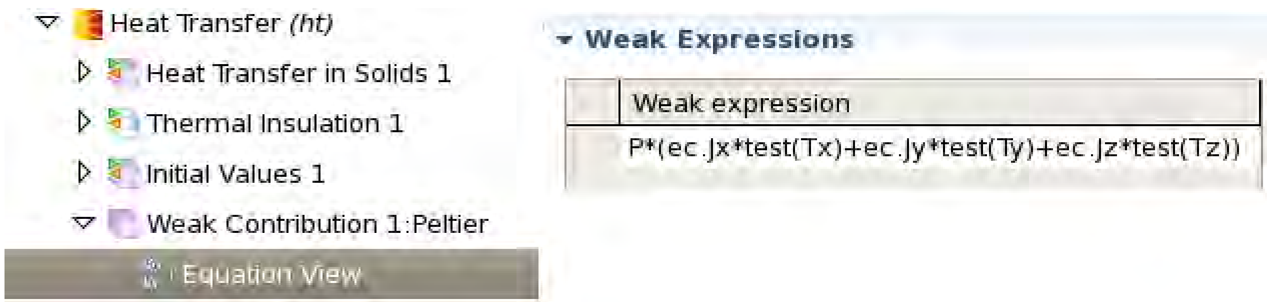
Weak form implementation

- **Implement weak Peltier contribution in Heat Transfer module:**



COMSOL Multiphysics analysis

- **Peltier contribution**
  - **Weak form**
- **Temperature dependent material properties**
  - **Peltier/Seebeck coefficients**
  - **Thermal conductivity**
  - **Electrical conductivity**

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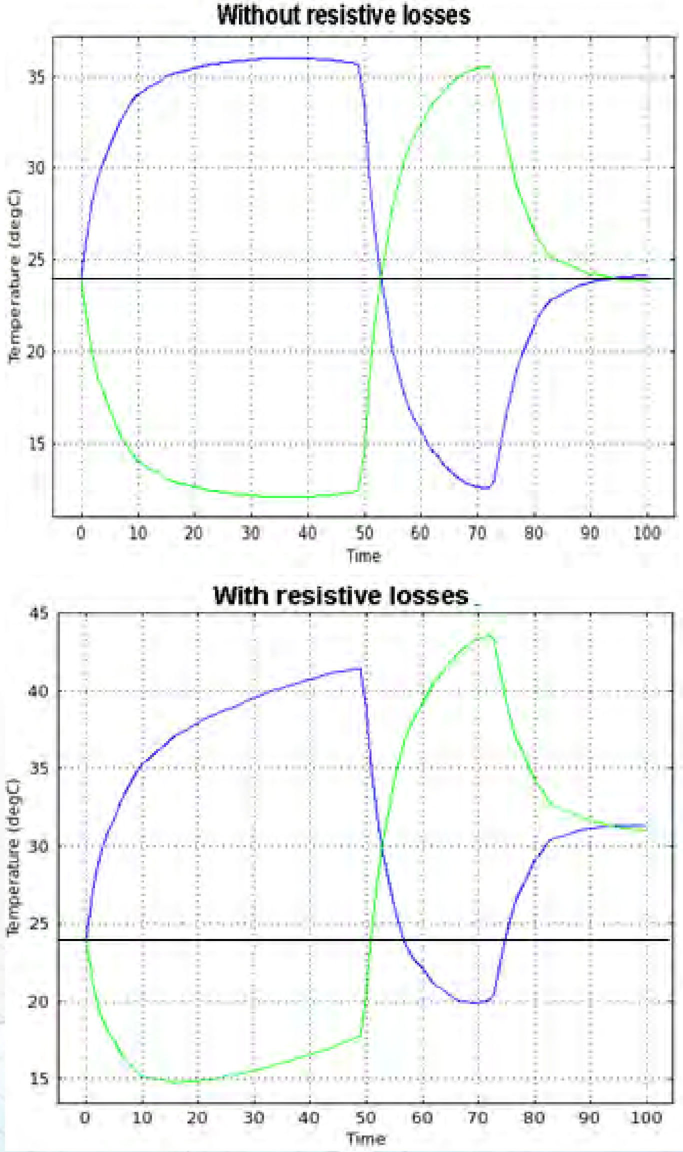
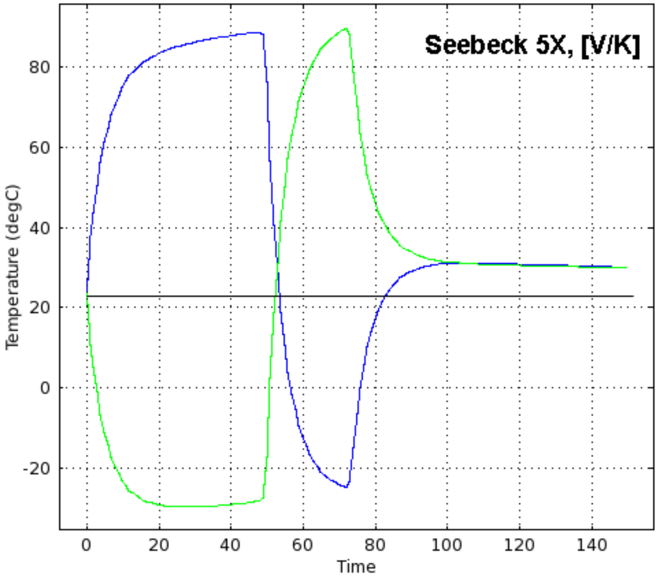
Property variations

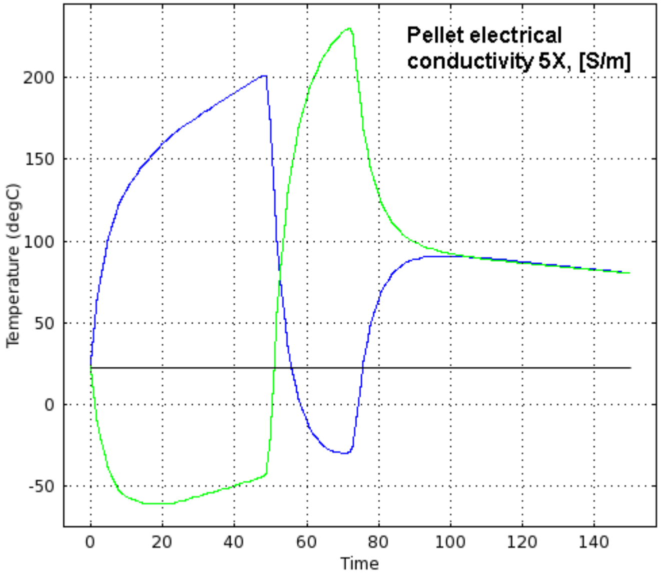
- **Effect of resistive losses**
- **TEM**
  - **Applied current vs time history**
  - **Effect on hot and cold sides**



Property variations

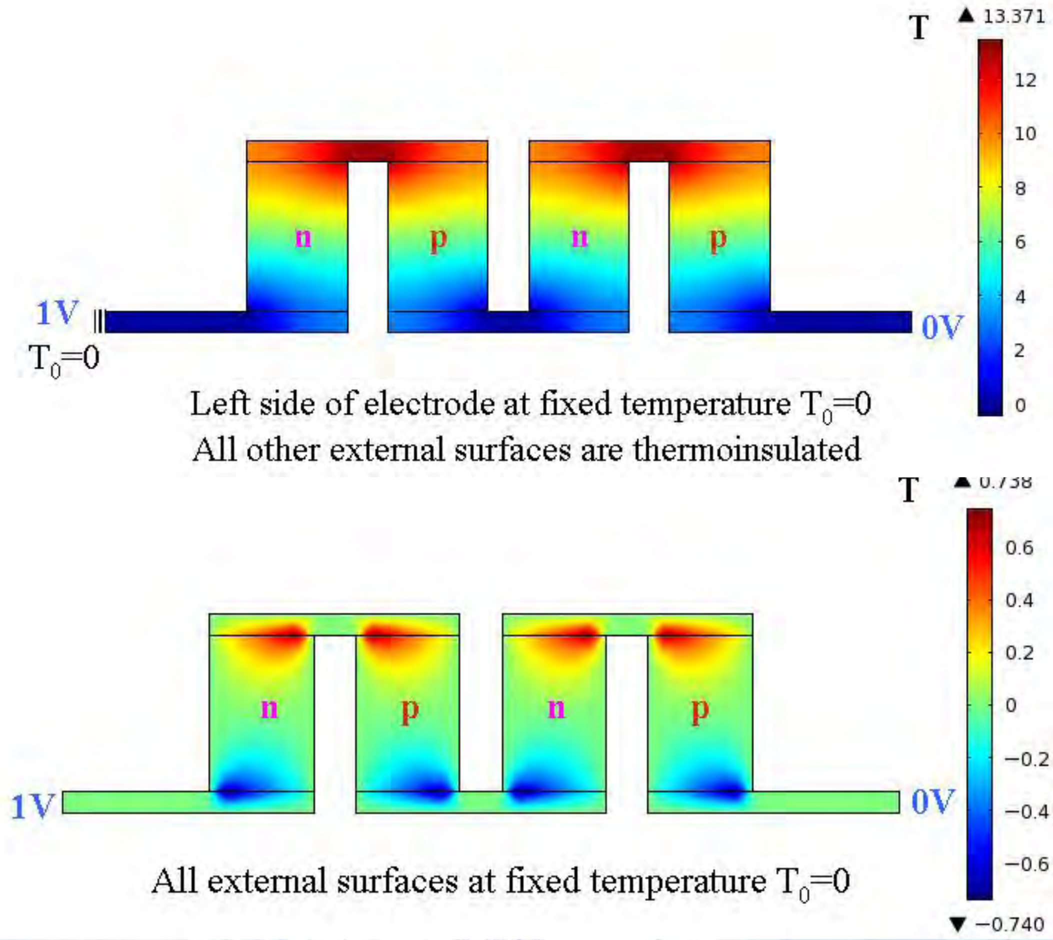
- **TEM: Applied current vs time history**
- **Effect of variation in Seebeck coefficient of 5x**
- **Effect of variation in electrical conductivity of 5x**





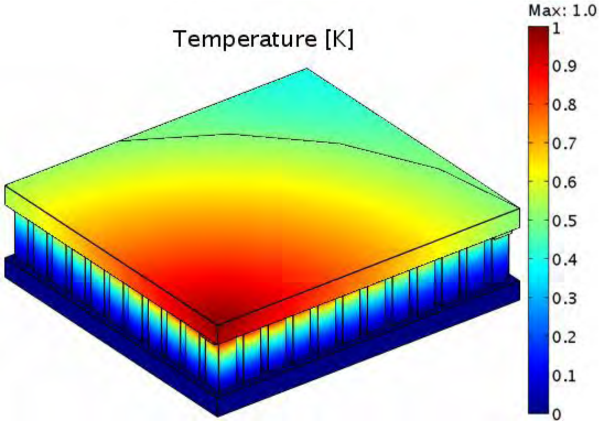
Analytical results: Peltier

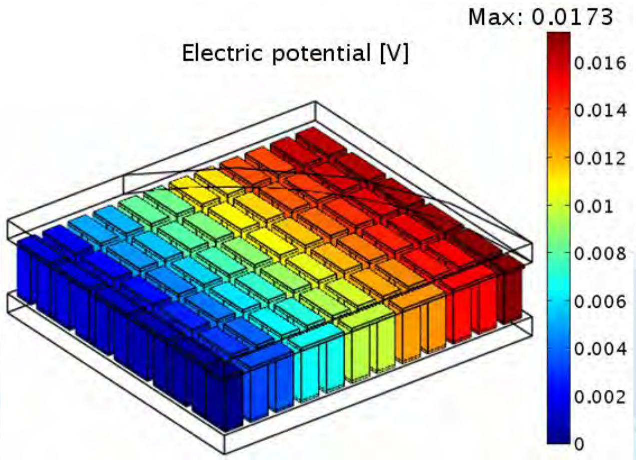
- BiTe3 p-n junctions subject to imposed voltage
- Temperature distribution developed
- Solid state heater/cooler



Analytical results: Seebeck

- **Imposed thermal gradient in BiTe3 TEM**
- **Current generated in array of cells**
- **Magnitude of generated current depends on temperature difference**





Summary

- Peltier/Seebeck terms implemented using weak form methods
- Fully coupled temperature dependent material properties
- Predict effect of imposed thermal gradients
- Predict effect of electric current flow

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