Multiphysics Analysis of Thermoelectric Phenomena

S.P. Yushanov, L.T. Gritter, J.S. Crompton and K.C Koppenhoefer

AltaSim Technologies, LLC

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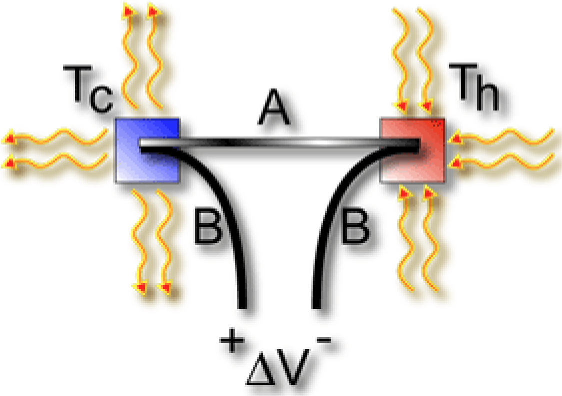
Thermoelectric materials

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

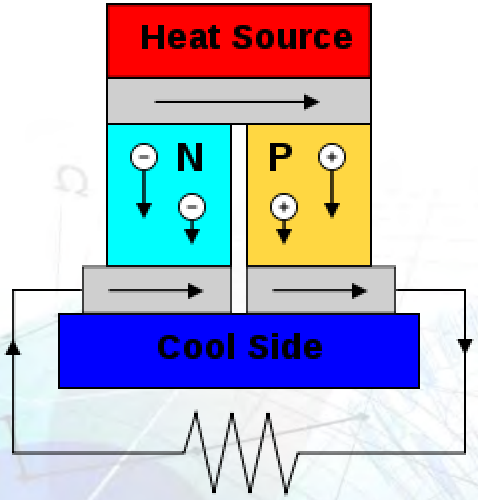
Thermoelectric materials

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



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

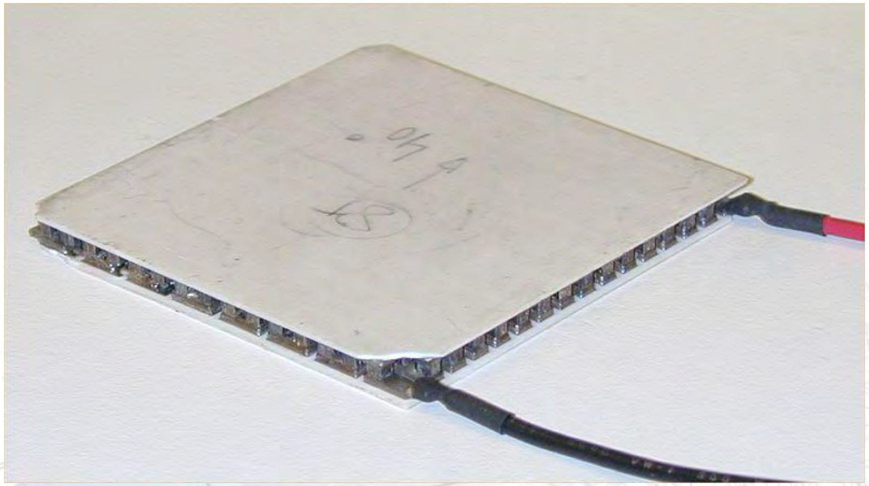


Thermoelectric materials

- **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**

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

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:**

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

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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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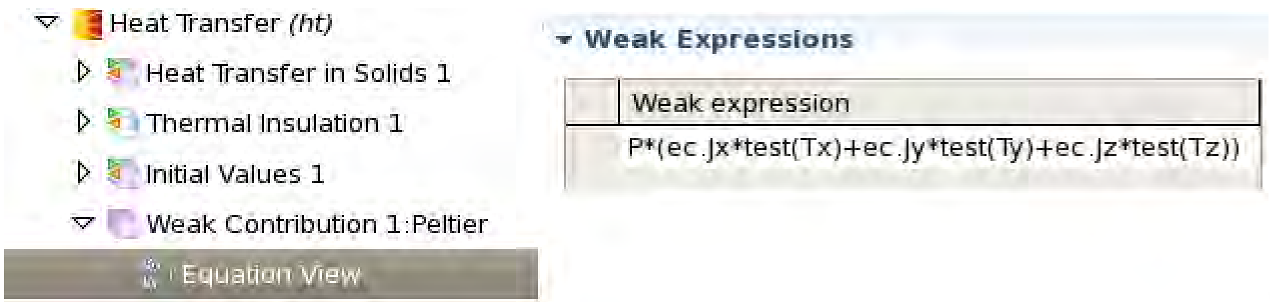
Weak form implementation

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

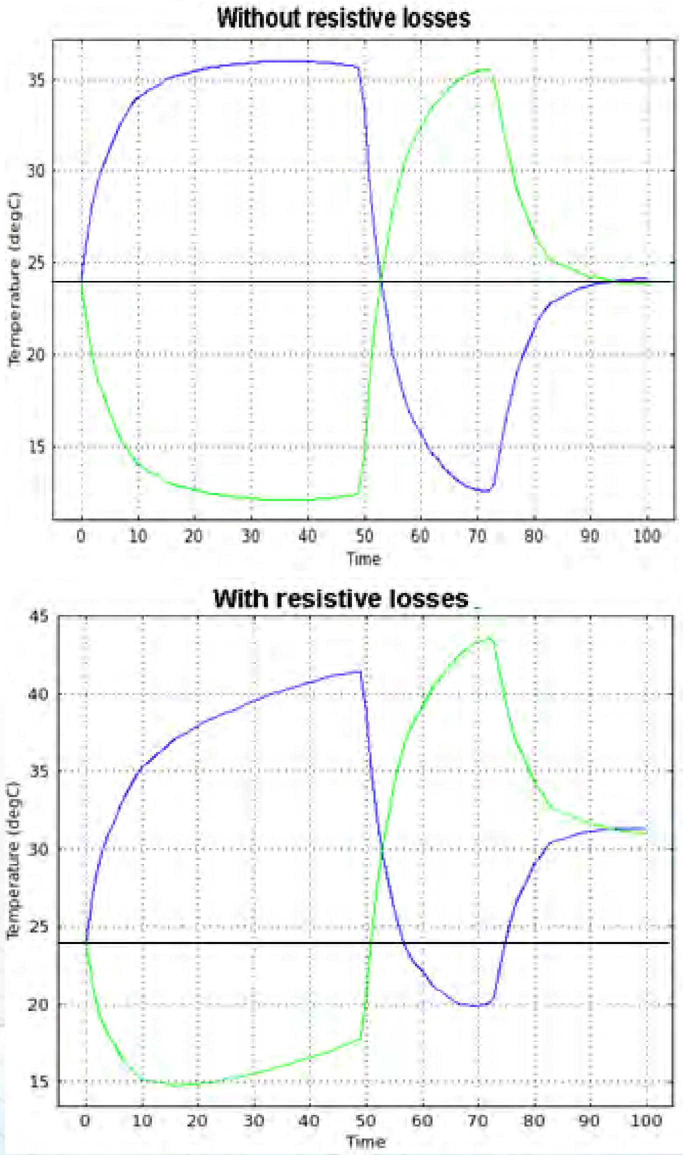


COMSOL Multiphysics analysis

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

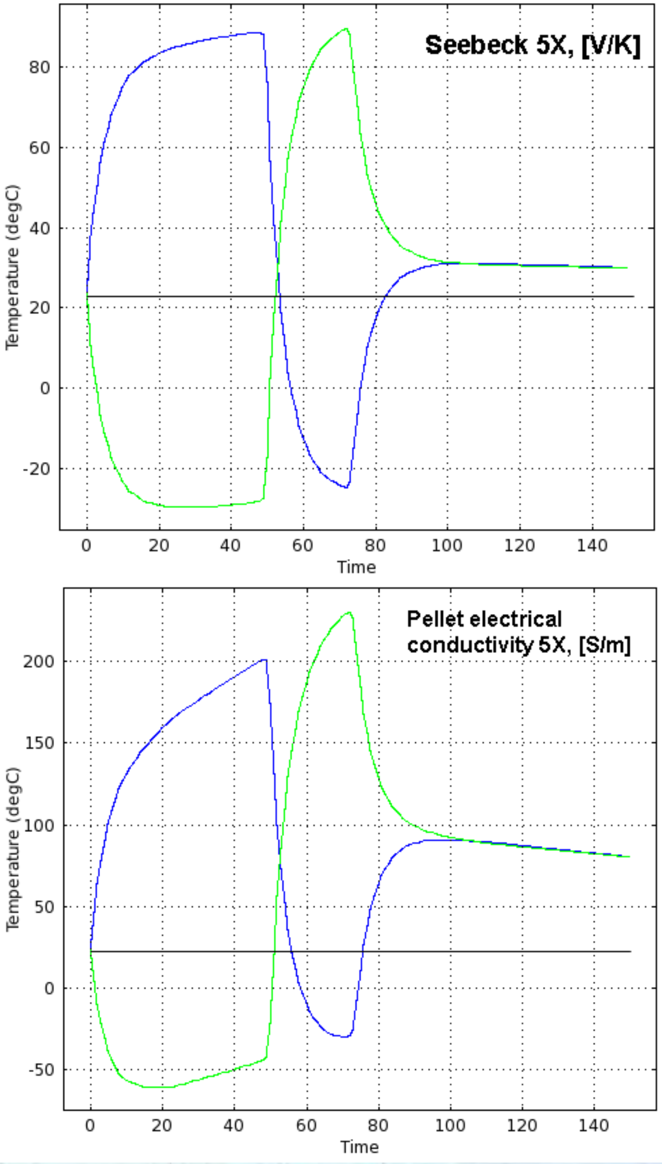
Property variations

- **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**



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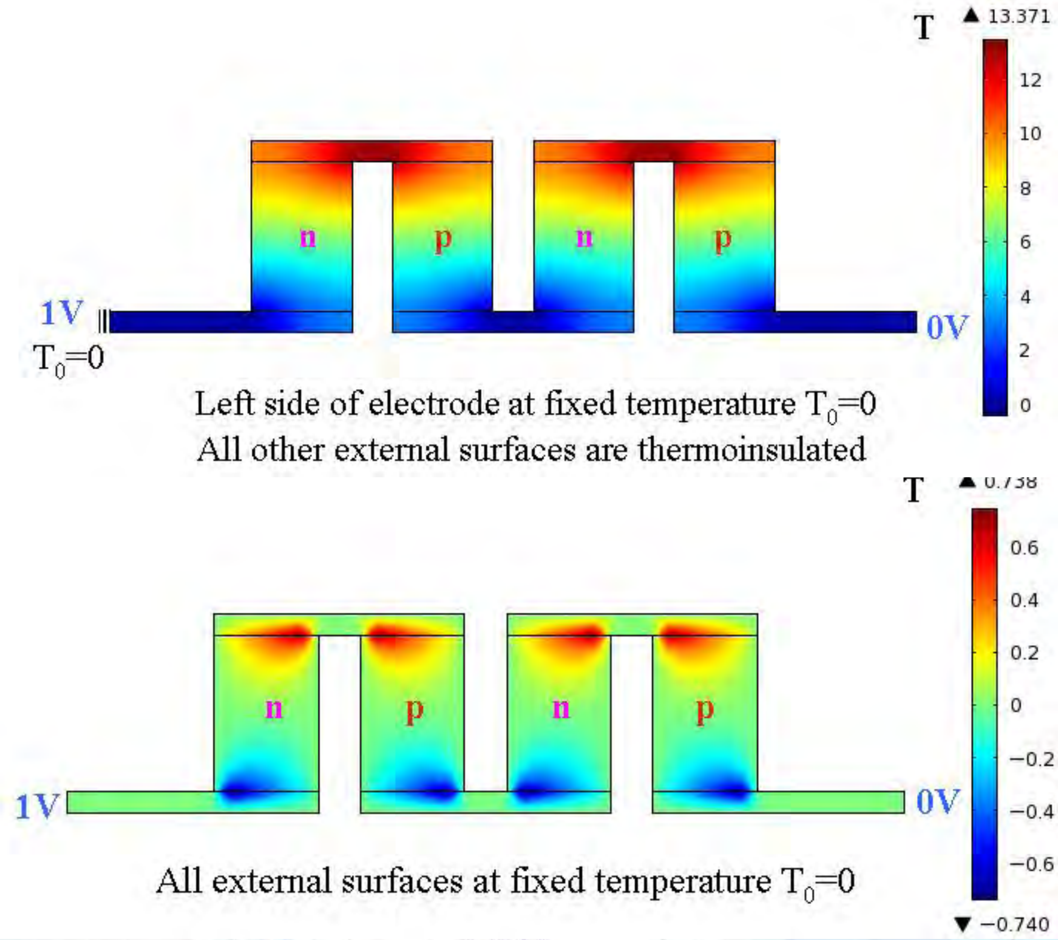
Analytical results: Peltier

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



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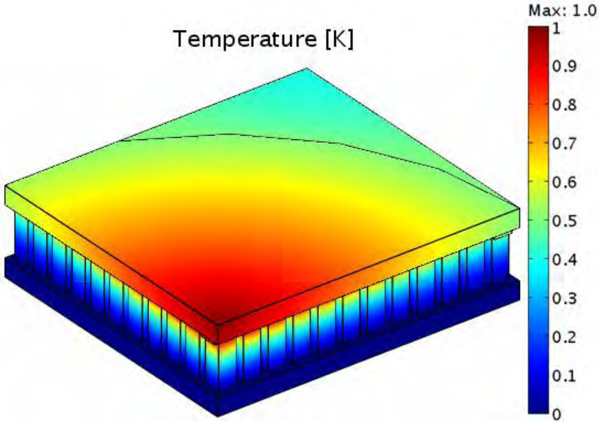
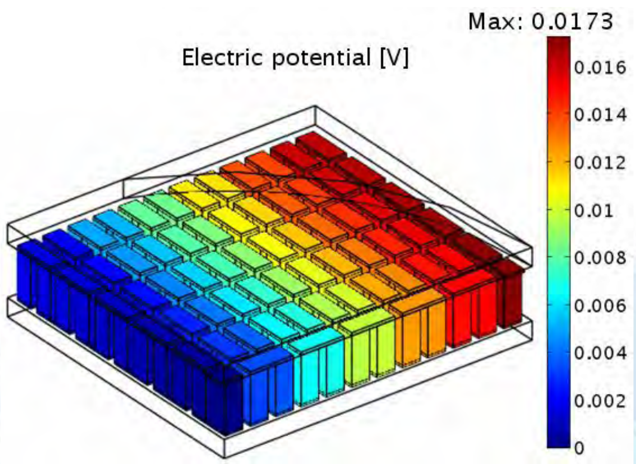
Analytical results: Seebeck

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





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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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