Multiphysics Simulation of Thermoelectric Systems

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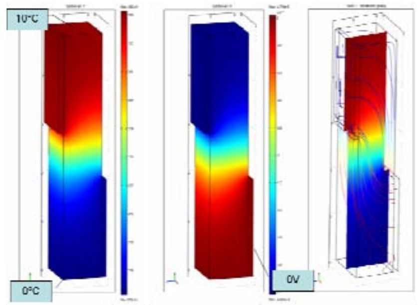
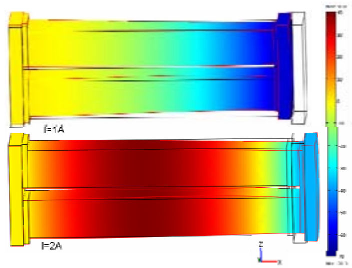
Contents

$$-\vec{\nabla}((\sigma\alpha^2 T+\lambda)\vec{\nabla}T)-\vec{\nabla}(\sigma\alpha T\vec{\nabla}V)=\sigma((\vec{\nabla}V)^2+\alpha\vec{\nabla}T\vec{\nabla}V)$$

$$\vec{\nabla}(\sigma\alpha\vec{\nabla}T)+\vec{\nabla}(\sigma\vec{\nabla}V)=0$$

$$\begin{aligned}
&e_a\frac{\partial^2 u}{\partial t^2}+d_a\frac{\partial u}{\partial t}+\nabla\cdot(-c\nabla u-\alpha u+\gamma)+\beta\cdot\nabla u+au=f && \text{in } \Omega\\
&n\cdot(-c\nabla u-\alpha u+\gamma)+qu=g-h^T\mu && \text{on } \partial\Omega\\
&hu=r && \text{on } \partial\Omega
\end{aligned}$$





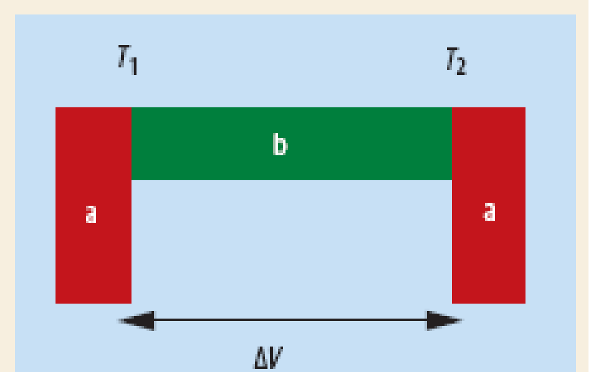
1. Introduction
2. Equations to solve
3. Implementation in COMSOL
4. Thermoelectric modeling
5. Thermo-electric-mechanic calculations

Introduction

Seebeck-Effect

T. Seebeck (1821)

$\alpha = \Delta V / \Delta T$



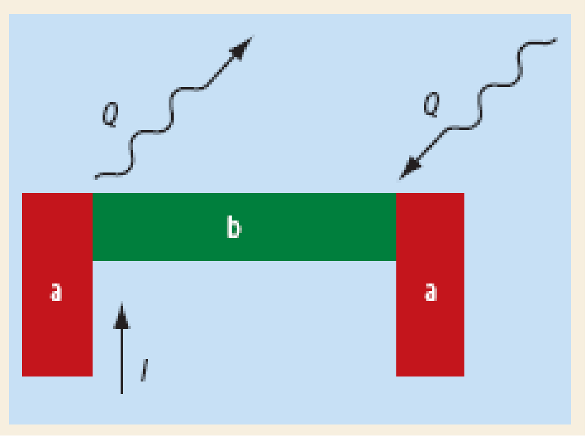
Physik Journal, Mai 2007,
Sommerlatte, Nielsch, Böttner

Peltier-Effect

J. C. A. Peltier (1834)

$Q = \Pi * I$

$\Pi = \alpha * T$



Thermoelectric Figure of Merit Z

$$Z = \frac{\sigma \alpha^2}{\lambda}$$

α: Seebeck Coefficient

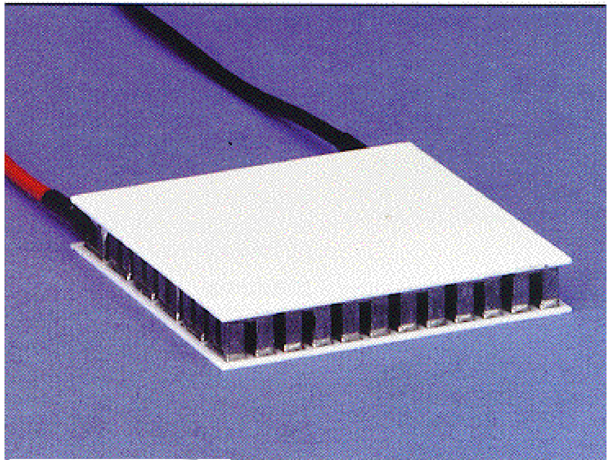
Π: Peltier Coefficient

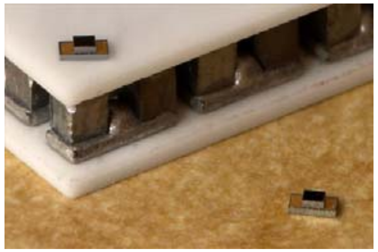
σ, λ: electrical and thermal conductivities

Introduction

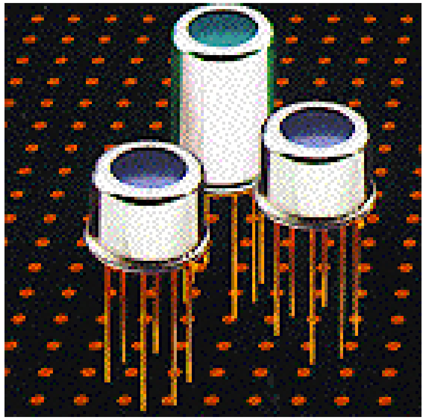
Applications of Thermoelectrics

Coolers

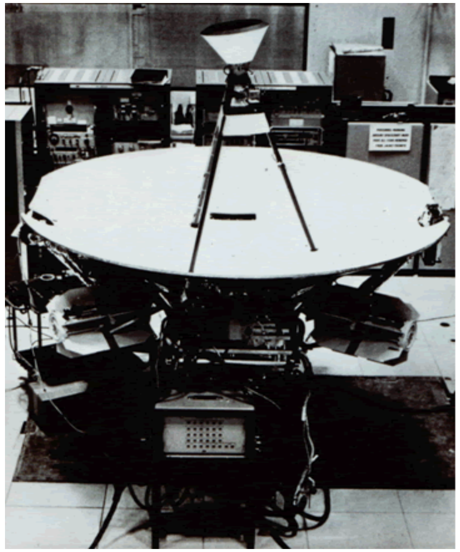


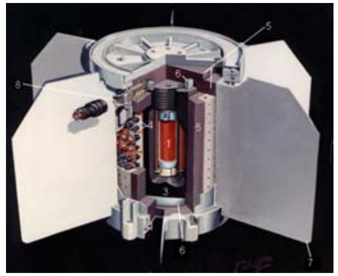


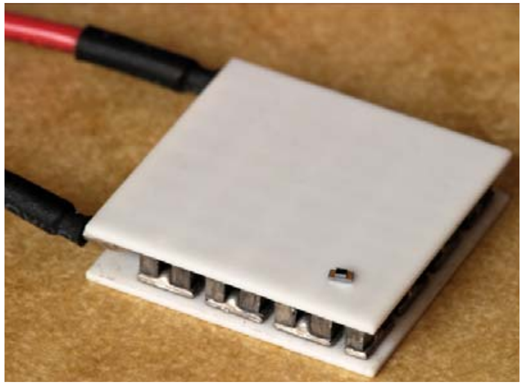
Detectors, Sensors



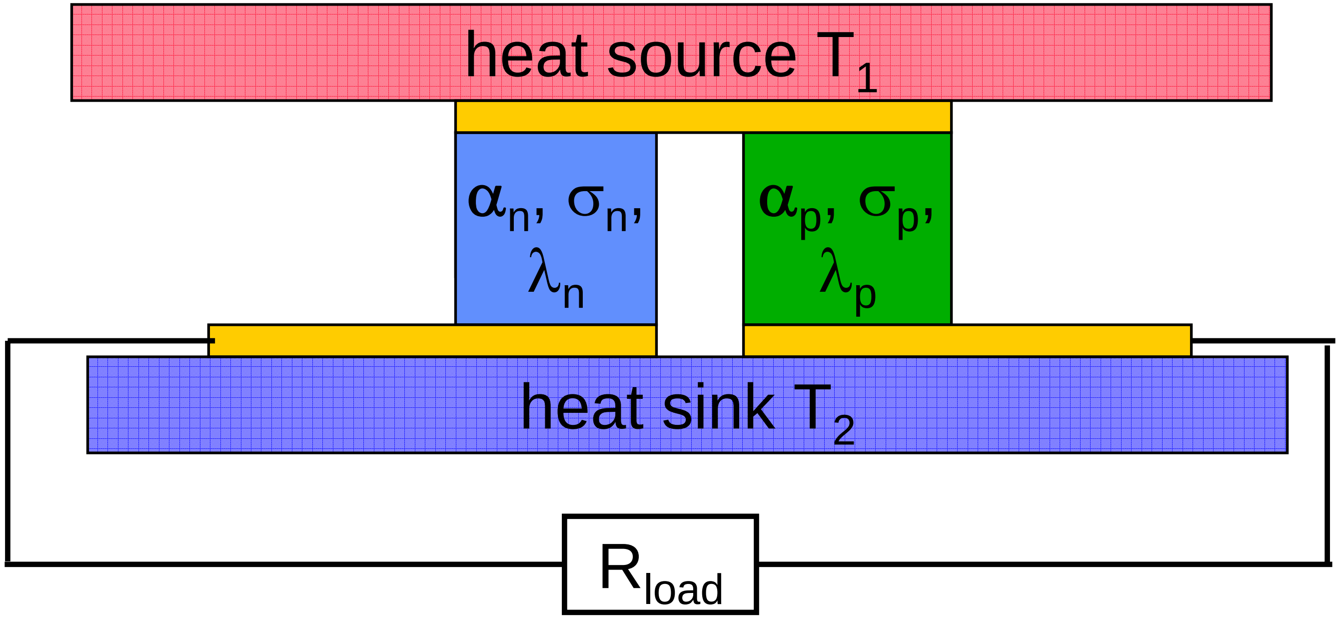
Generators







Introduction



Seebeck-Coefficient

α_n and α_p

Electrical Conductivity

σ_n and σ_p

Thermal Conductivity

λ_n and λ_p

Dimensionless Figure of Merit ZT

$$ZT = \frac{\sigma \alpha^2}{\lambda} T$$

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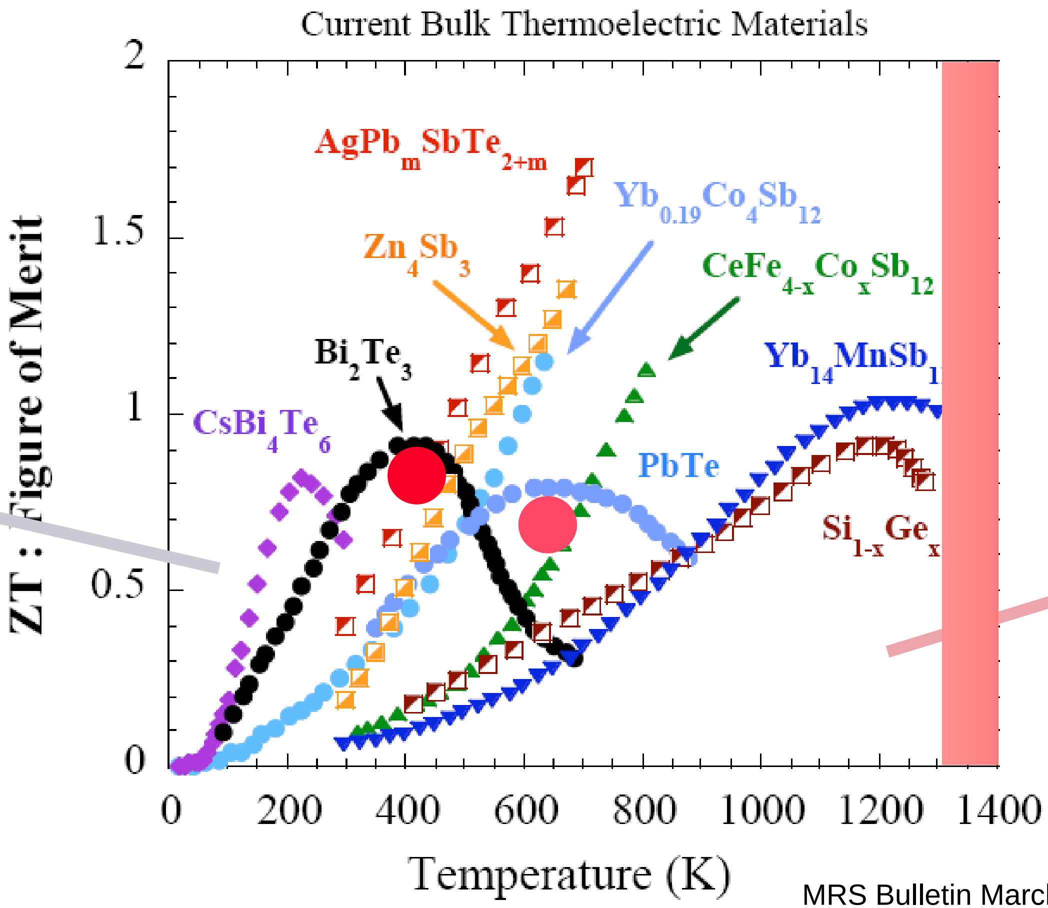
Introduction

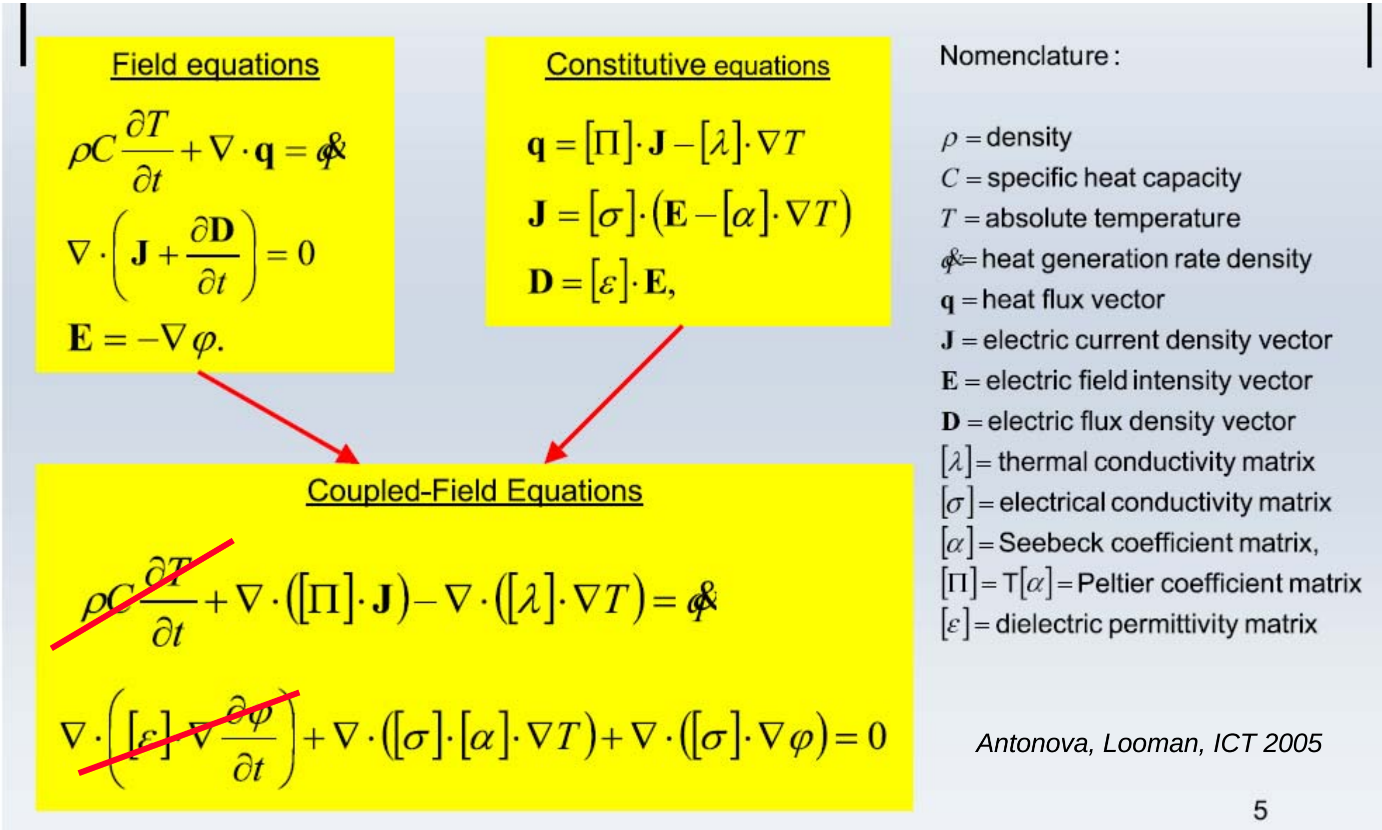
cooling



MRS Bulletin March, 2006

waste heat

Thermoelectric Effects in ANSYS 9 and higher (Antonova et al., ICT 2005)



Example for COMSOL implementation:

Rearrange equations …

$$-\vec{\nabla}((\sigma\alpha^2 T + \lambda)\vec{\nabla} T) - \vec{\nabla}(\sigma\alpha T \vec{\nabla} V) = \sigma((\vec{\nabla} V)^2 + \alpha \vec{\nabla} T \vec{\nabla} V)$$

$$\vec{\nabla}(\sigma\alpha\vec{\nabla} T) + \vec{\nabla}(\sigma\vec{\nabla} V) = 0$$

Thermoelectrics in COMSOL:

Rearrange equations … $$-\vec{\nabla}((\sigma\alpha^2 T + \lambda)\vec{\nabla}T) - \vec{\nabla}(\sigma\alpha T\vec{\nabla}V) = \sigma((\vec{\nabla}V)^2 + \alpha\vec{\nabla}T\vec{\nabla}V)$$

$$\vec{\nabla}(\sigma\alpha\vec{\nabla}T) + \vec{\nabla}(\sigma\vec{\nabla}V) = 0$$

… to match with PDE-application modes (coefficient form, different notation!)

$$c_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla\cdot(-c\nabla u - \alpha u + \gamma) + \beta\cdot\nabla u + au = f \qquad in \quad \Omega$$

$$n\cdot(-c\nabla u - \alpha u + \gamma) + qu = g - h^T\mu \qquad on \quad \partial\Omega$$

$$hu = r \qquad on \quad \partial\Omega$$

Thermoelectrics in COMSOL:

Thermoelectric coupled field equations

$$-\vec{\nabla}((\sigma\alpha^2 T+\lambda)\vec{\nabla}T)-\vec{\nabla}(\sigma\alpha T\vec{\nabla}V)=\sigma((\vec{\nabla}V)^2+\alpha\vec{\nabla}T\vec{\nabla}V)$$

$$\vec{\nabla}(\sigma\alpha\vec{\nabla}T)+\vec{\nabla}(\sigma\vec{\nabla}V)=0$$

… example: static thermoelectrics

$$\cancel{c_a\frac{\partial^2 u}{\partial t^2}}+\cancel{d_a\frac{\partial u}{\partial t}}+\nabla\cdot(-c\nabla u-\cancel{\alpha u+\gamma})+\cancel{\beta\cdot\nabla u}+\cancel{au}=f \qquad in \quad \Omega$$

$$n\cdot(-c\nabla u-\cancel{\alpha u+\gamma})+\cancel{qu}=g-h^T\mu \qquad on \quad \partial\Omega$$

$$hu=r \qquad on \quad \partial\Omega$$

Thermoelectrics in COMSOL:

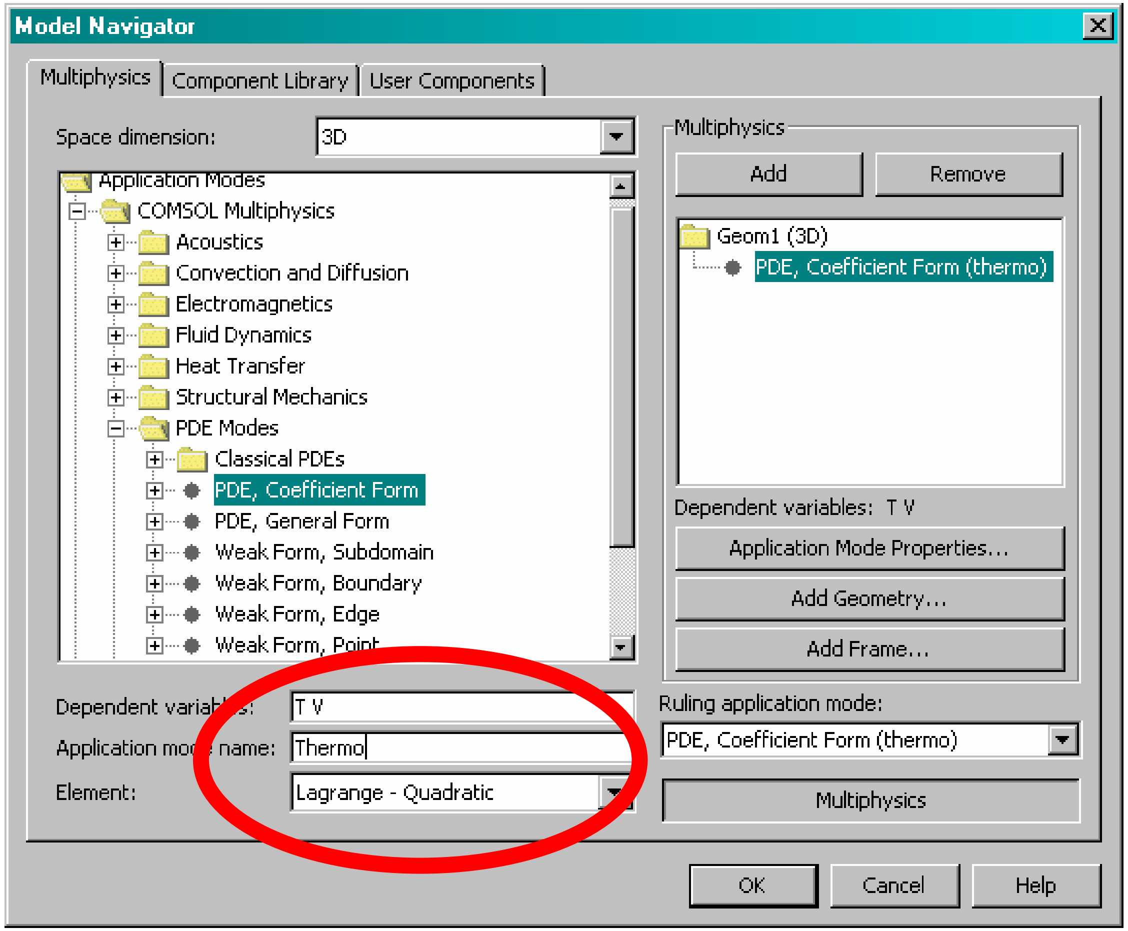
Defining

-Application mode

PDE-Mode, coefficient Form

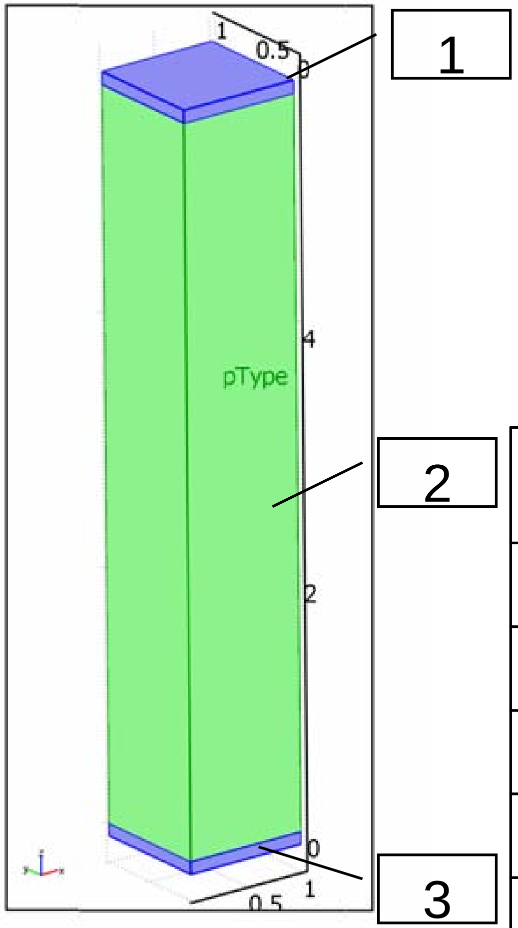
- Field Variable

$$\vec{u} = \begin{pmatrix} T \\ V \end{pmatrix}$$



Thermoelectrics in COMSOL:

Defining model geometry, example:
P-Type thermoelectric leg



		Thermoelectric Material, 2	Electrode (Copper), 1, 3
Seebeck Coefficient	**α, V/K**	**p: 200e-6 n: -200e-6**	**6.5e-6**
Electric conductivity	**σ, S/m**	**1.1e5**	**5.9e8**
Thermal conductivity	**λ, W/m/K**	**1.6**	**350**
Density	**ρ, kg/m³**	**7740**	**8920**
Heat capacity	**C, J/kg/K**	**154.4**	**385**

Antonova, Looman, ICT 2005

1, 3: Copper electrodes
wxlxh: 1x1x0.1mm³

2: p-type thermoelectric leg
wxlxh: 1x1x5.8mm³

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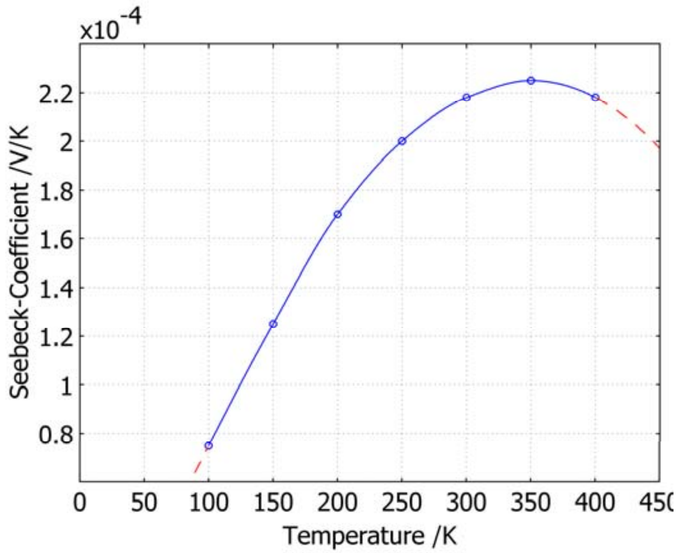
Thermoelectrics in COMSOL:

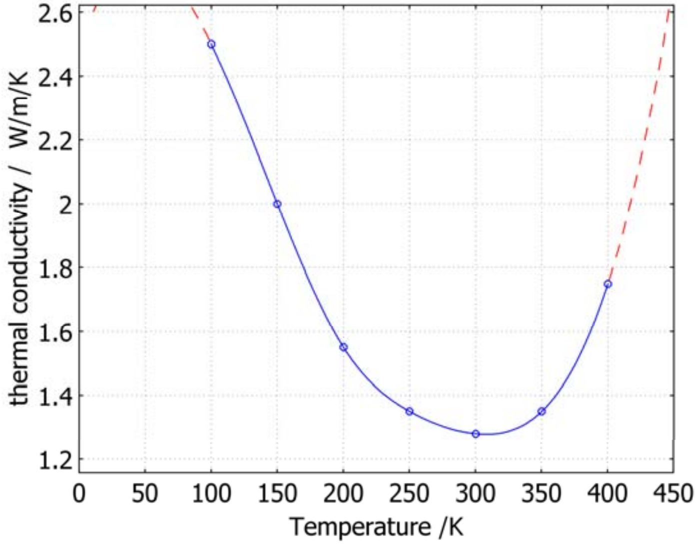
Temperature dependent material properties for p-Bismuth Telluride

T /K	α / 10^{-6}V/K	λ / W/m/K	σ / 10^{3}A/V/m
100	75	2.5	185
150	125	2	142
200	170	1.55	100
250	200	1.35	72
300	218	1.28	60
350	225	1.35	55
400	218	1.75	70

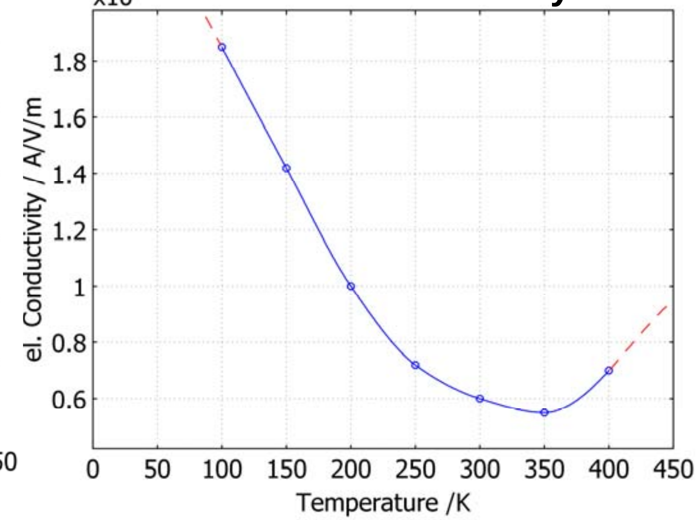
Seebeck-coefficient α



thermal conductivity λ

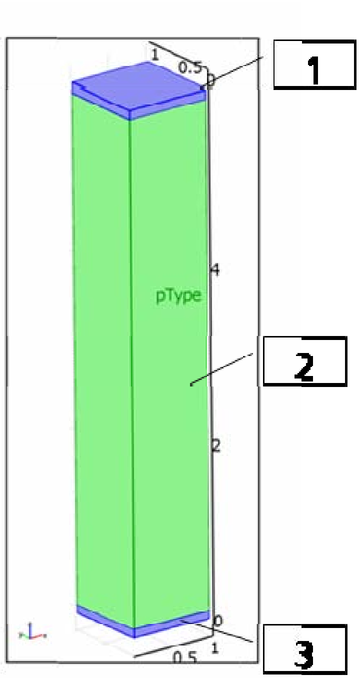


electrical conductivity σ



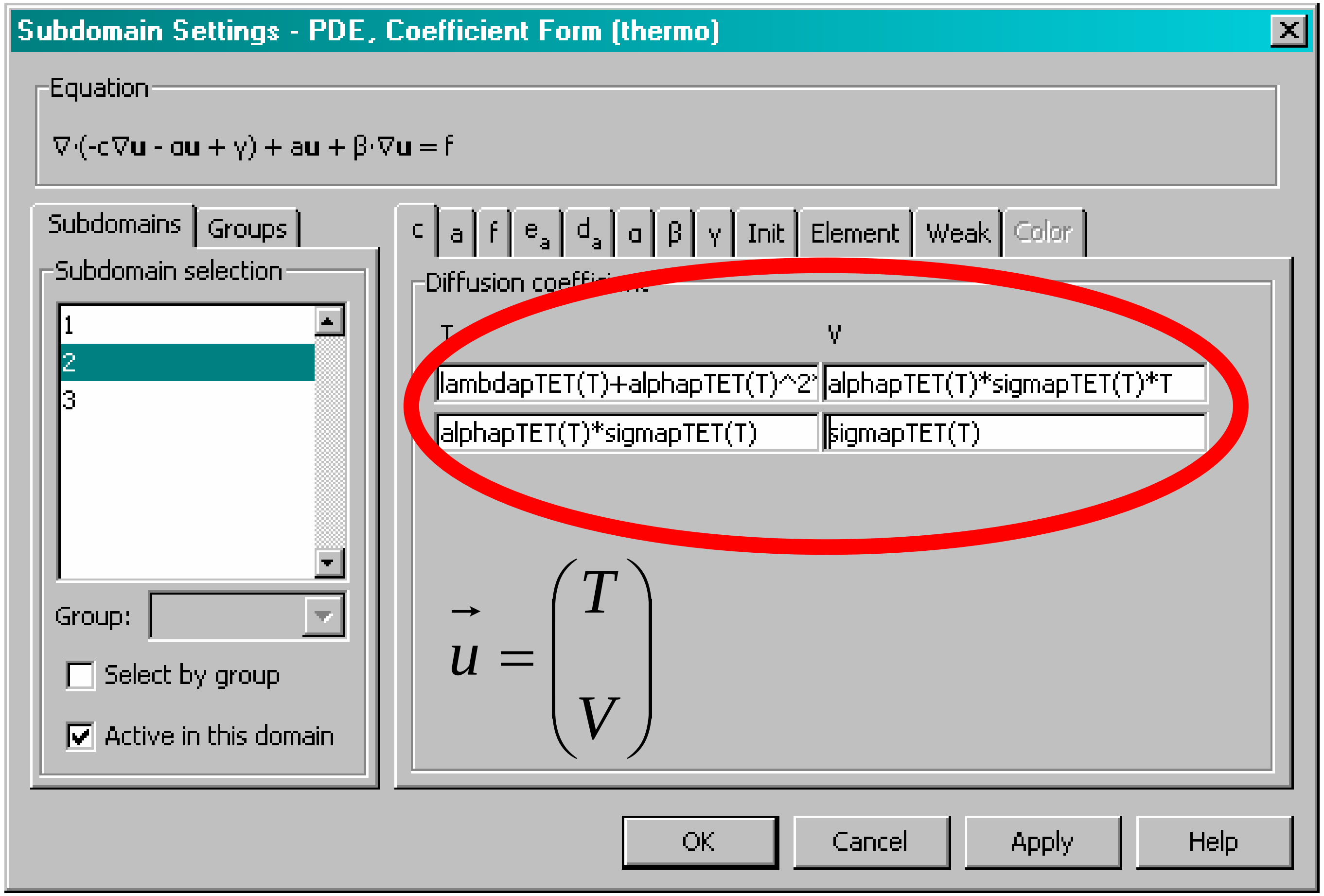
Seifert, W., Ueltzen, M., Müller, E.; One Dimensional Modelling of Thermoelectric Cooling; phys.stat.sol. (a) 194, No.1, pp 277 – 290; 2002

Thermoelectrics in COMSOL:



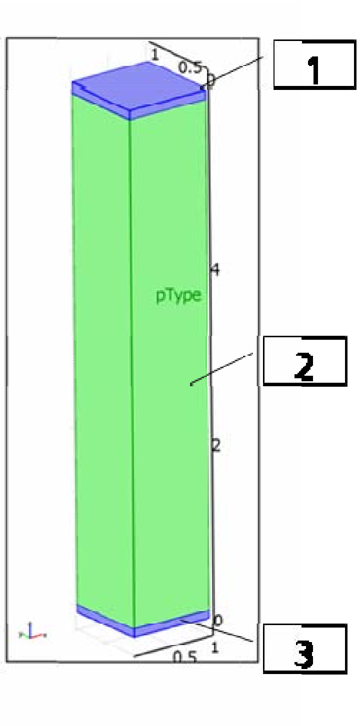
Defining coefficient c:

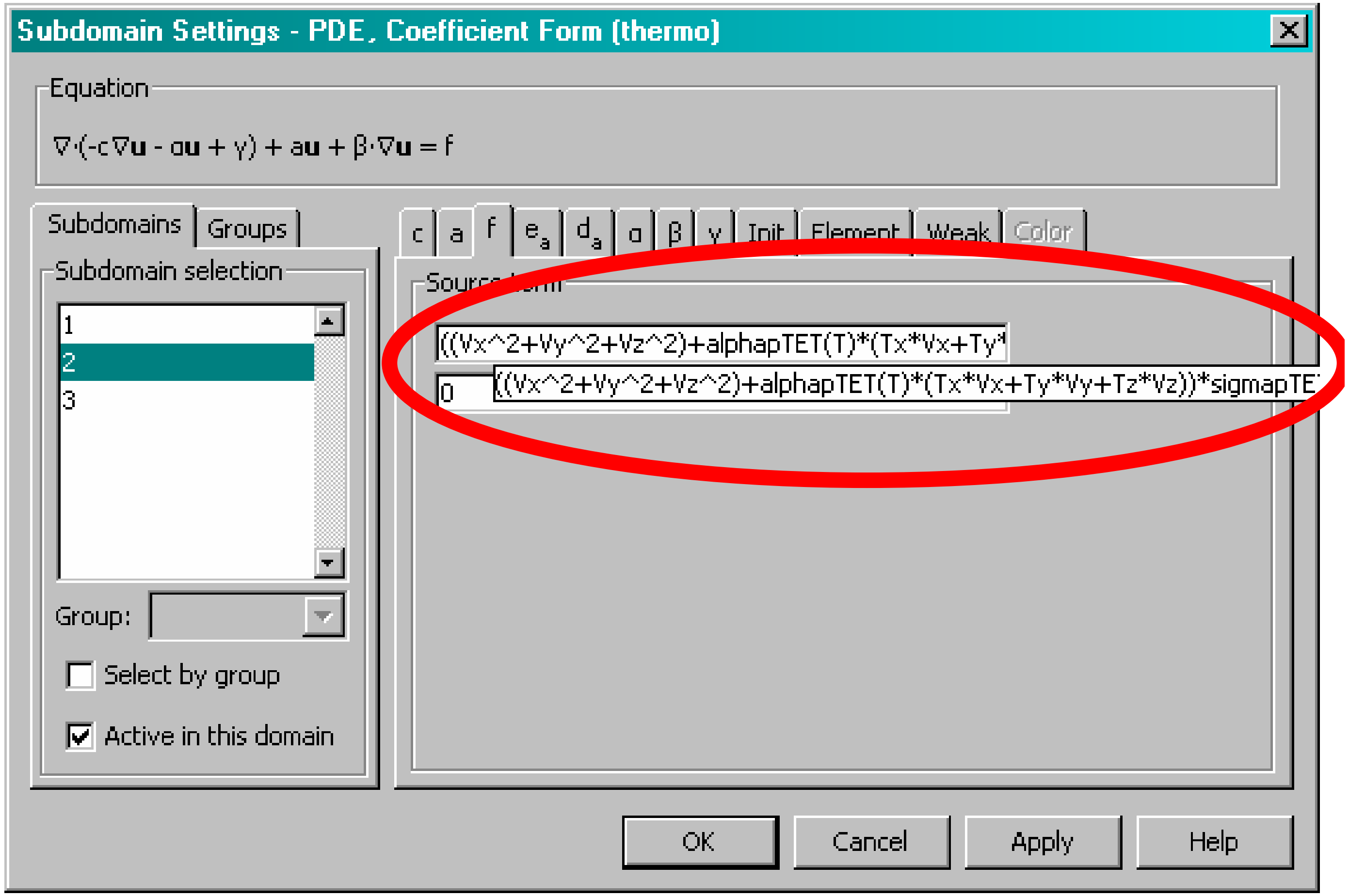
$$c = \begin{pmatrix} \lambda + \sigma\alpha^2 T & \sigma\alpha T \\ \sigma\alpha & \sigma \end{pmatrix}$$



$$\vec{u} = \begin{pmatrix} T \\ V \end{pmatrix}$$

Thermoelectrics in COMSOL:

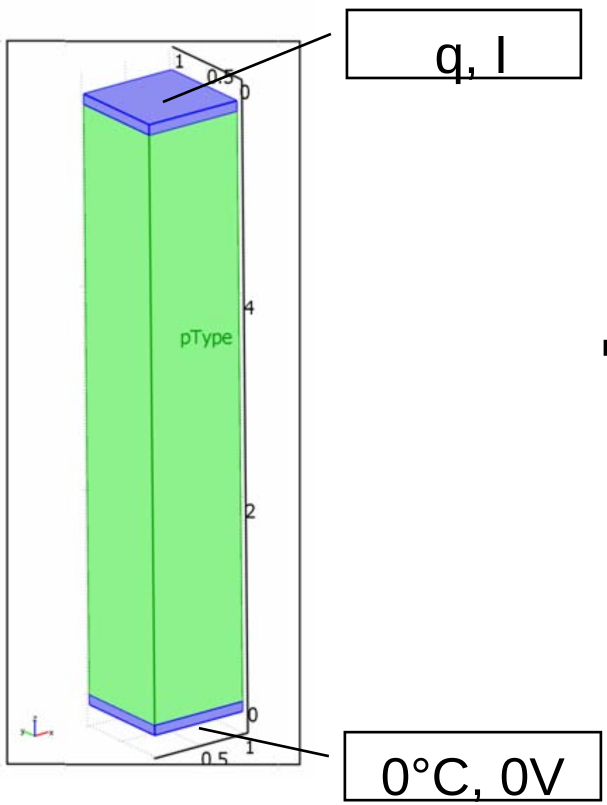




Defining coefficient f

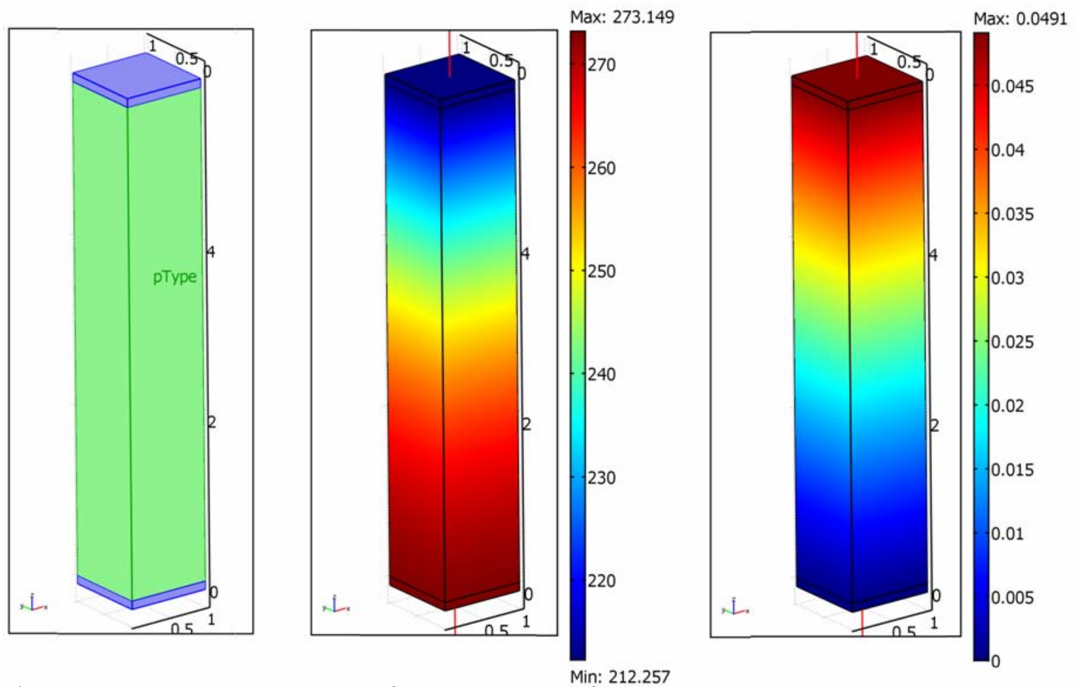
$$f = \begin{pmatrix} \sigma\left(\left(\vec{\nabla}V\right)^2 + \alpha\vec{\nabla}T\vec{\nabla}V\right) \\ 0 \end{pmatrix}$$

Thermoelectrics in COMSOL:



solve →

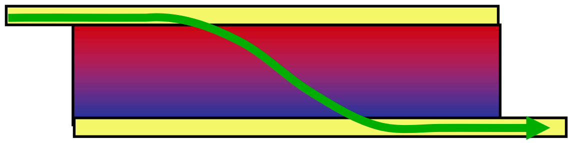
Geometry Temperature Voltage

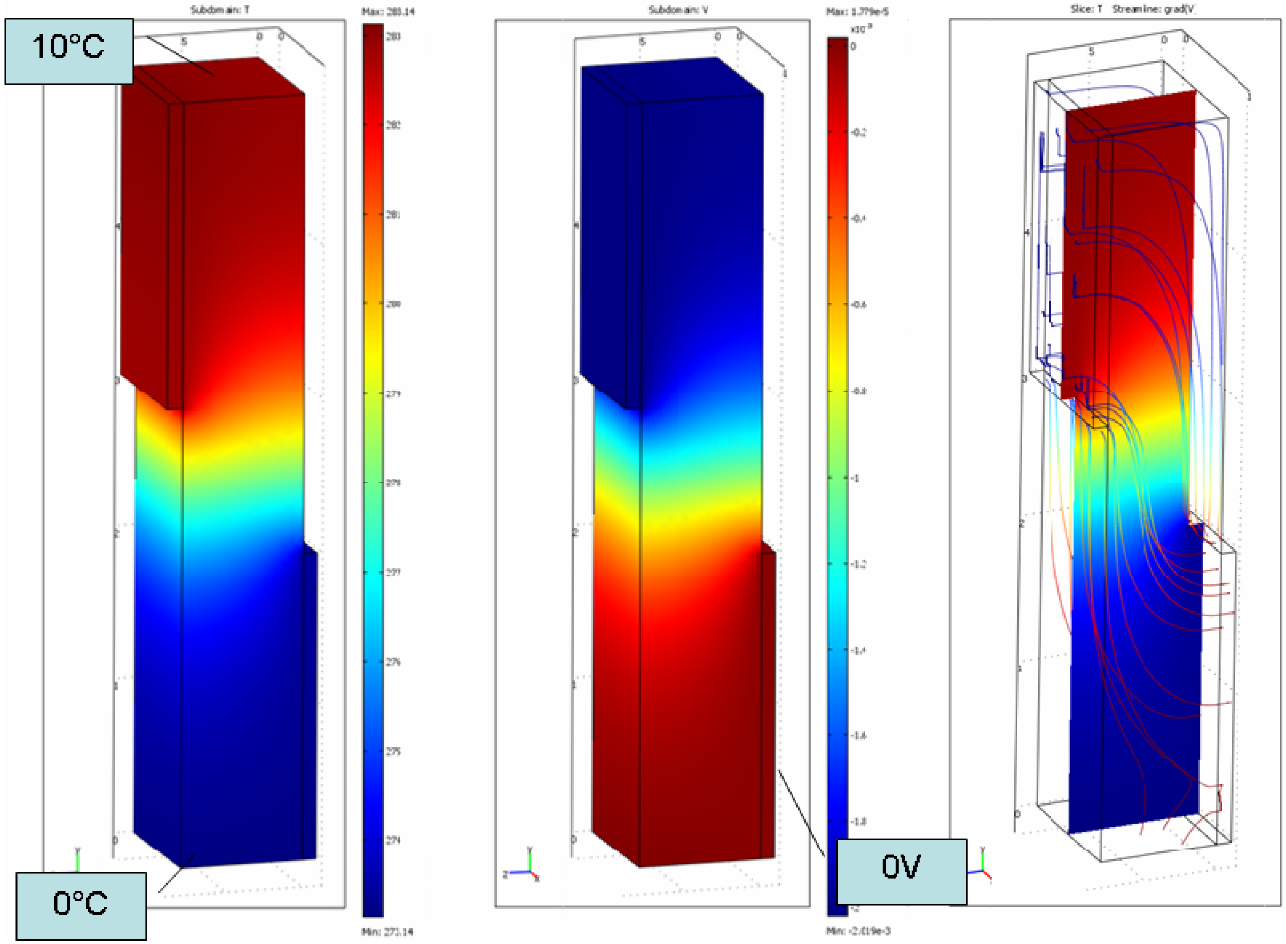


A p-type thermoelectric element is contacted by copper electrodes (left). The base is kept at 0°C and 0V. At the top 0.7A current was applied. Adiabatic boundary conditions were used. The resulting temperature distribution is shown in the center, the voltage is shown right. A temperature difference of nearly 61 K is achieved. The voltage at the upper electrode is 49 mV.

Boundary conditions:
Heat load q (here 0W), current I

„complex “ geometries

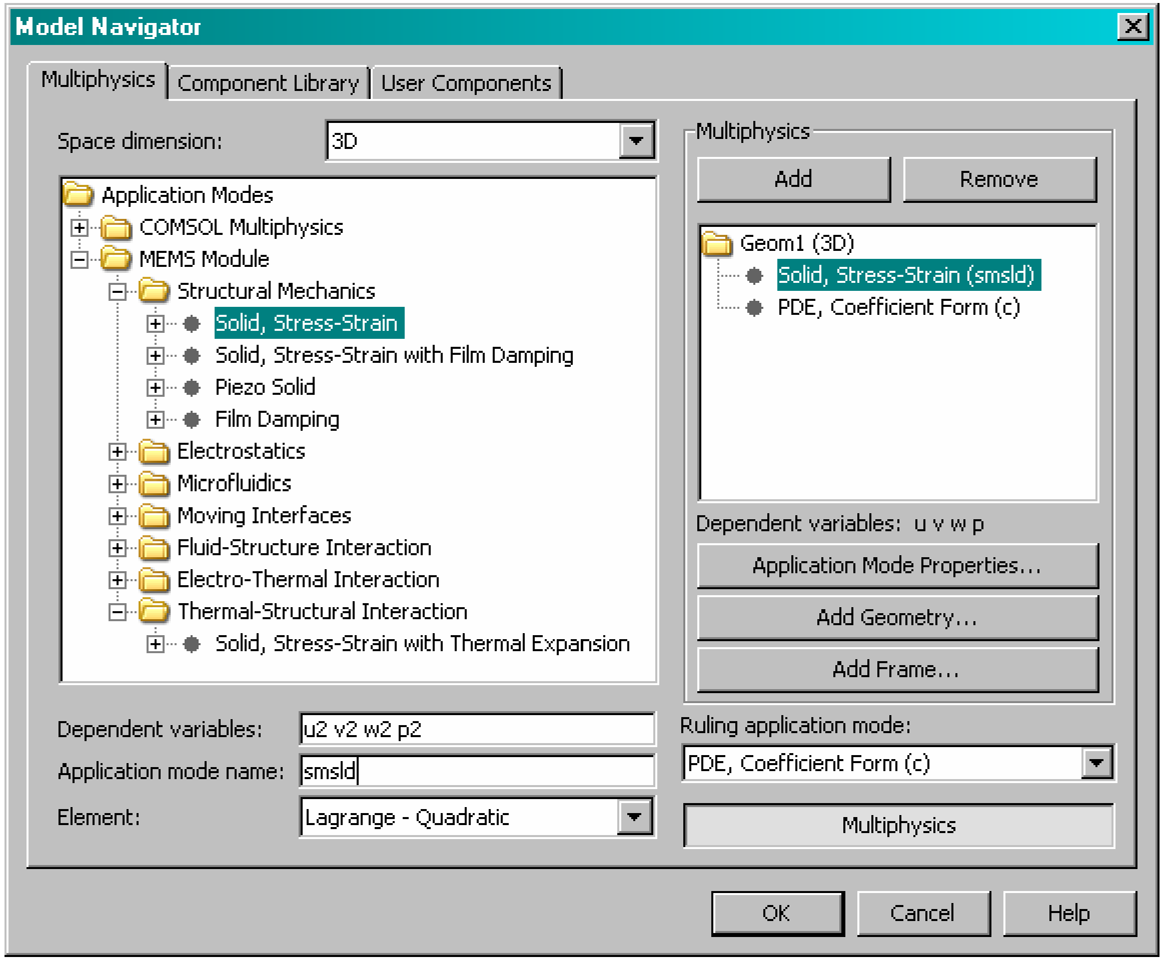




Example for a more “complex” element geometry: The copper electrodes are laterally connected (with respect to the temperature gradient). Left side: Temperature distribution, the top is set to 10°C, the base is at 0°C. The appropriate Voltage is shown in the middle; the left graph shows the voltage color coded electric streamlines and the temperature as a slice plot.

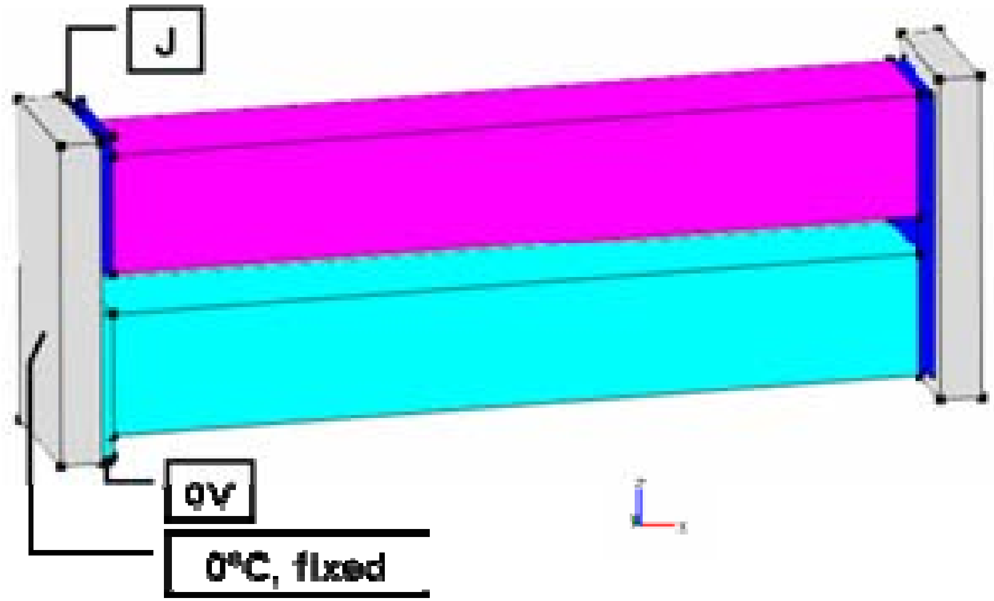
Thermal- electric- mechanic effects

Temperature
Voltage
Displacement
Stress



- thermoelectric effects
- strain
- thermal expansion
- no piezo-effect

Thermoelectric and thermomechanic effects



Elastic material properties of Bi_2Te_3 c_{ij} in 10^{11}dyn/cm² at 280K

c_{11}	c_{66}	c_{33}	c_{44}	c_{13}	c_{14}
6.847	*2.335*	*4.768*	*2.738*	*2.704*	*1.325*

Thermal expansion coefficient a_i / 10^{-6}/K at 300K of Bi_2Te_3

a_x	a_y	a_z
21.3	*14.4*	*14.4*

Landolt-Börnstein; Numerical data; ISBN3540121609; Vol 17f, pp.275, 1983

Thermoelectric material properties		Thermoelectric Material Bi_2Te_3 based	Electrode (Copper)
Seebeck Coefficient	*α, V/K*	*p: 200e-6 n: -200e-6*	*6.5e-6*
Electric conductivity	*σ, S/m*	*1.1e5*	*5.9e8*
Thermal conductivity	*λ, W/m/K*	*1.6*	*350*

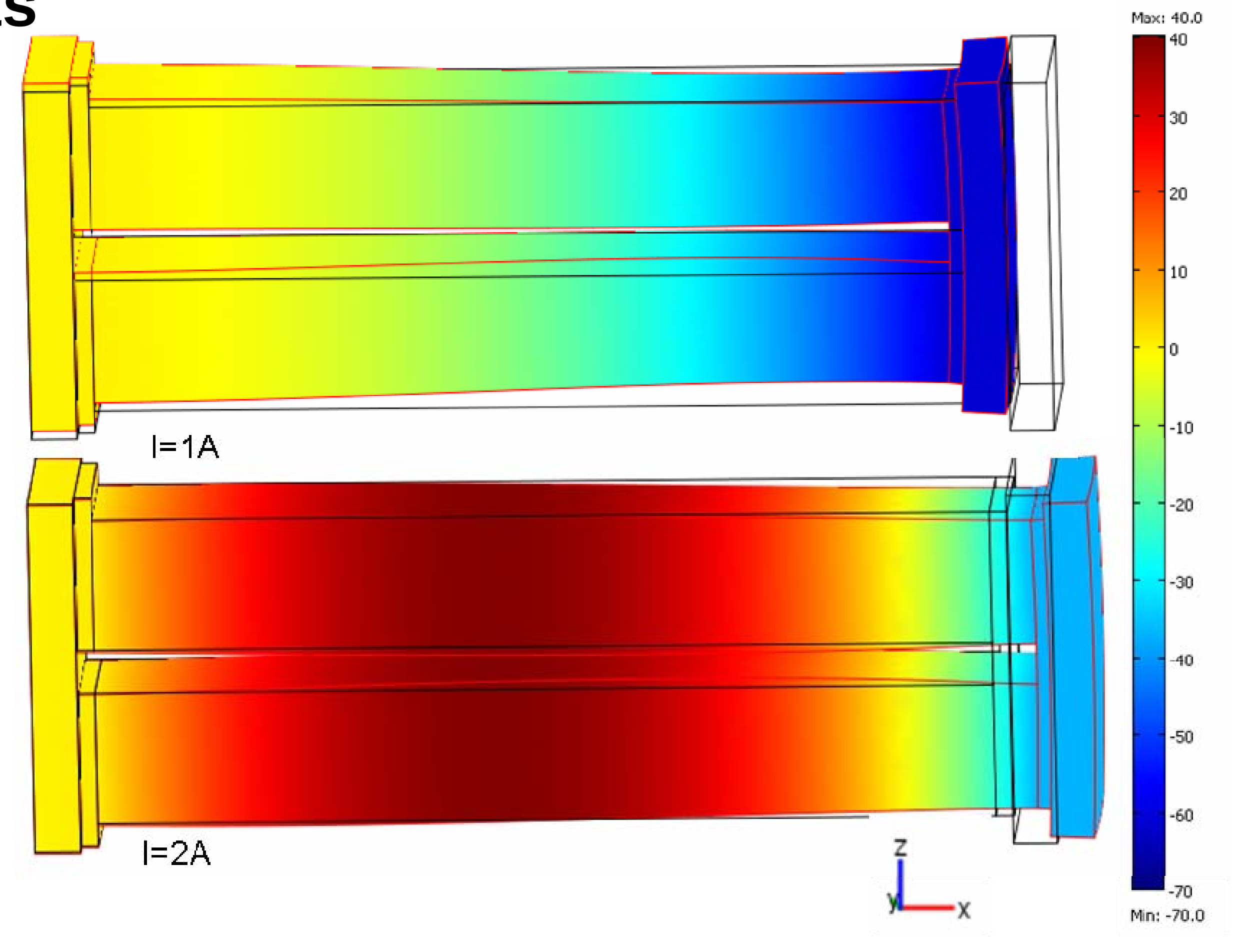
Antonova et al., ICT 2005

Thermoelectric and thermomechanic effects

Example:
Displacement due to thermal expansion

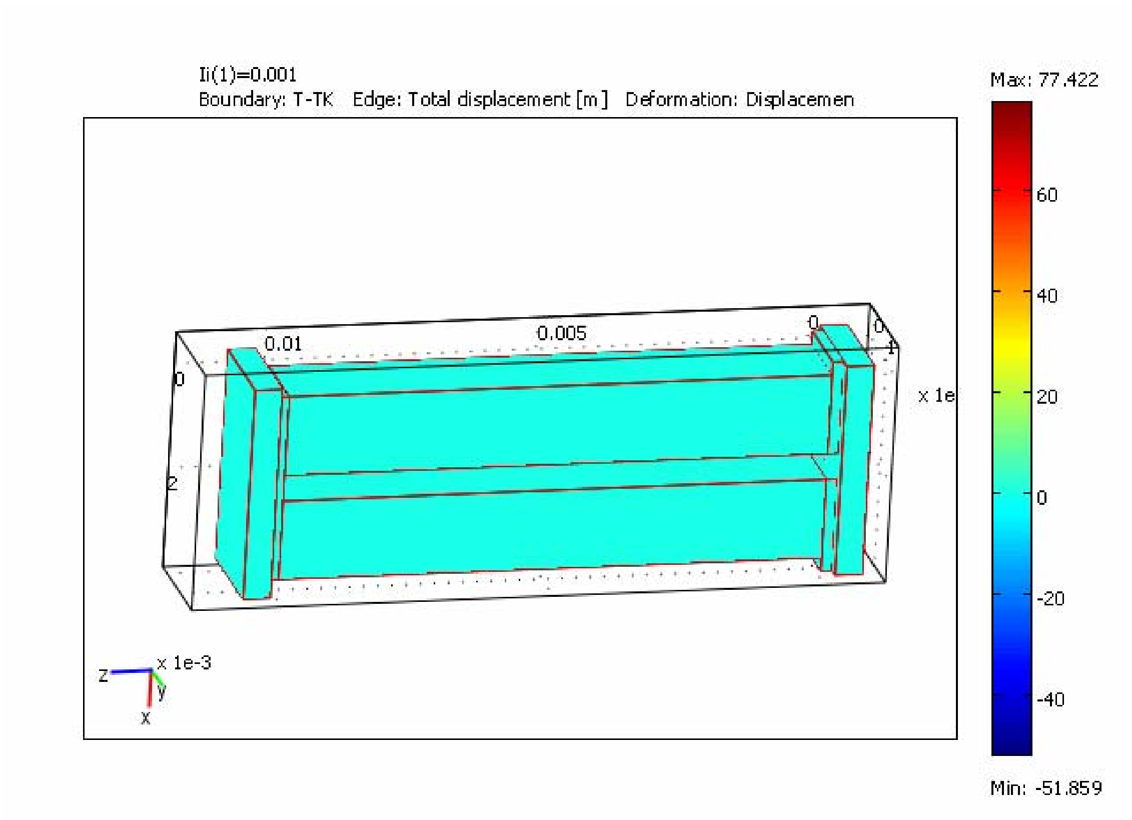
5 microns shrunken at 1A

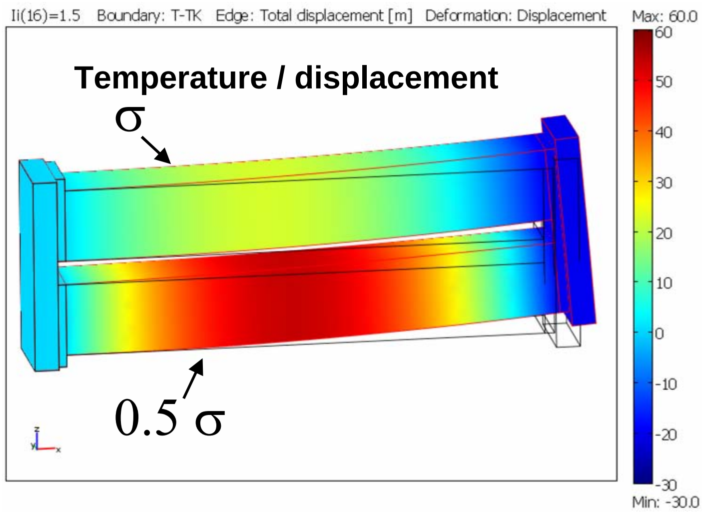
4 microns expanded at 2A
(still cooling)

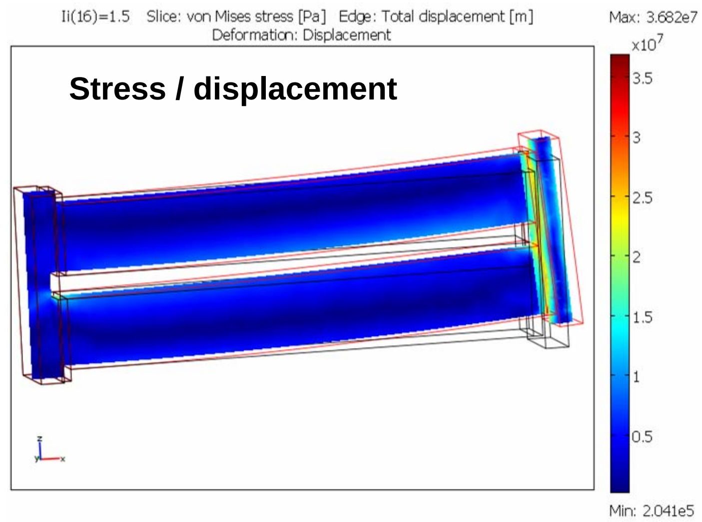


Thermoelectric and thermomechanic effects

Example: asymetric material properties







Summary

Thermoelectric effects in COMSOL for modeling of thermoelectric cooling, generation and sensing
Temperature and position dependent material properties
Anisotropic materials (not shown here for thermoelectrics)
Arbitrary geometries
Graded/ stacked materials
Determination of effective material properties (no quantum effects)

Simultaneous modeling of thermoelectric systems including
-Mechanical effects, strain, stress
-Thermomechanical effects
-Convection (not shown here)
-Radiation (not shown here)
-…

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