Simulating Thermoelectric Effects with Finite Element Analysis using COMSOL

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Abstract

An implementation of the thermoelectric effects in finite element analysis (FEA) using the COMSOL-Multiphysics platform is presented. It allows thermoelectric calculations with temperature dependent material properties on arbitrary geometries [1]. In addition, the calculations can be combined with structural analysis and also convection can be taken into account.

Introduction

The thermoelectric coupled field equations for the temperature T and electric potential V for steady state calculations can be written as

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

$$(1)$$

and

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

$$(2)$$

where the material properties α, σ and λ denote the thermopower (Seebeck-coefficient), the electric and the thermal conductivity, respectively. Usually those material properties depend on the temperature and may be unisotropic. Here only isotropic material properties are used, for anisotropic materials the appropriate matrices can be used. Also no transient magnetic fields are taken into account. The above equations can be derived from the coupled equations in [2] or the literature cited therein [3].

The FEA-Model

COMSOL- Multiphysics allows the implementation of common arbitrary partial differential equations (PDEs) of the field variable u on a one to three dimensional region Ω. Two PDE modes can be used: The "Coefficient-Form" and the "General Form". In the more didactical "Coefficient Form" PDE application mode, the program allows the definition of the coefficients for the following PDE:

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

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

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

$$(3)$$

Equation (3) follows the notation of the COMSOL-Multiphysics documentation. Please notice that some symbols from the equations (1) - (2) occur also here, but with a different meaning. The first line describes the PDE, the second and third lines define the coefficients for the generalized Neumann boundary condition and the Dirichlet boundary condition on the surface of the region Ω.

The thermoelectric field equations can now be transformed into the "coefficient form" as follows.

With the vector valued field variable

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

$$(4)$$

the coefficient c in (3) is

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

$$(5)$$

and f is

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

$$(6)$$

The other coefficients in equation (3) are zero for static calculations.

For transient calculations, capacitive influences have to be respected. Mostly it is sufficient to consider only the thermal capacity (heat capacity C, density ρ). Then d in equation (3) is

$$d = \begin{pmatrix} \rho C \\ 0 \end{pmatrix}$$

$$(7)$$

For fast transient calculations, also electric capacities can be included by setting γ in equation (3) to

$$\gamma = \begin{pmatrix} 0 & 0 & 0 \\ \varepsilon\frac{\partial^2 V}{\partial x\partial t} & \varepsilon\frac{\partial^2 V}{\partial y\partial t} & \varepsilon\frac{\partial^2 V}{\partial z\partial t} \end{pmatrix}$$

$$(8)$$

Here ε is the dielectric permittivity.

For the implementation of the PDE coefficients into COMSOL the notation for deviations is

$$\frac{\partial V}{\partial x} = Vx, \quad \frac{\partial V}{\partial t} = Vt, \quad \frac{\partial^2 V}{\partial x\partial t} = Vtx, \quad \vec{\nabla}V = \begin{pmatrix} Vx & Vy & Vz \end{pmatrix}$$

$$(9)$$

The following examples show results of calculations for typical thermoelectric applcations. The material properties for the calculations with temperature independent values are shown in table 1. Here typical values for Bismuth-Telluride and copper were taken from [2]. Temperature dependent material properties were taken manually from figure 7 in [4]. They were interpolated by cubic splines (figure 1-3). For the copper electrodes no temperature dependency was used.
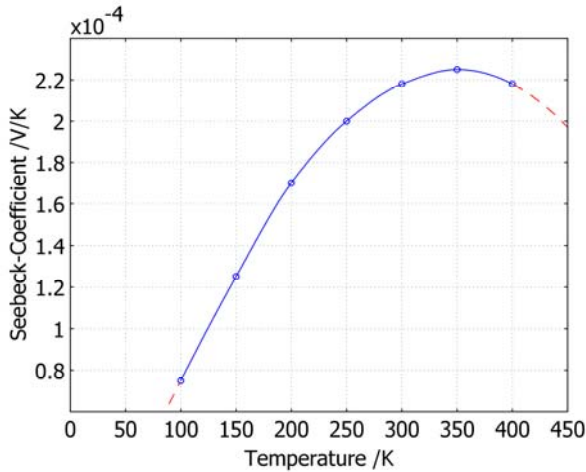
Figure 1: Temperature dependent Seebeck coefficient of $(Bi_{0.5}Sb_{0.5})_2Te_3$ taken from [4] and cubic spline interpolation.
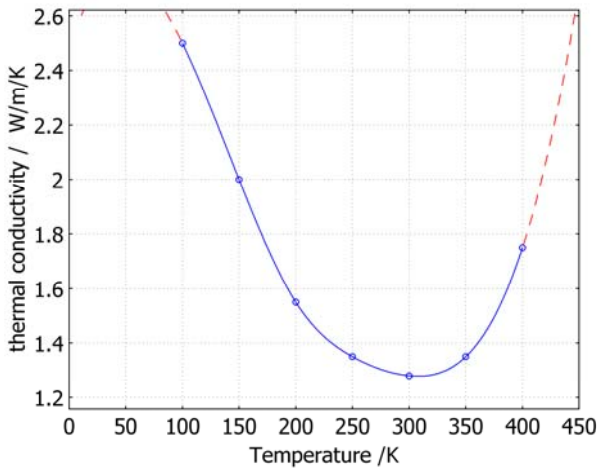

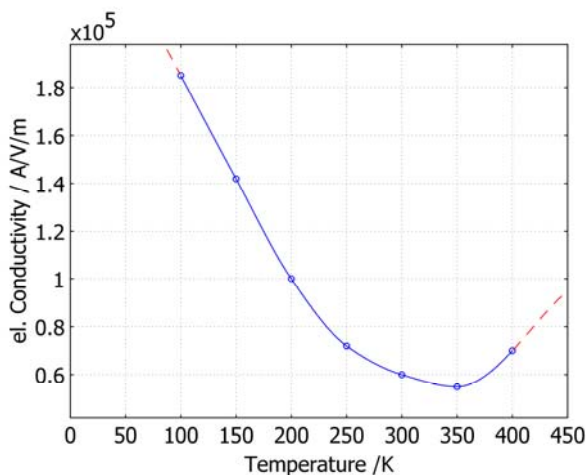**Figure 2: Temperature dependent thermal conductivity of $(Bi_{0.5}Sb_{0.5})_2Te_3$ [4].**

Figure 3: Temperature dependent electric conductivity of $(Bi_{0.5}Sb_{0.5})_2Te_3$ [4].

Table 1: Numerical material properties from [2]

		Thermoelectric Material	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
Density	ρ, kg/m³	7740	8920
Heat capacity	C, J/kg/K	154.4	385

Table 2: Temperature dependent material properties of $(Bi_{0.5}Sb_{0.5})_2Te_3$ from [4].

T /K	α / 10^{-6}V/K	λ / W/m/K	σ / 10^3A/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

Example 1: Thermoelectric Cooler

A simple cooler geometry consists of one p-type semiconductor element 1x1x5.8mm³ in size. It is contacted by two copper electrodes 0.1 mm in thickness (Figure 4).
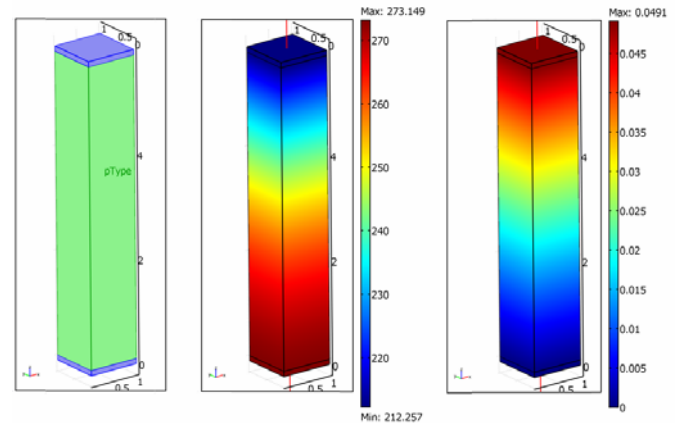

Figure 4: A p-type thermoelectric element is contacted by copper electrodes (left). The base is kept at 0°C and 0V. At the top 0.7A current was applied. Adiabatic boundary conditions were used. The resulting temperature distribution is shown in the center, the voltage is shown right. A temperature difference of nearly 61 K is achieved. The voltage at the upper electrode is 49 mV.

Table 1 sows the (constant) material properties. The boundary conditions were set to 0V and 0°C (273.15K) at the base of the lower electrode. Adiabatic boundary

conditions were taken on all other surfaces. At the top of the upper electrode a current of 0.7A was applied.

Figure 4 shows the result of the calculation. In the center, the temperature distribution shows that the cold side temperature is at 212.26K. The associated voltage is shown right. To drive the current, a voltage of 49.1mV is needed.
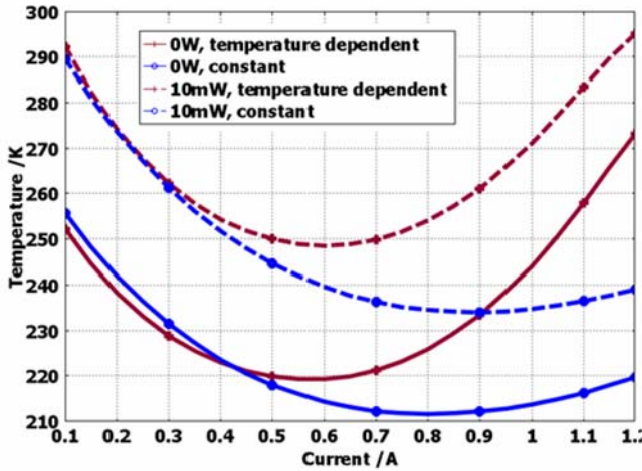

Figure 5: Calculated cold side temperatures versus current for constant (circle) and temperature dependent material properties (cross) without (solid) and with 10mW heat load (dotted), respectively
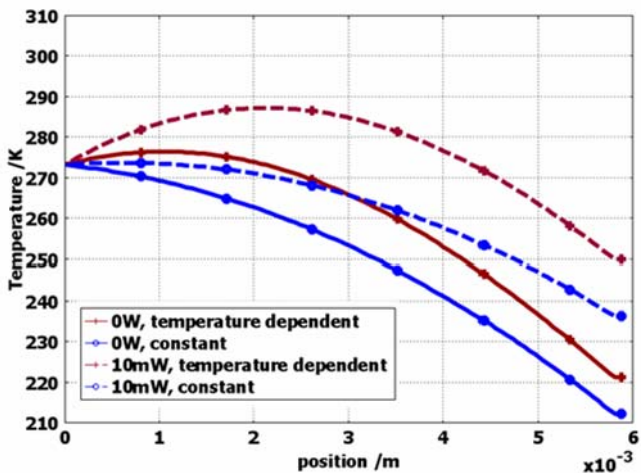

Figure 6: Temperature distribution along the element calculated with constant (circle) and temperature dependent material properties (cross) without (solid) and with 10mW heat load (dotted) on top of the element, respectively.

The same calculations were made with temperature dependent material properties. Figure 5 shows the cold side temperatures for temperature dependent (crossed curve) and constant material properties (circles). In addition, a heat load of 10mW was applied at the cold side. The elements have their maximum temperature difference at different currents according to the different material properties.

The temperature and voltage distribution along the element is shown in Figure 6 and 7 for a current of 0.7A.
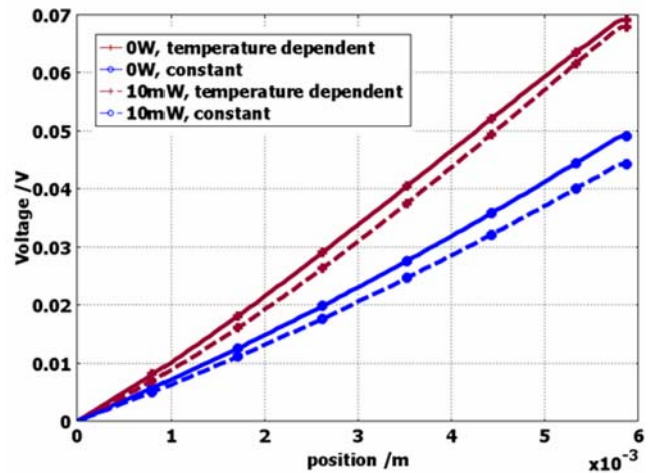

Figure 7: Voltage distribution along the element calculated with constant (circle) and temperature dependent material properties (cross) without (solid) and with 10mW heat load (dotted) on top of the element, respectively.

Example 2: Transient Operation

Figure 8 shows the result of a time dependent calculation. The above thermoelectric element is operated at 0.6 Ampere with no heat load at steady state temperatures. One second after the beginning of the calculation, the current is increased to 0.8A linearly within 0.1s. After 4 seconds the amperage decreases again linearly within 0.1s to 0.6A (figure 8, upper diagram). The lower diagram shows the transient cold side temperature with temperature dependent material parameters. The short current pulse causes a temporary temperature drop of about 3K. Such supercooling effects are also described e.g. numerically in [2] and, in addition, experimentallly in [5].
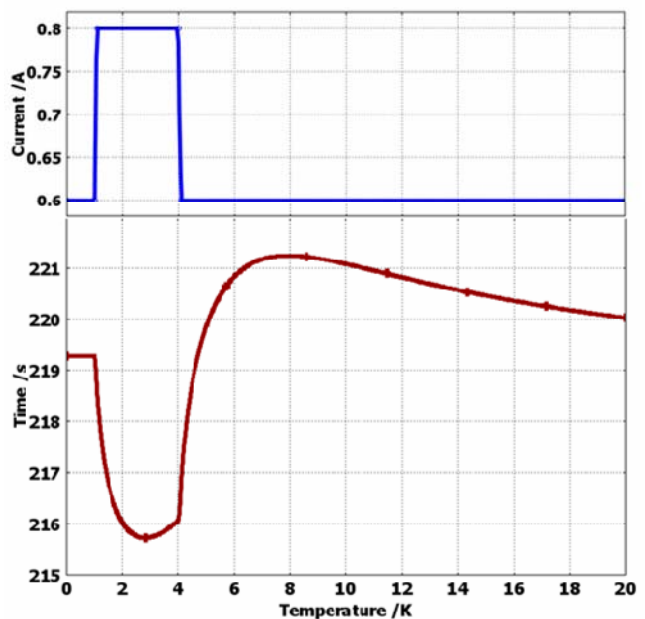

Figure 8: Transient calculation of Peltier-supercooling. A short current pulse generates temporarily lower cold side temperatures.

In this transient calculation, only the thermal capacities as described by equation (7) with the heat capacities and densities shown in table 1 were respected, electric capacitive effects according to equation (8) were neglected (set to zero).

Example 3: Thermoelectric generation

To simulate a thermoelectric generator, also the above shown semiconductor element was used, again with the variable material properties (figure 1 – 3). The top of the upper electrode was set to 100°C, the base of the lower electrode to 0°C, 0V. Figure 9: shows as a result the current-voltage and the current power characteristics of the generator.
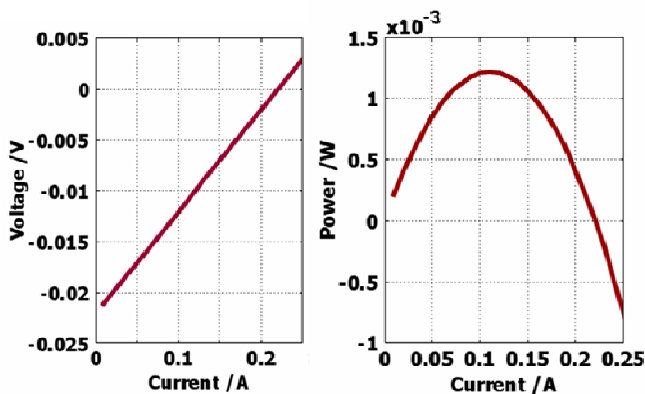

Figure 9: Current-voltage (left) and current-power characteristics (right) for the upper thermoelectric element

According to these characteristics, the open circuit voltage of the element is calculated to be about 21mV, the short-circuit current is about 220mA. The maximum power output is 1.22mW.

Example 4: Arbitrary Geometries

Many real life applications have more complex geometies like thermopile sensors or thin film devices. One typical example where FEA is advantagous is an electrode configuration which is in the direction of the temperature gradient. Thus, the often better thermal and electrical conductance of the electrodes will shorten both, the temperature differences as well as generated voltages. Figure 10 shows such a configuration. The size of the thermoelectric material is 1x5x0.8mm³, the electrode size is 1x3x0.1mm³. The temperature on top of the configuration is set to 10°C, the base is set to 0°C. The left figure shows the temperature distribution, the figure in the middle shows the voltage. The open circuit voltage at the upper left electrode is calculated to be -2.02mV. Both shortings of the field variables by the electrodes can be seen clearly, since the steepest gradient is between the electrodes. Figure 10 shows on the right side the electric current streamlines.
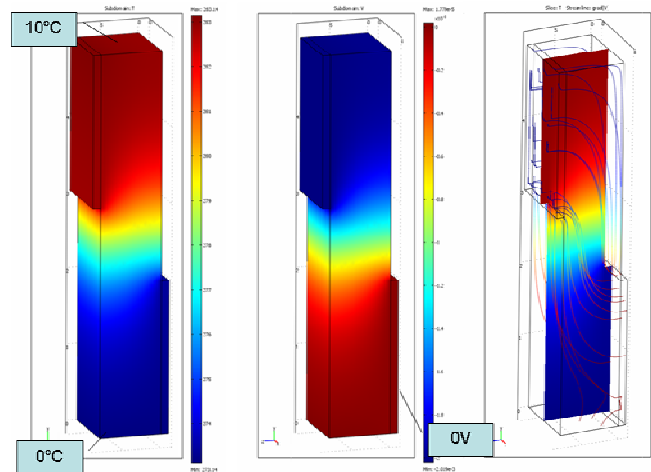

Figure 10: Example for a more "complex" element geometry: The copper electrodes are laterally connected (with respect to the temperature gradient). Left side: Temperature distribution, the top is set to 10°C, the base is at 0°C. The appropriate Voltage is shown in the middle; the left graph shows the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

Summary

An implementation of the thermoelectric field equations in COMSOL multiphysics 3.3a is shown. Thermoelectric calculations can be made for arbitrary geometries. Anisotropy (not shown) and temperature dependency of the materials can be included. Also transient calculations can be made. Structural analysis or convection can also be added easily (not shown here).

Literature

[1]: COMSOL Multiphysics 3.3a Documentation, www.comsol.com

[2]: Antonova E.E., Looman D.C; Finite Elements for Thermoelectric Device Analysis in ANSYS; Int. Conference on Thermoelectrics; 2005 pp. 200

[3]: Landau, L. D. and Lifshitz, E. M.; Electrodynamics of Continous Media, 2nd Edition, Butterworth Heinemann (Oxford, 1984)

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

[5]: Snyder, G.J. et al; Supercooling of Peltier cooler using a current pulse; J. Appl. Phys; Vol. 92, No. 3; pp. 1564-1569, 2002