Multiphysics simulation of thermoelectric systems

Martin Jaegle, Markus Bartel, Dirk Ebling, Alexandre Jacquot Harald Böttner
Fraunhofer-Institute for Physical Measurement Techniques
Heidenhofstrasse 8, 79110 Freiburg, Germany
Martin.Jaegle@ipm.fraunhofer.de, phone: +49 761 8857 345, fax +49 761 8857 224

Abstract

Examples for thermoelectric multiphysics finite element modeling are presented, where in addition to the thermoelectric field equations, thermo-mechanic effects are calculated simultaneously. The temperature dependency and anisotropy of the material properties can be respected. Thus, detailed modeling of thermoelectric systems are possible. The model is an extended version of a previously published model [1].

Introduction

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

$$-\vec{\nabla}((\sigma\alpha^2 T + \lambda)\vec{\nabla}T) - \vec{\nabla}(\sigma\alpha T\vec{\nabla}V) = \sigma((\vec{\nabla}V)^2 + \alpha\vec{\nabla}T\vec{\nabla}V) \tag{1}$$

and

$$\vec{\nabla}(\sigma\alpha\vec{\nabla}T) + \vec{\nabla}(\sigma\vec{\nabla}V) = 0\,, \tag{2}$$

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 at constant material parameters. The above equations can be derived from the coupled equations in [2] or the literature cited therein [3].

The FEA-Model

Only a view FEA-Programs can handle thermoelectric effects, like for example ANSYS version 9 and higher [2]. This paper shows an implementation of thermoelectricity into COMSOL Multiphysics, wich allows solving 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:

$$\begin{aligned}
&c_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla\cdot(-c\nabla u - \alpha u + \gamma) + \beta\cdot\nabla u + au = f && in \quad \Omega \\
&n\cdot(-c\nabla u - \alpha u + \gamma) + qu = g - h^T\mu && on \quad \partial\Omega \\
&hu = r &&
\end{aligned} \tag{3}$$

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 ∂Ω of the region Ω. The thermoelectric field equations can now be transformed into the “coefficient form” as follows.

With the vector valued field variable u, consisting of temperature T and voltage V,

$$\vec{u} = \begin{pmatrix} T \\ V \end{pmatrix}, \tag{4}$$

the coefficient c in (3) is

$$c = \begin{pmatrix} \lambda + \sigma\alpha^2 T & \sigma\alpha T \\ \sigma\alpha & \sigma \end{pmatrix} \tag{5}$$

and f is

$$f = \begin{pmatrix} \sigma\left(\left(\vec{\nabla}V\right)^2 + \alpha\vec{\nabla}T\vec{\nabla}V\right) \\ 0 \end{pmatrix} \tag{6}$$

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

$$d = \begin{pmatrix} \rho C \\ 0 \end{pmatrix} \quad \textbf{(7)}$$

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

$$\gamma = \begin{pmatrix} 0 & 0 & 0 \\ \varepsilon \dfrac{\partial^2 V}{\partial x \partial t} & \varepsilon \dfrac{\partial^2 V}{\partial y \partial t} & \varepsilon \dfrac{\partial^2 V}{\partial z \partial t} \end{pmatrix} \quad \textbf{(8)}$$

Here ε is the dielectric permittivity.

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

$$\frac{\partial V}{\partial x} = Vx, \quad \frac{\partial V}{\partial t} = Vt, \quad \frac{\partial^2 V}{\partial x \partial t} = Vtx,$$
$$\vec{\nabla} V = \begin{pmatrix} Vx & Vy & Vz \end{pmatrix} \quad \textbf{(9)}$$

Thermomechanic allpication modes can be combined with this thermoelectric model in order to study thermal expansion and strain at various temperatures. In this paper, the "solid, stress, strain" application mode of the MEMS-Module was taken. The calculations were made with COMSOL 3.4.

Dimensions and material properties

The following examples show results of calculations for a p-n thermocouple, contacted by copper electrodes on a alumina substrate, as shown in figure 1. The dimensions of the thermoelectric leg are 1.5x1.5x10mm³ with 0.5mm spacing. The electrodes are made from 0.2mm copper, the thickness of the alumina substratre is 0.5mm. The left side is kept at 0°C and is mechanically fixed. The current density J is applied at the upper left electrode, the lower left electrode is grounded.

For reasons of simplicity, neither temperature dependency of the material data, nor transient or unisotropic calculations were taken into account. Examples for temperature dependent materials and transient calculations with this FEA-model can be found in [1].

The thermoelectric material data are from [2] and are shown in table 1, they are typical values for bismuth telluride. The thermal conductivity of the alumina substrate was set to 29W/m/K.

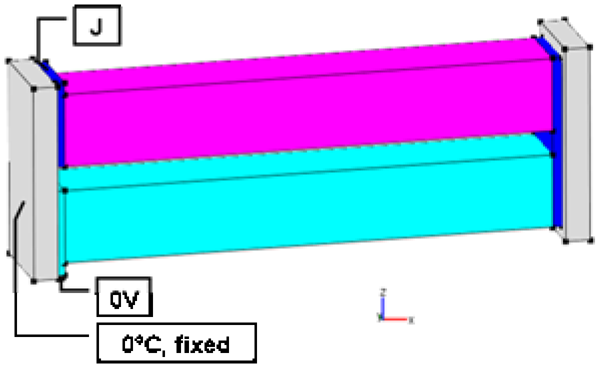

Figure 1: The thermocouple example consists of two 1.5x1.5x10mm³ legs. They are contacted with copper on a alumina substrate. The left side is kept at 0°C and mechanically fixed. The current density J is applied at the upper left electrode, the lower electrode is grounded.

Table 1: Thermoelectric material properties for a typical bismuth telluride based material, 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

The elastic moduli and thermal expansion coefficients for bismuth-telluride are are taken from [4] and are listed in table 2. The mechanic properties for copper and alumina are taken from the COMSOL material library., Young's modulus was 110GPa for copper and 300 GPa for alumina, Poissons ratio was 0.35 for copper and 0.22 for alumina. The temperature expansion coefficient was 17 10^{-6}/K for copper and 8 10^{-6}/K for alumina. Reference

Temperature for the thermal expansion was 0°C.

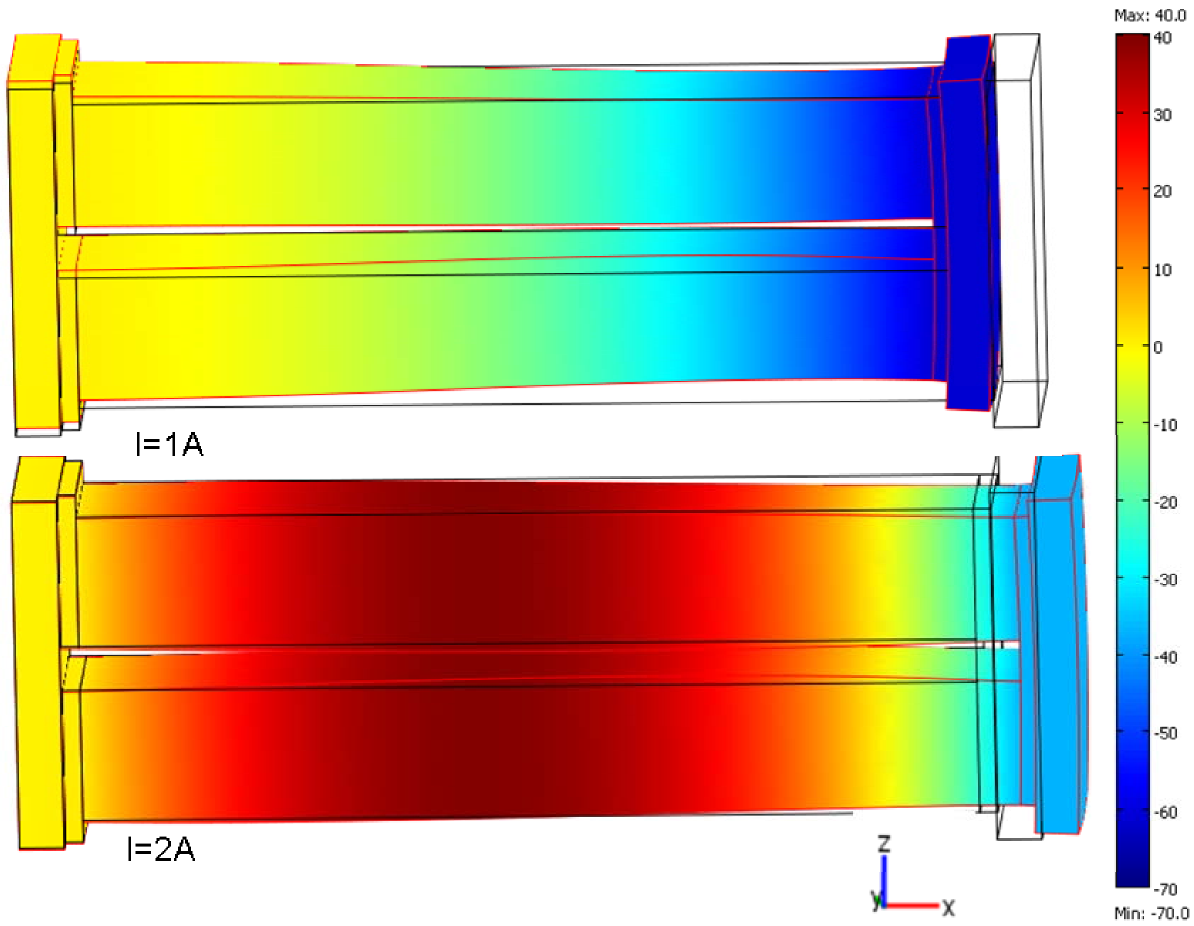

Figure 2: The thermal expansion of the thermocouple for 1A and 2A current. The initial geometry is shown as a black wireframe, the deformed frame is red and filled with temperature coded colors. At maximum cooling near 1A, the module shrinks about 5 microns (above). At 2A, the module is thermally expanded although it is still cooling.

Table 2: elastic material properties c_{ij} in 10^{11}dyn/cm² at 280K and temperature expansion coefficient a_i in 10^{-6}/K of Bi_2Te_3 at 300K, from [4]

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

a_x	a_y	a_z
21.3	14.4	14.4

Calculation results

To solve the PDEs, the "parametric segregated solver" in COMSOL was used. The current was varied from 0.001 - 2A. Figure 2 shows the result for two currents, 1A above and 2A below. The original geometry is shown as a black wireframe, the displacemend by thermal expansion is indicated by the red wireframe, filled with temperature coded color.

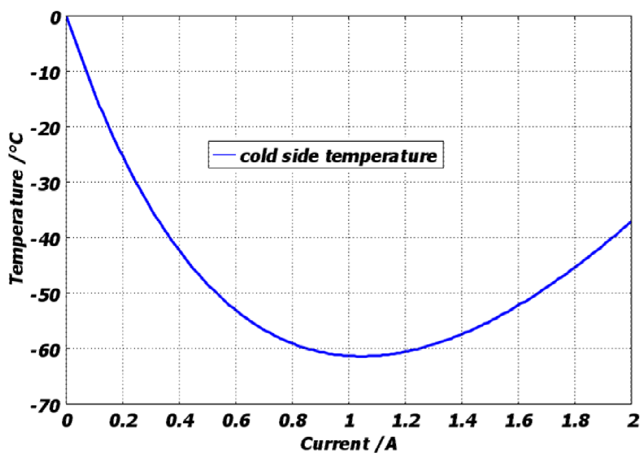

Figure 3: The calculated cold side temperature versus current shows a

maximum temperature difference of about 62°C.

At maximum cooling near 1A, the module shrinks about 5 microns (above). At 2A, the module is thermally expanded although it is still cooling.

Figure 3 shows the calculated cold side temperature versus the applied current for an operation as a peltier module. About 62°C temperature difference can be achieved at 1 A.

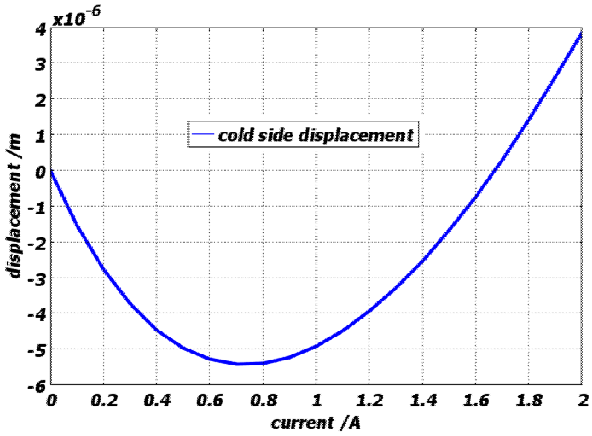

Figure 4: thermal expansion of the module in x-direction

The according change of the module length in x-direction is shown in figure 4. At low currents, the module shrinks due to the cooling. With higher temperatures the module expands. Minimum size and maximum cooling are not at the same current.

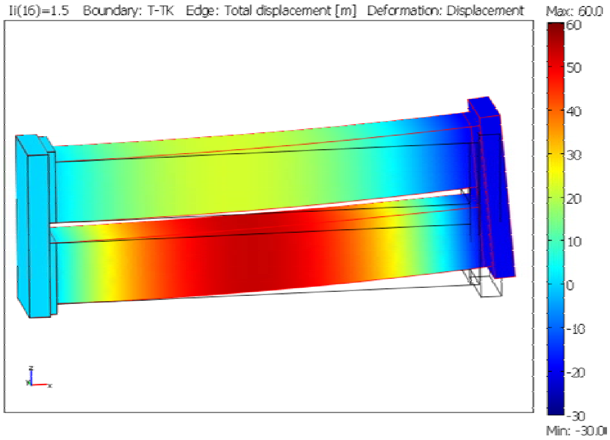

Figure 5: A doubling of the resistivity of the lower thermoelectric leg leads to higher temperatures and thus to asymmetric thermal expansion. Other parameters like in figure 2, the current is 1.5A.

With this model, thermoelectric and thermomechanic effects can be simulated simultaneously, and thus enabling thermomechanic studies of thermoelectric effects. As an example the effect of a changed electric resistivity is shown in the figures 5 and 6. The electric resistivity of the lower thermoelectric leg was doubled. Figure 5 shows the calculated temperature distribution and thermal expansion for a current of 1.5A. The different resistivities of the thermoelectric legs lead to an assymetric temperature distribution in the legs, causing a bending of them due to the thermal expansion. Figure 6 shows the von Mises stress within the module as a slice Plot. a maximum stress of about 37MPa was calculated.

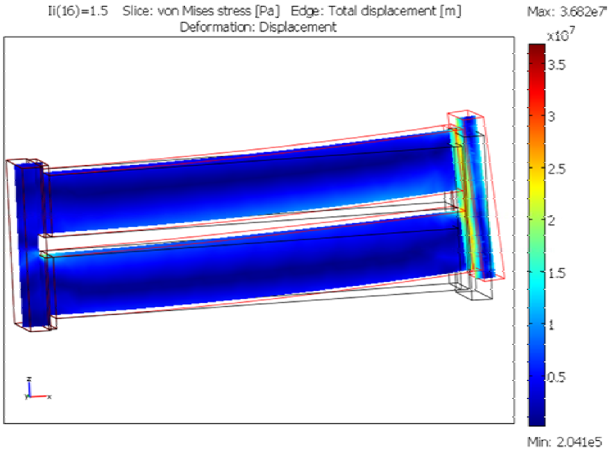

Figure 6: Von Mises stress in the asymetrically strained module of figure 5

Acknowledgment: I wish to thank Florian Schindler-Saefkow for helpful discussions.

Literature

[1]: Jaegle, Martin; Simulating Thermo-electric Effects with Finite Element Analysis using COMSOL; Proceedings ECT2007, Odessa; p.222

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