# 3D-Model of Asymmetric Thermo-Electric Generator Modules for High Temperature Applications

Marcel Dannowski, Wieland Beckert, Lisabeth Wagner, Hans-Peter Martin
Fraunhofer IKTS, 01277 Dresden, Winterbergstrasse 28
mail: Marcel.Dannowski@ikts.fraunhofer.de

**Abstract:**
This paper presents the modeling and simulation of an asymmetric thermoelectric module. The thermoelectric module is characterized by a novel module design and a lager temperature range than conventional high-temperature modules. The materials are boron carbide and titanium diboride which were specially developed for use in high temperature range.
Particularity of the model described here is the approach of equation based modeling in COMSOL Multiphysics. Feature of the presented model here is the level of detail and the implementation of temperature-dependent material properties. As a result thermal and electrical performance of the thermoelectric module is presented which includes the decoupled electrical power as well as the current-voltage behavior of the module.

**Keywords:** asymmetric thermoelectric modules, Seebeck effect, equation-based modeling

## 1. Introduction

Thermoelectric generators are characterized by a direct conversion of thermal energy into electrical energy. In recent years, thermoelectric generators have been mainly used in Aerospace or niche applications. However, thermoelectric generators are increasingly used in various application areas for example in the automotive industry. The aim is, to use the waste heat in the exhaust gas line of a car. The problem in this context is the efficiency of the thermoelectric generator, which is typically far below the Carnot efficiency. One way to increase the efficiency of novel thermoelectric systems is the use in high temperature applications. It can be shown that the ZT-value increases with higher temperatures and therefore an improvement in efficiency occurs. In this context, existing materials, such as bismuth telluride can be used only up to a temperature range of 250 ° C. The materials presented in this work are all suitable for high temperature applications. Furthermore shows this paper the implementation of the thermoelectric effects in COMSOL Multiphysics. Under the general term of the thermoelectric effects, the Seebeck, Peltier and Thomson effect is understood. The Seebeck effect influenced by a temperature gradient which generates an electrical voltage is the counterpart of the Peltier effect which creates a temperature gradient in current flow. The Thomson effect describes the change of the heat flow with simultaneous current flow. Furthermore, a model of a thermoelectric module is presented based on of new materials which are suitable for high temperature applications. The material for the thermoelectric legs based on boron carbide and titanium diboride. Depending on the material configuration, temperatures of up to 800 ° C can be realized. In the presented model of an asymmetric thermoelectric module, all significantly important component groups are integrated. The implemented model includes substrate layer, metallization layer and the actual thermoelectric material, where p/n-type material does not necessarily have the same Area size. The focus of the modeling is initially on the geometry integration into COMSOL Multiphysics to subsequently start the mesh generations. A first evaluation of the thermoelectric module can be done by evaluation of the voltage over-currrent diagram. Thereupon follows an assessment of the electrically decoupled performance of the thermoelectric module.

## 2. Model implementation

Thermoelectric modules are characterized by an alternating construction of p and n type thermoelectric legs. In the general, each thermoelectric leg pair has the same relationships. This thermoelectric leg pairs are assembled into a thermoelectric module. The presented thermoelectric module is characterized by an asymmetric design, which includes different size rations for the thermoelectric leg pairs. Figure 1 shows the asymmetric design of the thermoelectric module [2]. It is to recognize that the presented thermoelectric module design has no commonalities with the conventional thermoelectric module.

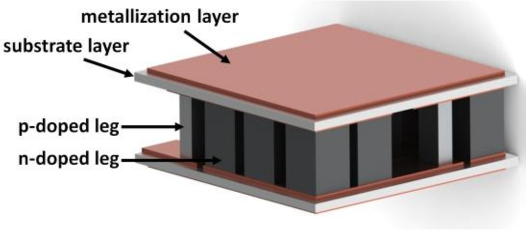
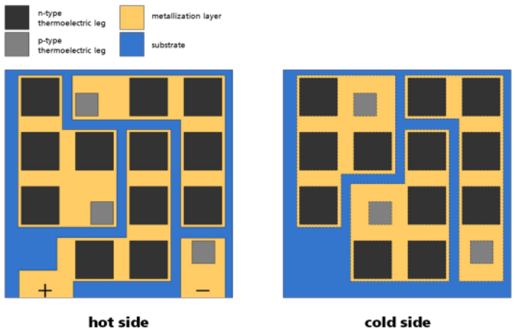


**Figure 1**. Asymmetric thermoelectric module

As well as in a classical module construction exists the asymmetrical design also of an alternating structure. This means that the p / n-doped material are alternately connected to each other. This Design consists of alternating metallization, substrate and electrode layer. In the middle of the packaging is the actual thermoelectric material which consists of boron carbide and titan diboride. The substrate layer was aluminum nitride and nickel used for the metallization layer.

From Figure 1 it can be seen that due to the different material properties and a previous estimate of the module design different cross-sections have been designed for p and n-doped material. In Figure 2, the thermoelectric module is shown again in a sectional view, what should make you a better insight on the geometrical structure.



hot side

cold side

**Figure 2**. Sectional illustration of the asymmetric module design

As seen in Figure 2, the thermoelectric module builds on three thermocouples. In this regard, the n-doped material was divided into 4 smaller legs. This fact follows from the ideal packing density, and the actual robustness of the thermoelectric module. In the following this geometry should be integrated into COMSOL Multiphysics. A rough overview of the geometric dimensions is given in table 1.

| Variable | size | unit |
|---|---|---|
| area p-doped leg | 2.5e-6 | m² |
| area n-doped leg | 9e-6 | m² |
| high p/n-doped leg | 0.0067 | m |
| modul Area | 0.0009 | m² |

**Table 1.** Rough overview of the geometric dimensions

Within COMSOL Multiphysics it possible to keep the geometry creation as variable as possible. Which means in this case important geometric variables can be changed directly via a parameter list. Here are especially mentioned outer body proportions and the layer thicknesses of the thermoelectric material. In Figure 3 can be seen how the thermoelectric module was implemented in COMSOL Multiphysics.

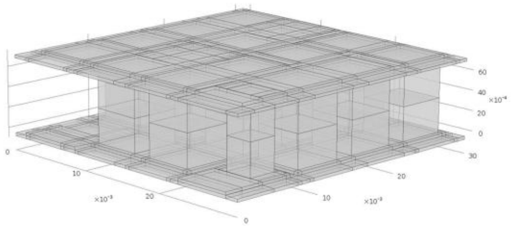


**Figure 3**. In COMSOL Multiphysics constructed thermoelectric module

Furthermore can be seen in figure 3 that the geometry was assembled over many individual blocks. Through this geometric construction is a better meshing of the computing domain possible. The goal here was to use in the mesh generation only hexahedral elements. In this context, a better convergence and less computation time of the model are expected.
As can be seen in figure 4, the entire meshing process could be implemented with structural elements.

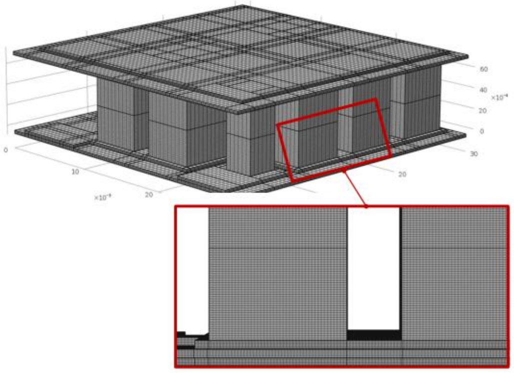


**Figure 4**. Structual mesh of the thermoelectric generator

For a better illustrative of the mesh, figure 4 shows a side view of the thermoelectric module. The detailed view in figure 4 also shows a further mesh refinement. Main focus of this mesh refinement was the metallization layer and the actual thermoelectric material. It is important to note that with an increasing current flow within the metallization layer a poor mesh quality can negatively affect of the simulations results.

## 3. Mathematical Model

Foundation for the modeling is the heat flow density [1]

$$\vec{q} = S \cdot T \cdot \vec{j} - \kappa \cdot \nabla T \qquad (1)$$

$$\nabla \cdot \vec{q} = \vec{j} \cdot \vec{E} \qquad (2)$$

and the electric current density [1]

$$\vec{j} = \sigma \cdot \vec{E} - \sigma \cdot S \cdot \nabla T \qquad (3)$$

$$\nabla \cdot \vec{j} = 0 \qquad (4)$$

for a description of thermoelectric systems. The material parameter $\sigma$ describing the electrical conductivity while S reflects the Seebeck-coefficient and $\kappa$ represents the thermal conductivity. Using the electric field [1]

$$\vec{E} = \frac{\partial T}{\partial x} \cdot S + \frac{\vec{j}}{\sigma} \qquad (5)$$

can be recorded for a description of the thermo-electricity following partial differential equation.

$$\kappa \frac{\partial^2 T}{\partial x^2} - \vec{j} \cdot \frac{\partial (ST)}{\partial x} + \vec{j} \cdot S \cdot \frac{\partial T}{\partial x} = -\frac{\vec{j}^{\,2}}{\sigma} \qquad (6)$$

Based on this partial differential equation can calculate all the important phenomenon of thermoelectric such as Seebeck or Peltier effect.

An important part in the modeling is the integration of this partial differential equation into the simulation environment of COMSOL Multiphysics. One way of the implementation is the approach of the equation based modeling. Here COMSOL Multiphysics provides the possibility to the implementation of a separate PDE mode. This kind of modeling offers a high maximum degree of flexibility. In our case, there are two PDE application modes, one for temperature and one for the electric voltage. Equation 7 shows the partial differential equation in coefficients notation as it is stored in COMSOL Multiphysics [3].

$$\begin{cases} e_a \frac{\partial^2 u}{\partial u^2} - d_a \frac{\partial u}{\partial t} - \nabla \cdot (c\nabla u + \alpha u - \gamma) + \beta \cdot \nabla u + \alpha u = f \rightarrow in \;\; \Omega \\ n \cdot (c\nabla u + \alpha u - \gamma) + qu = g - h^T \mu \rightarrow on \;\; \partial\Omega \\ hu = r \rightarrow on \;\; \partial\Omega \end{cases} \qquad (7)$$

where

- $\Omega$ is the computational domain
- $\partial\Omega$ in the domain boundary
- n the outward unit normal vector on $\partial\Omega$
- $u$ the dependent single variable

As mentioned above two PDE modes are introduced, each for the temperature and the electric voltage.

For a description of the temperature, it is necessary to integrate the following coefficients

$$c = k + \sigma \cdot S^2 \cdot T \qquad (8)$$

$$\alpha = -\sigma \cdot S \cdot \vec{E} \qquad (9)$$

$$f = \vec{j} \cdot \vec{E} \qquad (10)$$

In this case, the temperature is set for the single dependent variable u.

The individual coefficients of the electric voltage density can be implemented as follows

$$c = \sigma \tag{11}$$

$$\gamma = -\sigma \cdot S \cdot \vec{T} \tag{12}$$

In this case, the single variable is the electrical voltage. Now with this description for the resulting electric voltage, and for the temperature, the thermoelectricity can be calculated in each case of the declared area.

The integration of the temperature-dependent properties is realized by local functions. There is the possibility depending on the load case to deposit different material properties for each layer.

## 4. Results

All results presented here are based on a temperature gradient of 400 ° C and an applied voltage of 0.1 V.

Figure 5 shows a temperature distribution of the thermoelectric module. As indicated in Figure 5 cannot be expect of a homogeneous temperature distribution across the thermoelectric module. Due to different material characteristics of the thermoelectric materials is not assumed to be the same temperature distribution within the thermoelectric module.

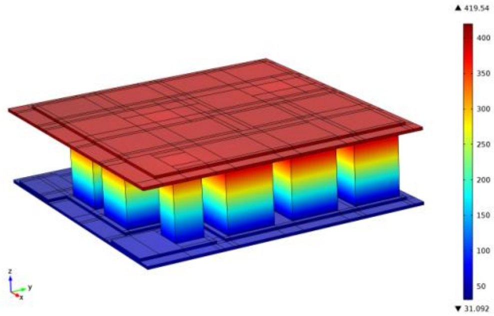


**Figure 5.** Temperature distribution of the thermoelectric module at a temperature gradient of 400°C and an applied voltage of 0.1 V

As can be seen in figure 5, the actual thermoelectric material causes the greatest temperature gradient. This fact can be explained by the poor thermal conductivity of the legs as compared to the example of the substrate layer. Figure 6 and 7 shows by a surface plot the different temperature gradients on the metallization layer.

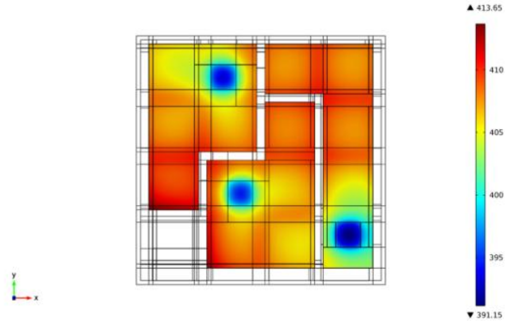


**Figure 6.** Surface plot for the temperature in the metallization layer of the hot side

Figure 6 shows the temperature distribution in the metallization layer. The direct counterpart, the cold side of the metallization layer is shown in Figure 7.

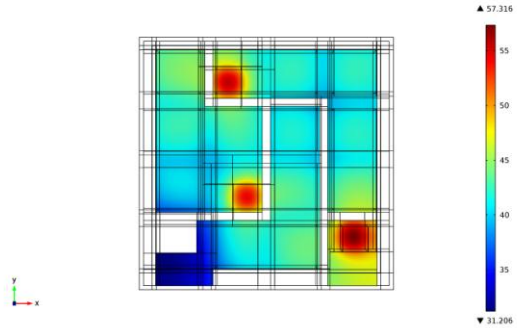


**Figure 7.** Surface plot for the temperature in the metallization layer of the cold side

As can be seen in figure 6 and 7 that different materials of the thermoelectric legs has a significant influence on the temperature distribution within the thermoelectric module. The better thermal conductivity of titanium diboride caused a smaller temperature gradient across the thermoelectric legs and thus also a lower share for thermoelectric converted energy. Diagram 1 illustrates once again based on a temperature gradient through the thermoelectric legs the influence of the different material properties.

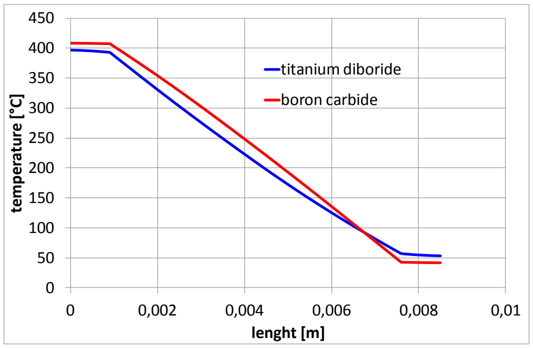


**Diagram 1**. Temperature profile through the thermoelectric legs

Once again can be seen in diagram 1 that the largest temperature gradient is obtained through thermoelectric leg. As expected metallization layer and substrate layer has a subordinate influence on the temperature distribution.

Another important point is the modeling of the electrical voltage distribution within the thermoelectric module. Figure 8 shows the electrical voltage distribution of the thermoelectric module.

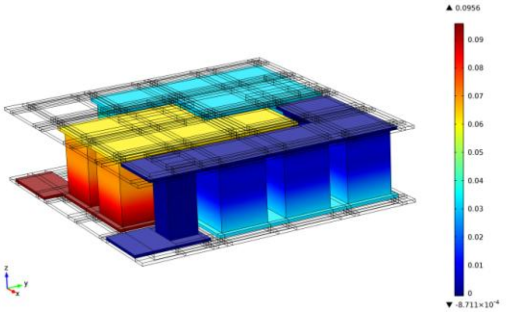


**Figure 8.** Voltage distribution of the thermoelectric module at a temperature gradient of 400°C and an applied voltage of 0.1 V

Depending on the material properties is to realize that the larger voltage drop is caused by the n-doped material. For a further assessment of thermoelectric systems with regard to power management are used power-current and voltage-current diagrams

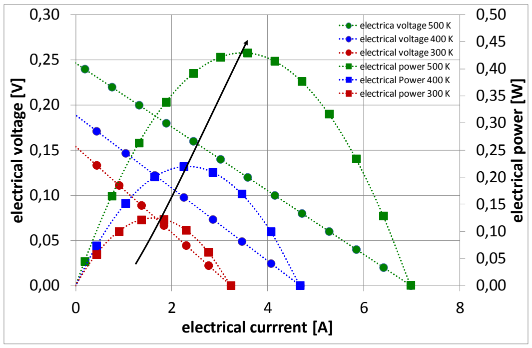


**Diagram 2.** Power-current and voltage-current diagram for a assessment of the thermoelectric module

As see in diagram 2, a first assessment on the thermal-electrical behavior of the thermoelectric module can be obtained from the model. Furthermore, there is the possibility for a determination of the working point under thermal load. In diagram 2 indicates the direction of the black arrow maximum power of decoupled electrical power.

## 5. Conclusion

In this work, we presented a model for the description of a asymmetric thermoelectric module. The implementing geometry is characterized by an innovative construction and could be described with a detailed 3D model. The model presented here allows a quick variation of the geometry, because the entire geometry was created from individual blocks (Figure 3). This fact allows a complete variation of the detailed 3D models which is also connected to a variation of the computational mesh.

On the foundation of the equation based modeling the partial differential equation [6] for the description of the thermoelectric effects could be integrated. For this, the PDE mode was used which is already integrated in COMSOL Multiphysics. The created model allows an accurate statement about the temperature distribution and the electrical voltage distribution. Furthermore details can be made about the converted electrical energy at different boundary conditions. Another important component of this model is the possibility of temperature-dependent material properties, which are interconnected via local functions. It has to be noted for the outlook that a comparison with measurements is desirable. Furthermore, a comparison between the various materials should be simulated. Especially the influence of different metallization layer materials and the electrical resistance caused thereby is in focus of the work outstanding. Another important aspect of the model expansion is the connection of the thermoelectric module to a heat reservoir as example a heat exchanger.

## 6. References

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## 7. Acknowledgements

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