COMSOL Multiphysics® Simulation Integrated into Genetic Optimization

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Abstract: The main topic of this paper is the development of an innovative tool that can be applied in a wide range of complex problems, to simulate, optimize and improve system design especially when dealing with huge numbers of parameters and constraints.

The new methodology is obtained by joining the power of Comsol multiphysics simulation with the modern optimization approach of genetic algorithms. It has been successfully applied within an industrial research program focused on the development of thermoelectric micro-generators (μTEGs) based on innovative proprietary materials.

This paper shows how this tool optimizes μTEG's element geometry in a simple case study. Values of the thermoelectric material physical variables can't be disclosed for confidentiality reasons.

Keywords: Seebeck effect, thermoelectric micro-generator, finite element analysis, genetic algorithm, multiobjective optimization.

1. Introduction

A thermoelectric micro-generator (μTEG) is a solid state device, able to generate an electric potential when it is exposed to a temperature gradient due to the thermoelectric Seebeck effect [1].

ZT is a common dimensionless figure of merit for thermoelectric (TE) materials which is a measure of their thermodynamic efficiency and it is defined as:

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

where α is the Seebeck coefficient (V/K), T is the absolute temperature (K), σ is the electric conductivity (S/m), κ is the thermal conductivity (W/m*K)[1].

The possibility of using μTEGs to convert waste heat into electricity has recently regained interest as a consequence of the discovery of high ZT values in a certain range of materials [2].

Besides the ZT of the material, to fabricate high efficiency μTEG, it is necessary to design the optimal geometry of the μTEG's element [3, 4].

For this reason, simulation of thermoelectric performance parameters by numerical methods is a significant part of μTEG development: it allows time and cost saving in assessment of materials and variations of design parameters, such as shape, thermoelectric material length/width and thermal coupling.

According to the different heat transferring directions, structures of μTEGs can be divided into two categories: vertical structures and horizontal structures. In vertical structures, heat transfers along thickness direction of TE elements; while in horizontal structures heat transfers along their surface [4].

This work describes the application of the tool for designing high performance μTEG's elements based on thin-film TE material, with horizontal structure.

2. Thermoelectric Model

2.1 Governing Equations

Heat flux Q and electric current flux J are the main quantities of interest in thermoelectric effect simulations [1]:

$$Q = \alpha T J - \kappa \nabla T$$
$$J = \sigma E - \sigma \alpha \nabla T$$

where E is the electric field.

Heat energy conservation and electric current balance are the governing equations for thermoelectric effect analysis, that in the stationary case assume the following form:

$$\nabla \cdot Q = J \cdot E$$
$$\nabla \cdot J = 0$$

Expliciting the thermoelectric equations in terms of electric potential V, they assume the form:

$$\nabla\cdot\left(\alpha T\left(-\sigma\nabla V-\sigma\alpha\nabla T\right)-\kappa\nabla T\right)=$$
$$=\left(-\sigma\nabla V-\sigma\alpha\nabla T\right)\cdot\left(-\nabla V\right)$$

$$\nabla\cdot\left(-\sigma\nabla V-\sigma\alpha\nabla T\right)=0$$

These equations are transformed to a weak form in order to be implemented in Comsol Multiphysics [5].

To simplify the simulation, Seebeck coefficient, electric and thermal conductivity, are considered independent from temperature.

2.2 Geometry Description

The model describes a single TE element that can be manufactured by standard front-end microelectronics processes. It is constituted by a thin film of TE material deposited onto a substrate and two metallic contacts that work as both thermal and electrical contacts. Figure 1 shows the geometry (not in scale) and the compound structure:

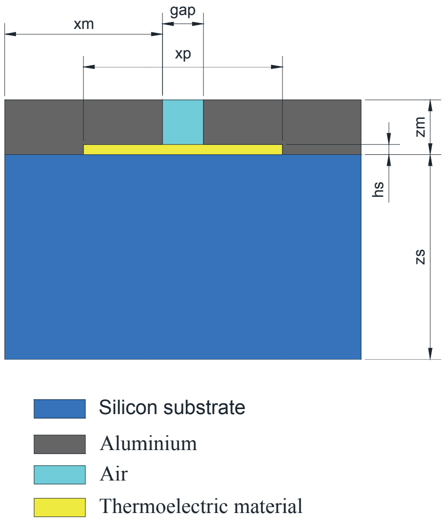

Figure 1. Cross section of the model (not in scale) and material composition.

The substrate is a silicon wafer, while the metal contacts are made of aluminium. The behaviour of materials used in the simulation are defined directly by a new Comsol physic interface, integrating all the governing equations described above.

2.3. Boundary Conditions

The following boundary conditions are applied in the model:

Heat exchange surfaces:

- Hot side, with a temperature of 493.15K
- Cold side, with a temperature of 293.15K

Electric exchange surfaces:

- Potential ground reference at 0V (on the cold side surface)
- Variable potential reference (on the hot side surface)

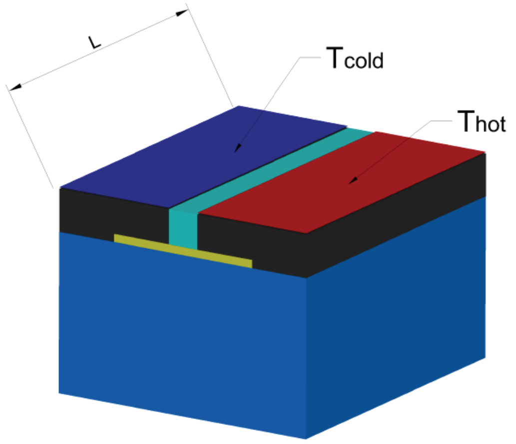

Figure 2. Boundary surfaces.

2.4. Electric Power Density Evaluation Method

The method, used to evaluate the electrical potential and current, is realized by the application of two different sets of boundary conditions, in two different runs. By means of this technique it is possible to simulate the open circuit and the short circuit to evaluate the electric potential and the amount of flowing current (through an optimized load) respectively. The generated electric power is evaluated using the following scheme:

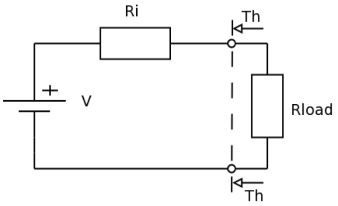

Figure 3. Electric power evaluation scheme.

where V is the open circuit potential of the TE element, defined as average value on the surface T_{hot}, while I is the short circuit current flowing in the same surface and integrated as follows:

$$I = \iint_{S_2} \vec{J} \bullet \vec{n} dS$$

The electric power is:

$$\mathrm{P}_{\mathrm{load}} = \mathrm{R}_{\mathrm{load}} \left(\frac{\mathrm{V}}{\mathrm{R}_{\mathrm{i}} + \mathrm{R}_{\mathrm{load}}} \right)^2$$

$$\mathrm{R}_{\mathrm{load}} = \mathrm{R}_{\mathrm{i}}$$

where R_i is the internal resistance of the TE element , evaluated as ratio between the potential in the open circuit and the current in the short circuit.

The Electric Power Density is:

$$\mathrm{P}_{\mathrm{d}} = \frac{\mathrm{P}_{\mathrm{load}}}{\mathrm{S}}$$

where S is the horizontal section area of the thermoelectric element:

$$\mathrm{S} = (2 \cdot \mathrm{x}_{\mathrm{m}} + \mathrm{gap}) \cdot \mathrm{L}$$

The physics used in this model allows to appraise also the thermal resistance (R_t), through the inverse of the ratio of the heat flux, flowing from the heat exchange surfaces (T_{hot} and T_{cold}), and the difference of the nominal temperature of these:

$$R_t = 1 \Big/ \frac{1}{T_{Hot} - T_{Cold}} \iint_{S_2} \vec{q} \bullet \vec{n} dS$$

The temperature of the previous named surfaces are fixed as:

$$T_{hot} = 493.15\ K$$
$$T_{cold} = 293.15\ K$$

All the materials used in the model have a thermal conductivity which is constant with the temperature variations, except for the silicon wafer, that is more sensitive to this variable, as represented in Figure 4.

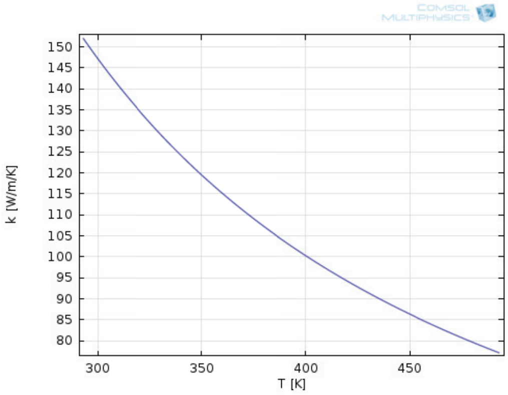

Figure 4. Silicon thermal conductivity versus temperature.

3. Genetic Algorithm

µTEG's element optimization is performed by genetic algorithm, an advanced mathematical technique that can be applied to solve complex problems characterized by many parameters and subjected to linear or non-linear constraints.

3.1. Optimization Problem Design

A generic optimization problem can be written in the following form:

max f(**x**) (*objective function*)

such that:

c(**x**) ≤ 0 (*non- linear constraints)*

$A \cdot \boldsymbol{x} \leq \mathbf{b}$ *(linear constraints)*

$\boldsymbol{l} \leq \boldsymbol{x} \leq \boldsymbol{u}$ *(lower and upper bounds)*

First step of the optimization design is represented by the definition of optimality criterion: the optimum element of the µTEG is the one with the higher power density.

This choice is related to the manufacturing processes of the microelectronics industry: that aims at the same time to maximize the electrical power and to minimize the area in order to reduce the probability of defect occurrence at wafer level.

Electrical power density is the objective function, called fitness function in genetic algorithm theory:

$$f : \frac{V * I}{4A} (W / cm^2)$$

Second step is represented by the identification of all variables that can be optimized and the definition of variability ranges for each variable.

At design level some parameters are fixed and the others are variables to be optimized; also upper and lower bounds of each variable must be defined. Referring to the described case study whose geometry has been shown in Figure 1, variable and fixed parameters are summarized in the following tables:

VARIABLES TO OPTIMIZE		
NAME	LOWER BOUND	UPPER BOUND
xm	10 μm	60 μm
xp	6 μm	10 μm
gap	4 μm	5 μm
zm	1 μm	6 μm

Table 1: Summary of variables to optimize

FIXED PARAMETERS	
NAME	VALUE
hs	500 nm
zs	375 μm
L	20 μm

Table 2: Summary of fixed parameters

Third step is represented by the definition of linear and non linear constraints. In the example described in this paper the choice of variables is subjected to the following linear constraint, that is connected to manufacturing requirements:

$$xp - gap > 2\mu m$$

3.2. Optimization Algorithm

A genetic algorithm is a heuristic search that simulates the process of natural selection [6]. The algorithm starts by creating a random initial feasible population; then it creates a sequence of new populations.

At each step, the algorithm scores each individual of the current population by computing its fitness value and selects members, called parents, based on their fitness, in order to create the next population.

Some of the individuals in the current population that have higher fitness are chosen as elite. These elite individuals are passed to the next population. Then the algorithm produces children from the parents by making random changes to a single parent or by combining a pair of parents.

The algorithm stops when one of the stopping criteria is met. In this case it stops when average cumulative change in value of the fitness function over 50 generations is less than 1e-6.

3.3. Optimization Tool

μTEG's element optimization is performed by interaction of Comsol Multiphysics and MathWorks MatLab, through the Comsol LiveLink module.

The genetic algorithm is implemented in MatLab, while electrical power density calculation is performed by two runs of Comsol Multiphysics: the first one evaluates μTEG's element electric potential and the second one evaluates μTEG's element electric current, as described in Paragraph 2.

At each generation, for each individual processed by genetic algorithm, MatLab sets new values into Comsol model's parameters and invokes Comsol simulations to evaluate fitness function.

4. Results

The result of the genetic optimization is the list of variables that maximize electrical power density.

Table 3 shows the difference between the initial values (project design) and the final values (optimized design).

Setting these optimal values in the model, the geometry, the thermal distribution and the current density change as shown in Table 3 and in the following maps (Figure 5-7).

Variable	PROJECT VALUE	OPTIMIZED VALUE
xm	55 µm	10 µm
xp	7 µm	7.36 µm
gap	4 µm	4 µm
zm	6 µm	2.12 µm

Table 3: Comparing Parameter values comparison before and after optimization

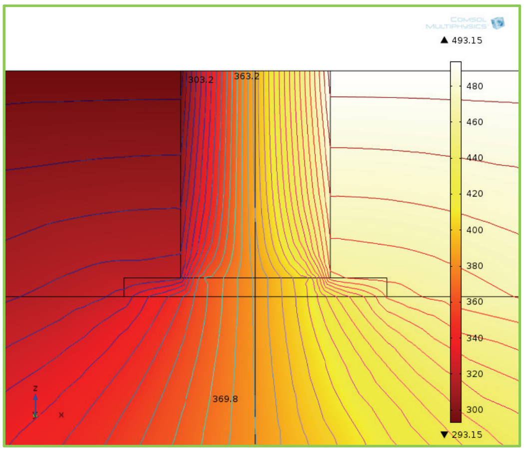

Figure 5. Heat map before optimization (detail view on the TE material).

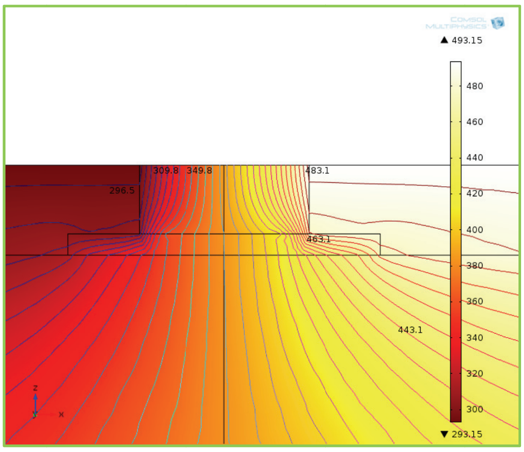

Figure 6. Heat map after optimization (detail view on the TE material).

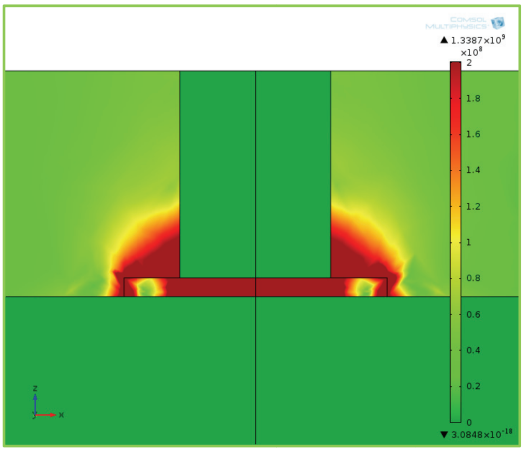

Figure 7. Electrical current density map before optimization (detail view on the TE material).

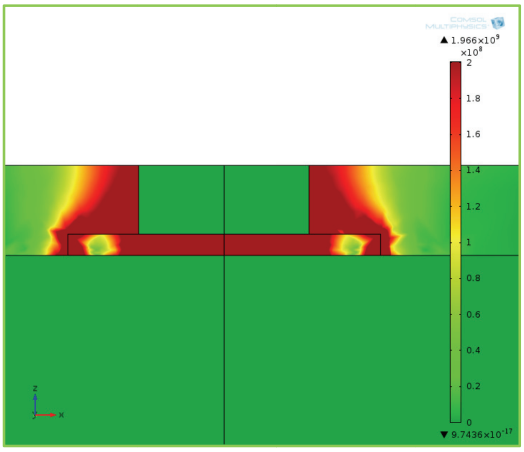

Figure 8. Electrical current density map after optimization (detail view on the TE material).

The behaviour of the two models (project design and optimized design) can be summarized in Table 4:

FEATURE	PROJECT VALUE	OPTIMIZED VALUE
Horizontal area (S)	2280 μm^2	480 μm^2
Electric Potential (V)	57.80 mV	69.92 mV
Electrical Current (I)	5.75 mA	7.10 mA
Heat flux	435.18 mW	274.33 mW
Electric Power generated (P_{load})	0.08 mW	0.12 mW
Electric Power Density (Pd)	3.64 W/cm^2	**25.86 W/cm^2**

FEATURE	PROJECT VALUE	OPTIMIZED VALUE
Max temperature difference at the two sides of the TE material	146.8 K	178.4 K
Thermal conductivity	2.96 mW/K	1538.17 mW/K
Electrical resistance	10.05 Ω	9.85 Ω
Thermal resistivity	2.30 K/W	3.65 K/W

Table 4: Comparison table of the two model behaviour

In optimum µTEG's element the electrical power density amounts to 25.8 W/cm^2. This high value is related to the usage of a simplified model, that doesn't take in account any kind of losses due to thermal interfaces and packaging.

A TE element in a real device can produce an electrical power density lower than the estimated one.

The computation time, to obtain results presented in the previous table, is less than 12 hours of run-time on a standard workstation machine: 16GByte RAM and Xeon 3GHz processor.

Figure 8 shows the fitness function evolution into generations of genetic algorithm: it quickly converges to the optimum value.

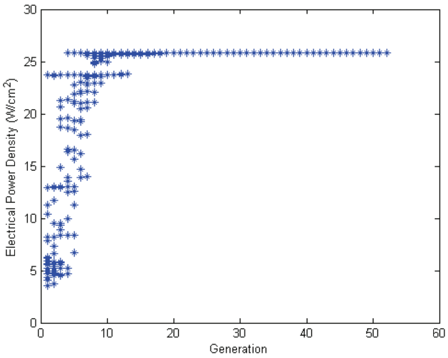

Figure 8. Fitness Function Evolution

5. Conclusions

This paper aims at demonstrating the power of interaction of multi-physics simulation with the optimization approach of genetic algorithms. It has been developed as a general purpose tool and has been applied on this case study in order to demonstrate that these optimization techniques can drive the design to greatly improve the µTEG's element performances.

Numerical results must be considered demonstrative and completely theoretical.

More generally, this tool can be a precious contribution to device designers, especially when device models have many variables to take in account and many complex geometrical or technical constraints.

6. References

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