Optimization Methodology of Thermoelectric Peltier-Modules, for Structural Design and Material Selection, using MCDM and FEM Modelling

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Abstract: Monitoring the temperature of medical products is essential, to ensure their safety and stability. The thermoelectric Peltier-modules can be used for either cooling or heating in this application. In this work, different geometries are applied and the resulting performance of the Bi2Te3-based module, characterized via finite element simulations and materials, is analyzed, where the primary objective was to reduce shear and torque stresses, which also depends operating conditions. In the first phase, Finite Element Analysis (FEM) analysis of the thermo-mechanical test unit for the Peltier-modules, is conducted. In the second phase, the best design concept selection phase, using multi-criteria decision theory is introduced, where the ranking of the criteria is weighted by the characteristics assigned to the selected values. The object is to choose the best design concept, from the alternatives generated during the first phase.

Keywords: MCDM methods; VIKOR algorithm; FEM

1 Introduction

Nowadays, the issue of thermoelectric materials is very important, due to the increase of global energy prices, but one of the main problems related to thermoelectric devices is the low efficiency of applications, where their performance is usually determined by the material properties of the constituent materials [1]. Improving the electrical performance, it is also important to extend the life and improve the reliability of the module. Thermal stress is a big problem in electronic systems. Thermal stresses and deformations are the main reasons for the limited lifetime of electronic devices [2]. Among other things, local differences in the coefficients of thermal expansion (CTE) of different materials, can be the cause of failure [3]. Regarding the mechanical failure criteria of Thermoelectric modules (TE-module) [4], the literature widely considers the von Mises stress, as the general stress, to determine the failure, it uses a FEM to calculate such stresses [5] [6]. Others highlighted the bending and shear stress responsible for mechanical failure [7]. The results of the examination show that the life expectancy can be improved by reducing the maximum thermal stress in the pellets. To verify the mechanical reliability of electronic devices, finite element software is now widely used to save analysis time. Looking at previous literature, most studies discussed the effects of changing parameters on mechanical and electrical performance. In Gao's research [8], he investigated the thermal stress distribution, mechanical properties, and thermoelectric properties of a TE-module using the finite element method. He found that the performance and efficiency of TE-module are not only influenced by material properties (Seebeck coefficient, electrical resistance, and thermal conductivity), but it is also determined by the mechanical properties of TE-module. However, few of these provided a practical way to take into account the values of mechanical and thermal stress on the entire structure, and to use them in the evaluation of new TE-modules constructions, in the initial design phase. Therefore, the aim of this work is to increase the lifetime of TE-module by exploring the potential stress-relieving effects of the geometry design at the initial design stage of TE-module by investigating the overall stresses and deflections. Using the values describing the behavior of the TE-module determined during the simulation of the finite element method (FEM) –the efficiency of the design concepts– was ranked with an interval-based target value VIKOR algorithm.

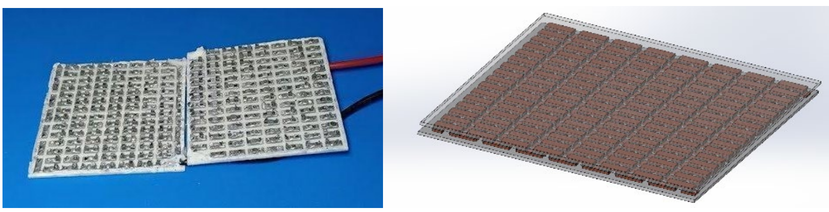

Figure 1

Structure of the TE-module (40x40x3.4 mm) (left side) and 3D model (right side) of the internal structure of the tested TE-module (Peltier 40x40 sealed Quick-Cool Quick-Ohm QC-127-1.4-8.5MS)

2 Research Methodology

The research discusses the extension of the evaluation of design concepts by taking into account weighted performance values, in the early stages of the product development process. In case of conflicting requirements, it is important to analyze the selection of materials, the selection of the design concept, the selection of production processes and the life cycles already at this design stage, since compromise solutions can be found based on the information obtained [9, 10, 11]. During the conceptual design of the development of TE-module, the best design concept is selected by using VIseKriterijumska Optimizacija I Kompromisno

Resenje (VIKOR) [12], which is a multi-criteria decision-making (MCDM) method. In order to compare the design concepts, we recorded the data obtained during the finite element analysis (FEA). The performance of the design concepts was predicted and estimated using the MCDM method, namely the interval-based target value VIKOR method, in order to obtain the concrete values of the individual sub-characteristics. The performance characteristics are the values of the maximum von Mises stress, the maximum deformation, the total deformation energy and the height, volume, surface and mass of the pellets in the TE-module. Finally, the collected data were compared using the VIKOR method, alternatively seven sub-criteria and ten design concepts. The details of each step are described in the following section.

3 Modelling of Thermoelectric Modules

In the early stages of design, numerical modelling techniques can be effectively applied to provide important information about the structural strength of new construction designs. Many literatures use the von Mises stress as a general stress to determine the failure of a TE-module, while others highlight the bending and shear stresses responsible for mechanical failure [6, 7, 8]. In this case, this work begins with the modelling of the TE-module, with the help of the SolidWorks three-dimensional (3D) computer design software and then with the finite element solver of the program, we model new designs with the operating conditions and analyses the obtained results. In addition to primary finite element analysis confirmed that soldered joints and pellets are components of the structure that suffer from plastic deformation and non-linear effects.

3.1 Thermoelectric Modules

The modelled thermoelectric module (Peltier 40x40 sealed Quick-Cool Quick-Ohm QC-127-1.4-8.5MS) contains 254 pellets of size 1.4x1.4x0.6 mm, the material is bismuth telluride (Bi_2Te_3). Based on the preliminary tests of the deformation and stress contours of this module, new pellet geometric designs were developed. Where the effect of increasing the height of TE-module pellets was investigated to determine their thermomechanical behavior under the same operating conditions. Initially analyzed results showed that the geometry of the pellets, and thus the change in their load, can have a significant effect on the von Mises stress, shear stress and total displacement arising in the TE-module. The distance between adjacent pairs of rows and columns between the pellets of the model is 0.5 mm. Figure 1 shows the structure and model of the TE-module, and Table 1 shows the dimensions of the elements for the TE-module. The 3D models of both the original and new designs were created to determine stresses (von Mises and shear) and total displacement. Previously analyzed results have shown that changing the load of semiconductor thermocouples, "pellets", has a significant effect on the von Mises stress, shear stress and total displacement. The distance between adjacent pairs of rows and columns between the pellets of the model is 0.5 mm. Figure 2 shows a model of the TE-module.

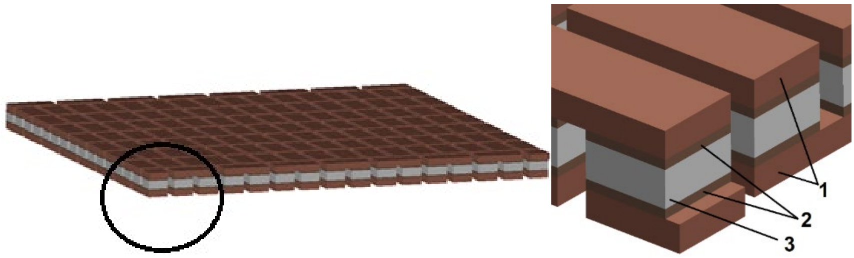

Figure 2
The structural elements of the TE-module: without the ceramic cover plate (left side), the elements of the TE-module and their enlarged detail (right side): 1: Cu elements, 2: SnPb solder layer, 3: Bi_2Te_3 semiconductor pellet

3.2 Material Properties

The modelled TE-module contain top and bottom ceramic cover plates, copper solder connectors and bismuth telluride (Bi_2Te_3) pellets. Material properties of the components at room temperature are listed in Table 2 and Table 3.

3.3 Boundary Conditions and Parameters used in the Numerical Simulation

Numerical simulation was performed using the finite element functions of SolidWorks. For the numerical simulation of the module behavior, the TE-module was placed between two rigid surfaces to perform the calculations, since under operating conditions, the load in the pellets continues to increase due to temperature changes, which hinders the thermal expansion of the TE-module, caused by the rigid surfaces under the effect of pressure. In the case of the examined TE-modul, a compressive load of 1200 kPa was applied as a load [13], specified on the surface of the aluminum oxide ceramic carrier on the warm side. During the constructional modelling of the TE-module, due to the sliding contact between the aluminum oxide ceramic and the interlocking surfaces, we characterized the contact with a friction coefficient of 0.6. For the numerical simulations, a temperature difference of 25°C was prescribed on the external aluminum oxide surfaces of the module, keeping the surface on the cold side at 20°C and applying 45°C on the warm side. Figure 3 illustrates the fit into the main structure. We present all the analyzed results for the TE-module to illustrate all the mechanical behavior and displacements during the application of the prescribed clamping force.

Table 1
Dimensions of the elements of the modelled TE-module

Elements	Size (mm)
Ceramic, (Electric insulator), Al_2O_3	40x40x0.8
Copper, (Electric conductor), Cu	3.3x1.4x0.45
Solder layer, SnPb	1.4x1.4x0.15
Pellets, Bi_2Te_3	1.4x1.4x0.6

Table 2
Material properties of the elements of the modelled TE-module

Material property	Ceramic (Electric insulator), Al_2O_3	Copper (Electric conductor), Cu	Solder layer, SnPb
Coefficient of thermal expansion, CTE, 50-190°C (10^{-6} K^{-1})	4.89-6.03	16.7-17.3	27.0
Density, ρ (kg/m^3)	3970	8940	7260
Young's modulus, *E* (GPa)	380	115	44.5
Poisson's ratio, μ	0.26	0.31	0.33

Table 3
Properties of isotropic bismuth telluride used for simulations [14]

Material property	p-type	n-type
Coefficient of thermal expansion, CTE, 50-190°C (10^{-6} K^{-1})	16.8	16.8
Density, ρ (kg/m^3)	6858.7	7858.7
Young's modulus, *E* (GPa)	47	47
Poisson's ratio, μ	0.4	0.4

3.4 Results

3.4.1 Stresses and Displacements

Simulation results presented in Table 4, the maximum and minimum values of the von Mises stress are given for a temperature difference of 25°C and a compressive load of 1200 kPa.

Based on the results of simulations, it can be said that the maximum stress is not always found in the same pellet element, but always at the corner of a pellet, at the point of contact with the welding material as illustrated in Figure 4. By reducing the temperature interval, the maximum mechanical stress level also decreases.

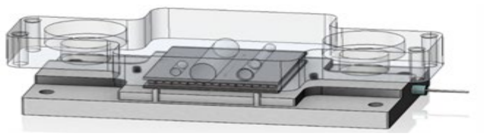

Figure 3
The assembled substructure

Table 4
The von Mises stress in the pellets (MPa) in the TE-module in the case of a maximum permissible load 350 N and the temperature difference of 25°C between the hot and cold side

Pellets height L (mm)	**von Mises stress (MPa)**	
	Min.	**Max.**
0.6	1.113	40.088
0.8	0.856	37.237
1	0.767	37.855
1.2	0.599	36.183
1.4	0.574	34.278
1.6	0.483	35.101
1.8	0.467	34.587
2	0.418	32.106
2.2	0.437	30.972
2.4	0.312	29.195

The ductile brazing alloy undergoes ductile deformation when the stress level exceeds the yield strength. This deformation reduces the stresses arising in the pellets. So, if Pb-Sn alloys were used instead of the more mechanically resistant Sn-Sb brazing alloy, the yield strength would be lower and the maximum stress level in the pellets would further decrease [14]. At the corners of the copper elements close to the ceramic surface, there are locally high stress regions, as large stress gradients develop in these areas, due to the difference between the coefficients of thermal expansion of the copper and the pellet. In addition, the tension decreases from the high stress area all the way to the base surface of the clamping element.

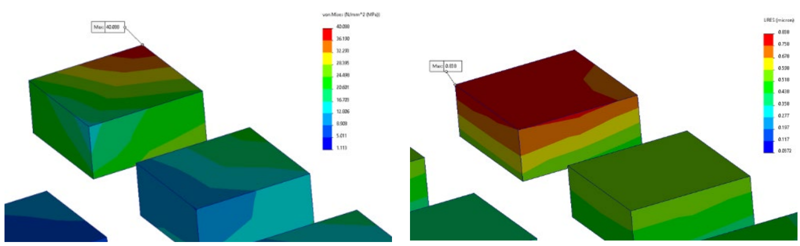

Figure 4
The von Mises stress (MPa) (left side) and displacement (micron) (right side) arising in the pellets (L=0.6 mm), in case of a temperature difference of 25°C between the hot and cold side in the TE-module

3.4.2 Summary of Results

This study examines the feasibility of improving the structural integrity of TE-module. For this purpose, FEA was carried out, where the deformation results a significant increase in the case of large temperature gradients, so it can be recommended that the thermoelectric module be installed with a damping spring, reducing the stresses arising in the elements of the general construction, which allows extending the life of the TE-module. With the use of the damping spring in the models, a significant reduction of stresses and total deformation was observed at the corners of the copper elements close to the ceramic surface, with lower von Mises stresses, shear stresses and smaller TE-module total deformation. In all cases, the maximum stresses occurred around the edge of the copper elements, near the ceramic plate. The higher stress levels around the corner zones were caused by stress concentrations. The mechanical stress distribution in the cross-sectional areas of the module varies uniformly. Based on the results, it is shown that with the variable pellet height in the design concepts, the maximum stress level and the total deflection can be reduced by changing the geometrical design and accordingly the mechanical performance/lifetime of the thermoelectric module can be improved.

4 Ranking of Design Concepts with Interval-based Target Value VIKOR Method

4.1 The Interval-based Target Value VIKOR Method

The interval-based target value VIKOR method is a possible solution to multi-attribute decision problems (MADM). To apply the VIKOR method, denote the number of criteria n and the number of materials that can be considered m.

Be it also $[x_i^L, x_i^U]$, the interval for the j^{th} criteria of the i^{th} material, $i = 1, \ldots, m$,

$j = 1, \ldots, n$

To make a decision we need a target value for what the ideal material would look like for us, so let's mark the target values for each characteristic $T_1, T_2, \ldots, T_n$, furthermore we also need a weighting of how important it is to be close to the target value for each characteristic, so let's mark the weights for each characteristic

$w_1, \ldots, w_n$, where:

$$w_j \geq 0,\ j=1, \ldots, \text{n and } \sum_{j=1}^{n} w_j = 1 \quad (1)$$

If a criterion is to be maximized or minimized (e.g., minimize cost), the maximum or minimum of the data for that criterion can be chosen as the target value. With the VIKOR algorithm, we determine for each material, one $[Q_i^L, Q_i^U]$, $i = 1, \ldots, m$ interval, which collectively indicates how far the given material falls from the target value, then a ranking can be established by comparing intervals in pairs. Next, we normalize the data. For this, let's introduce the following:

$$x_j^{L\,min} := \min\{x_{ij}^L : i = 1, \dots, m\} \tag{2}$$

$$x_j^{U\,max} := \max\{x_{ij}^U : i = 1, \dots, m\} \tag{3}$$

notations where j=1, …, n. These indicate the minimum and maximum values available for each criterion among the materials. We will use this, in addition to the target T_j, to determine the range of the data and use it to normalize the deviation from the target value. Let's introduce next:

$$V_{ij}^L := \frac{|x_{ij}^L - T_j|}{\max\{x_j^{U\,max}, T_j\} - \min\{x_j^{L\,min}, T_j\}} \in [0,\ 1] \tag{4}$$

$$V_{ij}^U := \frac{|x_{ij}^U - T_j|}{\max\{x_j^{U\,max}, T_j\} - \min\{x_j^{L\,min}, T_j\}} \in [0,\ 1] \tag{5}$$

where $i = 1, \dots, m$, $j = 1, \dots, n$ normalized quantities, the two quantities differ in that the target value for each criterion is compared with the lower or upper endpoint of the interval, so that characteristics moving on a larger scale do not excessively distort the results.) The following indicator numbers can then be calculated for each material:

$$S_i^L := \sum_{j=1}^{n} w_j \ \min\{V_{ij}^L, V_{ij}^U\} \tag{6}$$

$$S_i^U := \sum_{j=1}^{n} w_j \ \max\{V_{ij}^L, V_{ij}^U\} \tag{7}$$

$$R_i^L := \max\{\min\{V_{ij}^L, V_{ij}^U\} : j = 1,\ \dots, n\} \tag{8}$$

$$R_i^U := \max\{\max\{V_{ij}^L, V_{ij}^U\} : j = 1,\ \dots, n\} \tag{9}$$

$$\left[\frac{S_i^L - S^-}{S^+ - S^-}, \frac{S_i^U - S^-}{S^+ - S^-}\right] \tag{10}$$

$$S^+ = max\{S_i^U :\ i = 1,\ \dots, m\} \tag{11}$$

$$S^- = \min\{S_i^L :\ i = 1,\ \dots, m\} \tag{12}$$

interval, and

$$\left[\frac{R_i^L - R^-}{R^+ - R^-}, \frac{R_i^U - R^-}{R^+ - R^-}\right] \tag{13}$$

$$R^+ = \max\{R_i^U := 1,\ \dots, m\} \tag{14}$$

$$R^- = \min\{R_i^L := 1,\ \dots, m\} \tag{15}$$

it expresses individual regret. The two intervals can be combined according to how important we consider the individual indicators to be $v \in [0, 1]$ the weight of the majority of criteria (where $v = 0.5$ expresses a compromise solution). Then:

$$[Q_i^L, Q_i^U] = \left[v\frac{S_i^L - S^-}{S^+ - S^-} + (1-v)\left(\frac{R_i^L - R^-}{R^+ - R^-}\right), v\frac{S_i^U - S^-}{S^+ - S^-} + (1-v)\left(\frac{R_i^U - R^-}{R^+ - R^-}\right)\right] \quad (16)$$

indicates how far the material is from the target value. The minimum of these intervals is chosen to rank the materials. When comparing the intervals, we enter the last free parameter in the algorithm, the parameter α is the optimism level of the decision maker. The optimistic decision maker is characterized by larger α values, while the rational decision maker is characterized by α = 0.5. The value of v lies in the range of 0-1 and these strategies can be compromised by ν = 0.5 according to the suggestion of literature [16].

4.2 Ranking of Design Concepts

With the VIKOR selection method, we can specify an interval for each criterion of the design concepts, which describes the values between which, the given criteria of the given concept moves. This case study contains interval data, including language terms and target criteria. Here, we use an 11-point scale (Table 5) in order to better understand and display the quality criteria, as well as to convert the linguistic expressions into appropriate numbers.

Table 6 shows the weighting of the criteria. Determination of the most favorable values (target criteria) for each criterion:

Criterion 1: Pellet surface, (mm^2)

Criterion 2: Weight of pellets, (g)

Criterion 3: Displacement of pellets, (mm)

Criterion 4: Pellet volume, (mm^3)

Criterion 5: von Mises stress arising in pellets, (MPa)

Criterion 6: Pellet height, (mm)

Criterion 7: Total deformation energy arising in the pellets.

For this case, for all evaluated criterion, the lowest the value, the better. The goal is to select the most suitable concept based on the criteria, and to set up a ranking among the concepts, which one is the most appropriate based on the criteria examined. (Table 6) Table 7 presents the values of the criteria used for the evaluation and obtained during the simulations. Table 8 presents the relative importance of the criteria and the target values. Table 9 presents the ranking based on the criteria. Results presented in Table 9 show that the concept created with 1 mm high pellets received the highest ranking, and the design concepts implemented with 0.6 mm and 1.2 mm high pellets were the next best designs, i.e., these design concepts were close to the ideal solution based on the VIKOR method. We found that for the best-performing design concept in the TE-module, the cross-sections of the pellets were closer to the optimal ratio, the pellet height increased and the contact resistance decreased.

Table 5
Criteria value in 11-point scale format

Quality value of the material selection factor	
Exceptionally low	0.045
Extremely low	0.135
Very low	0.255
Low	0.335
Below average	0.410
Average	0.500
Above average	0.590
High	0.665
Very high	0.745
Extremely high	0.865
Exceptionally high	0.955

Overall, in the initial stage of the construction process, the selection evaluation supported by the interval-based target value VIKOR method of the proposals for changing the construction geometry, in this case the size of the pellets, in the design concepts of the TE-module, accelerates and supports the early design process of constructions.

Table 6
Comparison and quantitative value of the investigated criteria

Criteria	**Total**	**Relative importance, w_j**
1 Pellet surface (mm^2)	6	0.071
2 Pellet weight (g)	9	0.107
3 Pellet displacement (mm)	12	0.142
4 Pellet volume (mm^3)	9	0.107
5 von Mises stress in pellets (MPa)	15	0.178
6 Pellet height L (mm)	17	0.202
7 Total deformation energy in pellets	16	0.190

Table 7
The values of the criteria used for the evaluation and obtained during the simulations

Pellet Heigh L (mm)	Pellet surface (mm^2)	Pellet volume (mm^3)	Pellet weight (g)	Total Deformation Energy in pellets Max.	von Mises stress in pellets Max. (MPa)	von Mises stress in pellets Min. (MPa)	Pellet Displ. Max. (mm)	Pellet Displ. Min. (mm)
0.6	7.28	1.18	0.01	1.5784E-06	40.088	1.113	0.838	0.0372
0.8	8.4	1.57	0.01	2.0629E-06	37.237	0.856	0.896	0.0374
1	9.52	1.96	0.01	1.2117E-06	37.855	0.767	0.948	0.0368
1.2	10.64	2.35	0.02	1.3458E-06	36.183	0.599	1	0.0361
1.4	11.76	2.74	0.02	1.3323E-06	34.278	0.574	1.04	0.0326
1.6	12.88	3.14	0.02	1.5202E-06	35.101	0.483	1.1	0.0307
1.8	14	3.53	0.02	1.6015E-06	34.587	0.467	1.15	0.0295
2	15.12	3.92	0.03	1.5710E-06	32.109	0.418	1.19	0.0252
2.2	16.24	4.31	0.03	2.4016E-06	30.972	0.437	1.22	0.0233
2.4	17.36	4.7	0.03	2.3845E-06	29.195	0.312	1.26	0.0219

Table 8
Determining the relative importance of criteria

Criteria	1 Pellet surface (mm^2)	2 Pellet weight (g)	3 Pellet displacement (mm)	4 Pellet volume (mm^3)	5 von Mises stress in pellets (MPa)	6 Pellet height L (mm)	7 Total deformation energy in pellets
Relative importance of criteria, w_j	0.071429	0.1071429	0.1428571	0.1071429	0.1785714	0.202381	0.190476
Target value, T_j	0.6	7.28	1.18	0.01	0.312	0.0219	1.2117
Max, $x_j^U max$	2.4	17.36	4.7	0.03	40.088	1.26	2.4016
Min, $x_j^L min$	0.6	7.28	1.18	0.01	0.312	0.0219	1.2117

Conclusions

Previous publications [10] [11] have concentrated on VIKOR decision methods. This study adds a systematic analysis to the foregoing, while at the same time, basing the decision maker's decision process, on two different supporting methods. First, a brief overview of the relevant design process for TE-module design concepts was described.

Table 9
Ranking of design concepts

Weighting for the strategy α	**0.5**	**Optimism level *v***	**0.5**				
Pellet Height L (mm)	**S_i^L**	**S_i^U**	**R_i^L**	**R_i^U**	**Q_i^L**	**Q_i^U**	**Rank**
0.6	0.064797	0.3706723	0.3081772	1	0.0552567	0.6730919	2
0.8	0.176903	0.4805804	0.7153542	0.9283236	0.380453	0.6892103	7
1	0.075817	0.3912661	0.2222222	0.9438606	0.0062357	0.6486562	1
1.2	0.185655	0.5029667	0.5	0.9018252	0.2469637	0.6848438	3
1.4	0.218479	0.534461	0.5	0.853932	0.2655384	0.6718777	4
1.6	0.283913	0.614117	0.5568182	0.8746229	0.3390932	0.7302556	5
1.8	0.332329	0.668666	0.6676136	0.9111542	0.4377167	0.7846088	6
2	0.415764	0.7484379	1	1	0.698609	0.8868662	9
2.2	0.584168	0.9168668	1	1	0.7939075	0.9821786	8
2.4	0.61631	0.9483594	1	1	0.8120963	1	10

This is followed by Section 2, which describes the distinguishing features of the steps of the adequacy assessment process. Section 3 of this work presents the research steps and the applied materials. The authors used interval-based target value VIKOR analysis, to analyze the case study results. The study illustrates, that individual assessments, by experts, are very beneficial in the evaluation process.

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