

International Journal of Advanced Engineering Research and Science (IJAERS) Peer-Reviewed Journal ISSN: 2349-6495(P) | 2456-1908(O) Vol-8, Issue-8; Aug, 2021 Journal Home Page Available: <u>https://ijaers.com/</u> Article DOI: <u>https://dx.doi.org/10.22161/ijaers.88.35</u>



Thermoelectric Effects on MoSi₂ with Finite Element Analysis using COMSOL

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Received: 05 Jul 2021,

Received in revised form: 08 Aug 2021,

Accepted: 15 Aug 2021,

Available online: 24 Aug 2021

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Keywords— *Thermoelectric effect, peltier effect, COMSOL simulation, thermoelectric cooler thermoelectric generator.* Abstract— Realization of the thermoelectric effects within finite element analysis (FEA) by means of the COMSOL-Multiphysics platform is offered. It lets thermoelectric calculations among temperature dependent material traits on random geometries. Further, the calculations can be pooled with structural analysis plus convection can also be taken in report. Thermoelectric cooler employs Peltier effect for dissipating heat in an electronic casing structure. It shows exceptional rewards over conservative cooling skill via quiet process, extended life span, and effortless integration. Nevertheless, Joule heating results in the accumulation of internal heat thereby exposes thermoelectric cooler towards the risk of thermo-mechanical breakdown all through continuous operations in pragmatic thermal surroundings. In this paper, a 3D module of thermoelectric material MoSi2 is designed on the way to examine the thermoelectric effect of the material taking into consideration the temperature reliant TE material traits. The transient behavior is also observed. The results can be openly used intended for consistent design considerations and optimized thermoelectric devices in engineering.

I. INTRODUCTION

The thermoelectric effects within finite element analysis (FEA) can be realized by means of the COMSOL-Multiphysics platform. It lets thermoelectric calculations among temperature dependent material traits on random geometries [1]. The field equations in thermoelectric coupled intended for temperature as well as electric potential under steady state calculations are described as

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

and

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

where the material traits α indicate the seebeck-

coefficient, σ indicates the electric conductivity and λ indicates the thermal conductivity. Generally the material traits rely on the temperature moreover may perhaps be anisotropic. At this juncture simply isotropic substance traits are worn. For anisotropic resources, the appropriate matrices are taken in consideration. The transient magnetic fields are also not taken in consideration. The projected equations are as a consequence to the coupled equations in [2] or the text referred within [3].

II. GEOMETRICAL MODEL

COMSOL Multi-physics allows the execution of ordinary random partial differential equations (PDEs) intended for the field variable **u** over a one to 3D section Ω . Two PDE modes are worn: The "Coefficient-Form" as well as the

"General Form".

$$c_{a}\frac{\partial^{2}u}{\partial t^{2}} + d_{a}\frac{\partial u}{\partial t} + (-c\nabla u - \alpha u + \gamma) + \beta \cdot \nabla u + au = \beta$$
(3)

The thermoelectric field equations at this instant are altered into the "coefficient form" as follows. In the midst, the vector value of the field variable is defined by

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

the coefficient c in (3) is

$$\begin{pmatrix} \lambda + \sigma \alpha^2 T & \sigma \alpha T \\ \sigma \alpha & \sigma \end{pmatrix}$$
 (5)

Intended for transient calculations the capacitive influence need to be neglected. Generally it is satisfactory to mull over merely the thermal capacity (heat capacity C, density ρ). Then d in equation (3) is

$$d = \begin{pmatrix} \rho C \\ 0 \end{pmatrix} \tag{6}$$

The subsequent examples show outcomes of calculations for characteristic thermoelectric applications. The material traits for the calculations with temperature independent values are depicted in table 1. Here characteristic values for Molybdenum Silicide MoSi₂ were taken from [4] and Copper was taken from [2]. Temperature dependent material traits were interpolated by means of cubic splines (figure 1-3).



Fig.1: Temperature dependent Seebeck coefficient of MoSi2 and cubic spline interpolation.



Fig.2: Temperature dependent thermal conductivity of MoSi2.



Fig.3: Temperature dependent electric conductivity of MoSi2.

Table.1 Numerical material properties. [4]

Material Properties	MoSi ₂
Density	6240 Kg / m ³
Thermal Conductivity	66.2 W / (m.K)
Electric conductivity	3.28e ⁶ S/m
Seebeck Coefficient	3.9e ⁻⁶ V/K
Heat capacity at constant pressure	430 J / (kg.K)

T (K)	α (10 ⁻⁶ V/K)	λ (W/m/K)	σ(10 ⁵ A/V/m)
100	80	2.7	2
150	130	2.3	1.55
200	180	1.6	1.05
250	210	1.4	0.75
300	228	1.35	0.65

Table 2: Temperature dependent material properties.

350	230	1.4	0.58
400	228	1.8	0.73

III. THERMOELECTRIC COOLER

The geometry of a straightforward thermoelectric cooler comprises of solo p-type semiconductor component with dimensions $1 \times 1 \times 6 \text{ mm}^3$. It is sandwiched by two copper electrodes of 0.1 mm in thickness (Figure 4).



Fig.4: A p-type thermoelectric element.

The base is kept back at temperature 300 K along with 0V of voltage. At the top of the upper electrode, a current of 0.7A was applied. The resultant distribution of temperature is revealed in the middle. A temperature difference of nearly 70 K is achieved. Table 1 shows the (constant) material properties. Figure 4 shows the result of the calculation. In the center, the temperature distribution shows that the cold side temperature is at 230K. The associated voltage is shown right. To drive the current, a voltage of 50 mV is needed.

IV. TRANSIENT OPERATION

Figure 5 shows the outcome of a time reliant computation. The chart reveals the transient cold side temperature with temperature dependent material parameters. The short current pulse leads to a momentary temperature plunge of about 3K. Such super cooling effects are also described in [5].



Fig.5: Transient calculation of Peltier super cooling.

A tiny current pulse leads to momentarily lesser temperatures at the cold end. In such transient computation, barely the thermal capacities as suggested by equation (6) in the midst of the heat capacities in addition to densities are represented in table 1.

V. THERMOELECTRIC GENERATION

In order to simulate a thermoelectric generator, the earlier mentioned semiconductor component was worn yet again by means of the changeable material traits (figure 1 - 3). The top side of the higher electrode was adjusted to 373K, whereas the base of the lower electrode was adjusted to 273K along with 0V. Figure 6 displays the outcome of the current - voltage characteristics of the thermoelectric material and Figure 7 displays the outcome of the current power characteristics of the material.



Fig.6: Current-voltage characteristics of the thermoelectric material



Fig.7: Current- -power characteristics of the thermoelectric material

In accordance to the properties, it was observed that the open circuit voltage of the component is computed to be about 21mV, whereas the short-circuit current is computed around 220mA. The highest power output is observed as 1.22mW.

VI. SUMMARY

The accomplishment of the thermoelectric field equations using COMSOL multi physics 5.2 is projected. Thermoelectric computations may perhaps be finished for arbitrary geometries too. Anisotropy (not revealed here) as well as temperature reliance of the materials can also be incorporated. In addition, transient computations were made. It is probable in adding the structural analysis or convection effortlessly (not exposed here).

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