Multi-physics analysis for the design and development of micro-thermoelectric coolers

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Abstract: A rigorous research is underway in our team, for the design and development of high figure of merits (ZT= 1.5~2.0) micro-thermoelectric coolers. This paper discusses the fabrication process that we are using for developing the Sb$_2$Te$_3$/Bi$_2$Te$_3$ micro-thermoelectric cooling modules. It describes how to obtain the mechanical properties of the thin film TEC elements and reports the results of an equation-based multiphysics modeling of the micro-TEC modules. In this study the thermoelectric thin films were deposited on Si substrates using co-sputtering method. The physical mechanical properties of the prepared films were measured by nanoindentation testing method while the thermal and electrical properties required for modeling were obtained from existing literature. A finite element model was developed using an equation-based multiphysics modeling by the commercial finite element code FEMLAB. The model was solved for different operating conditions. The temperature and the stress distributions in the P and N elements of the TEC as well as in the metal connector were obtained. The temperature distributions of the system obtained from simulation results showed good agreement with the analytical results existing in literature. In addition, it was found that the maximum stress in the system occurs at the bonding part of the TEC i.e. between the metal connectors and TE elements of the module.

Keywords: Multi-Physics Analysis, Thermoelectric coolers, Phonon, Nanoindentation test, Von misses stress

1. INTRODUCTION

TEC (Thermo Electric cooler) modules show excellent cooling performance for the applications where temperature stabilization, temperature cycling or cooling below ambient is required. Due to their excellent performance, TEC are widely used in numerous products, including CCD (charge coupled device) cameras, laser diodes, infrared detectors, microprocessors, blood analyzers, portable picnic coolers as well as many other applications in aerospace [1], bioengineering [2, 3] and semiconductor industries. Recent suggestion by Dresselhause et al. [4] that nanoengineering of thermoelectric (TE) materials could result in higher values of ZT (thermoelectric figure of merit), and the findings of Venkatasthabramanian et al. [5] that a ZT value of 2.4 can be achieved in Sb$_2$Te$_3$ / Bi$_2$Te$_3$ thin films near 1 nm thickness, have given enormous momentum to the research on micro-TEC. Although TEC modules in the range of millimeter and centimeter sizes are widely commercially available these days, the micro-TEC devices are still in the research and development stage. Some of the recent works on fabrication of thin film for micro-TEC include those of H. Zou et al. [6, 7], Min and Rowe et al. [8], J.P. Fleural et al. [9] and so on. Numerical study on micro-TEC has also gained attention of researchers. One of the example of which is the study of Alexandru et al. [1], where they have performed FEM analysis of thermoelectric phenomena in semiconductor materials.

In this paper, we have developed an equation-based multiphysics model using the FEM code FEMLAB, for exploring the physical insights of micro-TEC. The fabrication process of the micro-TEC has been discussed. Various properties required for FE modeling have been obtained and thermal and structural analysis of the TEC have been performed. The model developed in this study will be helpful in reducing the time and cost of the design and development of micro-TEC significantly in our ongoing research.

2. WORKING PRINCIPLE OF A TEC

Fig. 1 shows the schematic picture of a typical TEC. In general a TEC consists of a series of P type and N type thermoelectric (doped semiconductor) materials sandwiched between two ceramic wafers. The TE materials are connected electrically in series and thermally in parallel through metal connectors on both sides. When a DC current passes through these materials, three different effects take place simultaneously, namely: the Peltier effect, Joule heating effect and heat transfer by conduction due to the temperature difference between the hot and the cold junctions.

It is generally known that electrons in P-type materials have lower energy state and those in N-type materials have higher energy state. As the electrons move from the P type to the N type material through an electrical connector the electrons jump to a higher energy state absorbing thermal energy from the cold side plate, but when these high energy electrons move from N type to P type material through the metal connector attached to the hot plate, they release their extra thermal energy. Thus the electrons, as they pass through the P and N

![Fig. 1 Schematic picture of a TEC module.](image-url)
4. MULTIPHYSICS MODELING

4.1 Model geometry

A simplified 2D model which consisted of a single pair P and N column of thermoelectric alloys along with metal (Cu) connectors on top and bottom of the TE columns as shown in Fig. 3(a) was developed for validation of the multiphysics modeling approach used in this study. The approach was then extended to three dimensions. The 3D model developed in this study consisted of three pairs of TE couples connected electrically in series through top and bottom metal connectors and thermally in parallel as shown in Figs. 3(b) and (c). The thermoelectric couples along with the metal connectors were sandwiched between two silicon substrates, which served as the hot and cold plate of the TE cooler. The dimensions of the substrates, connectors and TE elements were 700x600x200 µm, 140x515x2 µm and 65x500x10 µm respectively.

4.2 Governing equations

The transport of electrons in a thermoelectric material can be modeled using the Boltzmann transport equation (BTE). However, the boundary resistances in the metal-thermoelectric boundary interfaces hinder the phonon heat flow differently than the electronic heat flow and cause electron-phonon thermal non-equilibrium near the interfaces. Moreover, the mutual interaction of electron and phonon affects the thermal and electrical transport processes and hence the temperature distributions of both the electrons and phonons in the TE material. Therefore, to obtain the electron and phonon temperature distribution in TE materials of a TEC we need the coupled Boltzmann transport equation given by

\[-V \cdot (k_e \nabla T_e) = P(T_e - T_p)\]  
\[-V \cdot (k_p \nabla T_p) = \rho j_e^2 - P(T_e - T_p)\]

where \( p = \frac{n k_B}{\tau_e} \).

Descriptions of the symbols used in above equations and of those that will come forward are provided in the nomenclature section at the end of the paper. For simplification, as well as for proving the validation of our approach we used a one-dimensional approach as followed by Da Silva and Kaviany [16]. The coupled BTE then reduced to the form

\[-k_e \frac{d^2 T_e}{dx^2} = \rho_j j_e^2 - P(T_e - T_p)\]  
\[-k_p \frac{d^2 T_p}{dx^2} = P(T_e - T_p)\]

The boundary conditions for the model are

\[\frac{T_e - T_p}{(A_e R_p)_{h,e}} \bigg|_{x_0} = -k_e \frac{dT_e}{dx} \bigg|_{x_0}\]  
\[\frac{T_e - T_p}{(A_p R_p)_{h,p}} \bigg|_{x_0} = -k_p \frac{dT_p}{dx} \bigg|_{x_0}\]  
\[\frac{T_e - T_p}{(A_e R_p)_{w,e}} \bigg|_{x_0} = -k_e \frac{dT_e}{dx} \bigg|_{x_0} + \Delta x \cdot j_e \bigg|_{x_0} - (A_e R_p)_{w,e} \frac{j_e^2}{2}\]
The non-linear coupled set of equations (3) and (4) was modeled in the FEMLAB by selecting the general form of the PDE (Partial Differential Equation) given by

\[
\nabla \cdot (-e \nabla u - au + \gamma) + \beta \nabla u + au = f
\]

The \( \alpha \), \( \beta \) and \( \gamma \) in Eqn. 9 represents the conservative flux convection coefficient, the convection coefficient and the conservative flux term respectively. Considering \( \alpha = 0 \), \( \beta = 0 \) and \( \gamma = 0 \), the Eqn. 9 becomes

\[
-c \nabla^2 u + au = f
\]

A comparison between Eqn. 3 and Eqn. 10 yields \( T_e = u \), \( k_p = c \), \( a = P \) and \( f = P \beta_2 \). Similarly, by comparing Eqn. 4 with Eqn. 10 we obtain \( T_e = u \), \( k_p = c \), \( a = P \) and \( f = PT_2 \). Thus the governing equations (Eqn. 3 and Eqn. 4) were implemented in the FEMLAB through Eqn. 10 by using the constants as mentioned.

### 4.3 Electrical and thermal properties

The electrical and thermal properties of the Bi\(_2\)Te\(_3\) and Sb\(_2\)Te\(_3\) used in the model, obtained from ref. [16] are shown in Table 1. The boundary thermal and electrical resistances for the electron and phonon [16] are presented in Table 2.

### 4.4 Mechanical properties

For structural analysis of the model the mechanical properties are required. The Young’s modulus and the Poisson’s ratios were obtained using the nanoindentation method. Hardness of the materials were also measured from nanoindentation test results. The tests were performed using a nanoindentation XP with the Berkovich tip indenter, as shown in Fig. 4. Maximum indentation depth was 1000 nm. Fig. 5 shows a typical modulus versus displacement curve and hardness versus displacement curve as well as the nanoindentation mark on a Bi\(_2\)Te\(_3\) sample. Results obtained from the nanoindentation test are shown in Table 3.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Modulus (GPa)</th>
<th>Hardness (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sb(_2)Te(_3) (Bulk)</td>
<td>44.823</td>
<td>1.23</td>
</tr>
<tr>
<td>Bi(_2)Te(_3) (Bulk)</td>
<td>41.799</td>
<td>1.259</td>
</tr>
<tr>
<td>Bi(_2)Te(_3) (film)</td>
<td>48.325</td>
<td>2.750</td>
</tr>
<tr>
<td>Cu</td>
<td>229.706</td>
<td>6.654</td>
</tr>
</tbody>
</table>

### 5. RESULTS AND DISCUSSION

The phonon and electron temperature distributions in the...
2D simplified model for $T_e = 285$ K, $T_p = 300$ K and $I_e = 30$ mA are shown in Figs. 6(a) and (b), while the total displacement and stress developed in the model are shown in Figs. 6(c) and (d) respectively. Figs. 7 and 8 represent the variations of electron and phonon temperatures along the height of the Bi$_2$Te$_3$ (N type) and Sb$_2$Te$_3$ (P type) TE columns for different current (0, 15 and 30 mA) inputs.

It can be noticed that for $I_e = 0$ i.e. for no thermoelectric effect, the electron and phonon temperatures ($T_e$ and $T_p$) are same. But as $I_e$ increases, the difference between $T_e$ and $T_p$ near the junction increases.

The deviations of $T_e$ and $T_p$ at the hot junctions are higher than those at the cold junction. The reason is quite clear: at the cold junction (i.e. at $x = -2$ µm) the values of $T_e$ and $T_p$ decreases with peltier cooling and increases with Joule heating, but at the hot junction (i.e. at $x = 2$ µm) both the peltier effect and Joule heating effect raises the values of $T_e$ and $T_p$. Thus the deviations at hot junction are always higher than those at the cold junction. All these trends of the curves as well as their pattern and values are similar to those obtained by L.W. da Silva et al. through analytical solutions for same operating conditions. These consistencies prove the validation of our model and approach of study.

The Von misses equivalent stress developed in the model is shown in Fig. 6(d), while the variation of Von misses stress along the length of P and N type TE columns are shown in Fig. 9. It is evident from Fig. 9 that the maximum stress in the model occurs at the interface between the hot connector and the P type TE column. The curves for both the N type and P type columns show that the most vulnerable location for failure due to thermal stress are the end points of the column-metal connector interfaces. While the maximum stress developed at the N-type column-metal connector interface was 80 Mpa, the maximum stress for the P-type column was 125 Mpa. The higher stresses in the N-type thermoelectric column are due to the higher temperature in the Sb$_2$Te$_3$ column compared to Bi$_2$Te$_3$ column as noticed in Figs. 7 and 8. In the
6. CONCLUSIONS

Thermoelectric thin films were prepared using co-sputtering method. Properties required for finite element analysis were obtained through nanoindentation test on the thin films and bulk materials, in conjunction with other means. An equation-based multiphysics model was developed for analyzing the insights of micro-thermoelectric coolers. Simulation with the developed model showed fascinating results. The developed model will be used for the design and development of micro-thermoelectric cooler in our ongoing research.

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NOMENCLATURE

- \( k_p \) = Phonon thermal conductivity (W/mK)
- \( k_e \) = Electron thermal conductivity (W/mK)
- \( K_B \) = Boltzmann constant \( 1.3006 \times 10^{-23} \) J/K
- \( T_p \) = Phonon Temperature
- \( T_e \) = Electron temperature
- \( \tau_e \) = Electron/hole energy relaxation time
- \( \rho_e \) = Electrical resistivity (Ωm)
- \( J_e \) = Current (A)
- \( A_{ce} \) = Cross sectional area of thermoelectric column (m²)
- \( R_c \) = Contact resistance (W/mK)
- \( \delta \) = Electron-phonon cooling length (m)

REFERENCES


