ABSTRACT

Thermoelectric generators (TEGs) are solid state devices that convert thermal energy into electrical energy using the Seebeck effect. They can be used for energy harvesting in trucks and passenger vehicles by taking advantage of the temperature difference between the exhaust pipes and ambient environment. The key issue with thermoelectric devices today is the demand for increased operating temperatures while maintaining adequate reliability and low cost. Since TEGs are subjected to sub-critical thermal cyclic loading, ensuring satisfactory reliability is important for commercially viable products. TEGs used in passenger vehicles should be able to withstand extreme environmental conditions such as high temperature, shock and mechanical vibration [1]. Since the operating temperatures of TEGs can reach temperatures higher than 500 °C, aluminum brazes offer a good high temperature solution for die attach applications. The thermoelectric materials of TEGs are prone to oxidation and sublimation. A solution to minimize these phenomena is to enclose the TEG device in a hermetic package. This paper analyzes the reliability of aluminum alloy braze Al 718 (12% Si, 88% Al) used in TEG packages under fatigue loading. A power cycling temperature fluctuation method was employed to simulate the operating conditions of the TEGs for passenger vehicle. Low cycle fatigue simulations were performed using the direct cyclic approach embedded in the finite element software ABAQUS. Direct cyclic approach uses an extrapolation technique, which allows for efficient and computationally inexpensive simulations. The numerical model was validated using experimental test data. A validated damage model was used to analyze the cyclic damage evolution in the aluminum alloy braze for the hermetic TEG packages.

INTRODUCTION

The development of highly efficient thermoelectric materials enables the opportunity to utilize TEGs in passenger vehicles and cars under fluctuating temperature conditions. TEG packaging can be a challenging task in such loading conditions. The role of electronic packaging of TEG is not only to prevent the thermoelectric devices from shock and vibration, but also to create a hermetic atmosphere in which the TEG can function without ingress of atmospheric air. Thus, the design of the electronic package contributes to the overall efficiency of the TEGs. TEG packages which allow peripheral and vertical heat losses can reduce the efficiency significantly.

TEGs functioning principle is described by use the Seebeck effect, in which temperature differences result in a voltage, as shown in FIGURE 1. When a p-type and n-type semiconductors are connected in series, and a temperature difference is applied in the opposite sides, an electric current is generated as a result of the movement of the electrons and holes for the thermal excitation. Based on this principle, TEGs are constructed by connecting an array of p-type and n-type semiconductors using conductive metal pad as shown in FIGURE 2. The p- and n-type
semiconductors are referred to as thermoelectric (TE) materials. TE materials are connected electrically in series and thermally in parallel.

In the automotive application, TEGs are encapsulated using ceramic materials having high thermal conductivity to ensure a direct thermal path from the hot side to the cold side of the TEG. Since the operating temperature can exceed 500 °C, braze materials are used to bond different components of TEGs such as metallization, ceramic housing, and semiconductors. From perspective failure standpoint, the braze layers represent one of the weak links in the TEG package. Aluminum brazes are ductile materials and have a significant coefficient of thermal expansion (CTE). The interfaces bonded by brazes experience thermal stresses due to CTE mismatch. A thermal fluctuation during the operation of the TEGs results in cyclic fatigue loading in the aluminum braze. According to automotive standard AEC-Q101, electronic components used in the automotive application must withstand 5000 power cycles at temperature fluctuations higher than 100 K [2]. In order to assess the reliability of a thermoelectric device package assembly, accelerated lifetime testing is often used with higher temperature fluctuations for short time period.

At elevated temperature, the deformation of the braze material is likely to be predominantly plastic. The accumulation of plastic strain with number of cycle reversals can cause crack initiation and propagation, and eventually failure of the brazing joint [3]. Since the deformation of braze at elevated temperature usually exceeds the yield strength, a low-cycle fatigue (LCF) model should be considered while predicting the fatigue life of the TEG packages. Several failure models have been introduced to predict the fatigue life of solder/braze materials [3-15]. Dissipated energy-based constitutive models have been widely used. The continuum damage mechanics approach can be used to model the failure since the braze material is highly ductile. Damage initiation and evolution can be evaluated from the stabilized stress-strain response. A computationally efficient and inexpensive approach is the direct cyclic method utilizing an extrapolation of the stabilized stress-strain response of the material over many load cycles and checking the status of the critical elements at periodic intervals [16].

This paper describes an efficient modeling technique to simulate and validate the low cycle fatigue analysis of an aluminum alloy braze (12% Si, 88% Al) using the direct cyclic approach. Damage nucleation life by crack initiation was modeled using a power law of the accumulated plastic hysteresis energy during cyclic loading. Calibration of the damage model was performed using both experimental testing and finite element simulations. The validated model then can be used to predict the fatigue life of the TEG package at different operating conditions. To validate the FEA damage model, experimental specimens were fabricated in the clean room, and then thermally shocked. Shear tests were conducted to evaluate the decrease in strength due to material degradation during thermal cycling. Three-dimensional (3-D) computer aided design (CAD) models of test specimens were used in the finite element method.

EXPERIMENTAL TESTING Experimental specimens were fabricated in a clean room. Aluminum alloy braze was used to attach Silicon Germanium (SiGe) dies with Direct Bonded Aluminum (DBA) substrates. A
A brazing profile was determined, and Transient Liquid Phase (TLP) bonding technique was used for brazing. Several brazing profiles were investigated and a strong bond was achieved at 625 C reflow temperature. The brazing profile used in the fabrication process was shown in FIGURE 3. Experimental specimens fabricated in the laboratory is shown in FIGURE 4.

Shear tests were conducted using an XYZTEC series (S00249095) bond tester. Specimens were subjected to cyclic thermal loading in a thermal shock chamber for a total number of cycles that varied between 100 and 1200 cycles. Thermal shock of the TEG package is commonly used for microelectronics devices, whereas the device is placed in an oven and the temperature is varied over time. In the current study, thermal shock was applied to the TEG package, with temperature fluctuating between -40 °C to 200 °C, with a 3 minute ramp time and 10 minute dwelling time. The thermal shock temperature profile is shown in FIGURE 5. The braze strength was determined from a shear test of a batch of specimens every 100 cycles. The following relationship between strength and damage was used to convert the strength degradation data in terms of a scalar damage variable [17]:

\[ \bar{\sigma} = (1 - D)\sigma \]  

(1)

where, \( \bar{\sigma} \) is the damaged strength, \( \sigma \) is the effective (or undamaged) stress tensor, and \( D \) is damage.

VALIDATION MODEL

A. Finite Element Analysis Geometry and Meshing

FIGURE 6 shows a CAD model for 3-D full scale experimental shear test specimen. To reduce the computational time, a quarter model was used in the FEA simulation [18]. The finite element mesh employed 8-node linear hexahedral elements (C3D8R) [19]. To increase the simulation accuracy, a finer mesh was chosen near the braze area, as shown in FIGURE 6. A mesh refinement study was performed on the assembly of TEG package model to ensure adequate number of elements for the analysis. A thermo-mechanical analysis on the TEG package assembly was used in the study. The maximum equivalent plastic strain in the model was monitored while increasing the number of elements in the mesh. FIGURE 8 demonstrated insignificant changes in the maximum accumulated plastic strain for models having more than 200,000 elements. Therefore, from the mesh refinement study, meshes with a number of elements between 200,000 and 300,000 were found to be adequate enough to produce mesh independent results with optimized computation cost.
B. Material Modeling

Different layers of the materials used to fabricate shear test specimen are demonstrated in FIGURE 9. Mechanical and thermal properties of the materials used in the FEA are listed in TABLE 1. For SiGe, alumina (Al$_2$O$_3$) and aluminum (Al) only elastic properties were used. Elastic-plastic properties were used for the aluminum alloy braze. The kinematic hardening components of the plastic model were evaluated from the stabilized cyclic response. The data points used in the plasticity model were calculated from the stabilized response are listed in TABLE 2. A damage nucleation and evolution model was applied only to the braze layers anticipating the failure would take place in that area. For the low cycle fatigue analysis, a power law defining the damage initiation and evolution were considered. The damage initiation equations is

$$N_0 = c_1 \Delta w^{c_2} \quad (2)$$

and the damage evolution equation is

$$\frac{dD}{dN} = \frac{c_3 \Delta w^{c_4}}{L} \quad (3)$$

In the above equations, $N_0$ is the number of cycles to initiate damage, $\Delta w$ is the accumulated inelastic hysteresis energy per cycle and $L$ is the characteristic length of the element.

### TABLE 1: MATERIAL PROPERTIES OF DIFFERENT MATERIALS OF TEG PACKAGE

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal conductivity, W/m-K</th>
<th>Coefficient of thermal expansion, ppm/°C</th>
<th>Young’s modulus, GPa</th>
<th>Poisson’s ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum (Al)</td>
<td>210</td>
<td>23.6</td>
<td>68</td>
<td>0.36</td>
</tr>
<tr>
<td>Alumina (Al$_2$O$_3$)</td>
<td>20</td>
<td>7.7</td>
<td>303</td>
<td>0.21</td>
</tr>
<tr>
<td>Aluminum alloy braze (12% Si, 88% Al)</td>
<td>210</td>
<td>20</td>
<td>72</td>
<td>0.44</td>
</tr>
<tr>
<td>Silicon Germanium (SiGe)</td>
<td>4.8</td>
<td>2.7</td>
<td>130</td>
<td>0.28</td>
</tr>
<tr>
<td>Low Temperature Co-fired Ceramic (LTCC)</td>
<td>3.3</td>
<td>5.8</td>
<td>120</td>
<td>0.25</td>
</tr>
</tbody>
</table>

### TABLE 2: STRESS-STRAIN DATA OBTAINED FROM THE STABILIZED CYCLIC RESPONSE OF ALUMINUM ALLOY BRAZE [20]

<table>
<thead>
<tr>
<th>Stress, $\sigma_i$, MPa</th>
<th>Equivalent Plastic Strain, $\varepsilon_{pl}$, mm/mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>67.9</td>
<td>0</td>
</tr>
<tr>
<td>78.41</td>
<td>0.17</td>
</tr>
<tr>
<td>80.04</td>
<td>0.28</td>
</tr>
<tr>
<td>81.65</td>
<td>0.37</td>
</tr>
<tr>
<td>82.46</td>
<td>0.57</td>
</tr>
<tr>
<td>84.89</td>
<td>0.67</td>
</tr>
</tbody>
</table>

C. Direct Cyclic Modeling

The direct cycling approach was used to simulate fatigue loading over thousands of cycles. This method allows the finite element simulation to be performed in cycle increments, as opposed to cycle-by-cycle approach that is extremely computationally intensive. In the direct cyclic method, a truncated Fourier series of a displacement function $\bar{u}(t)$, as in equation (4), is used to determine the structural response within a load cycle

$$\bar{u}(t) = u_0 + \sum_{k=1}^{n}[u_k^s \sin k\omega t + u_k^c \cos k\omega t] \quad (4)$$

where $n$ is the number of Fourier terms, $\omega = 2\pi/T$ is the angular frequency, and $u_0$, $u_k^s$ and $u_k^c$ are unknown displacement coefficients which are solved by using modified Newton method. In addition, the residual vector $\bar{R}(t)$ is expanded in the same way as displacement function where each residual vector coefficient $R_0$, $R_k^s$ and $R_k^c$ corresponds to the displacement coefficient mentioned above.
\[
\ddot{R}(t) = R_0 + \sum_{k=1}^{n} [R_k^s \sin k\omega t + R_k^c \cos k\omega t]
\]  

(5)

The residual vector coefficients are obtained by integration over the load cycle employing standard element-by-element calculations [21].

\[
R_0 = \frac{2}{T} \int_0^T R(t) \, dt
\]

(6)

\[
R_k^s = \frac{2}{T} \int_0^T R(t) \sin k\omega t \, dt
\]

(7)

\[
R_k^c = \frac{2}{T} \int_0^T R(t) \cos k\omega t \, dt
\]

(8)

The residual vector coefficients are then used to determine the displacement correction to obtain the updated displacement solution in the subsequent iteration. The parameters used for the direct cycling procedure to determine the updated displacement coefficients are shown in TABLE 3.

### TABLE 3: PARAMETERS FOR DIRECT CYCLE PROCEDURE

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial number of terms in the Fourier series</td>
<td>25</td>
</tr>
<tr>
<td>Maximum number of terms in the Fourier series</td>
<td>30</td>
</tr>
<tr>
<td>Maximum number of iterations allowed in a step</td>
<td>100</td>
</tr>
<tr>
<td>Minimum increment in number of cycles over which the damage is extrapolated forward</td>
<td>50</td>
</tr>
<tr>
<td>Maximum increment in number of cycles over which the damage is extrapolated forward</td>
<td>100</td>
</tr>
<tr>
<td>Total number of cycles allowed in a step</td>
<td>3001</td>
</tr>
<tr>
<td>Damage extrapolation tolerance</td>
<td>1.1</td>
</tr>
</tbody>
</table>

D. Boundary Conditions

Both thermal and mechanical boundary conditions were applied to the TEG model. A thermal shock temperature profile for each cycle, was applied as shown in FIGURE 5. Mechanical boundary conditions included fixing the x- and z- symmetrical cutting planes. The bottom node on the intersecting line of the symmetry planes was fixed in y- direction, as indicated FIGURE 9.

E. Results

The progressive damage due to thermal loading was calculated for 1200 cycles. Low cycle fatigue analysis using direct cyclic approach reduced the simulation time significantly. Direct cyclic simulations were performed considering different number of cycles as the increment over which the damage was calculated. The considered number of cycle increments were 50, 100 and 500 cycles. Each simulation gave almost identical results, thus the 500-cycle increments were chosen for all the analyses. The damage contour plot for the shear test specimen is shown in FIGURE 10. The CTE mismatch is larger between the SiGe and the braze layers, which caused significant damage. The damage was computed by averaging the values for the entire cross-section of the braze (FIGURE 11).

The damage calculation depends on the material coefficients \( c_1, c_2, c_3 \) and \( c_4 \) from the equations (2) and (3). A parametric study was conducted to determine the best set of values for \( c_1, c_2, c_3 \) and \( c_4 \) that describes the damage behavior in the aluminum alloy braze. A best fit data with the experimental results was obtained, and a comparison between the experimental and simulation data is shown in FIGURE 13. The damage initiation criteria determined the number of cycle to initiate damage. Once the calculated damage value reached the initiation criteria, the damage evolution process started. Therefore, no zero damage existed up to the 271st cycle. An initiation life was found to be approximately 300 cycles from the experimental observations, which is close to the computed value. The material coefficients determined from this procedure are listed in TABLE 4.

### TABLE 4: DAMAGE COEFFICIENTS OF ALUMINUM ALLOY BRAZE

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_1 )</td>
<td>275</td>
</tr>
<tr>
<td>( c_2 )</td>
<td>-0.014</td>
</tr>
<tr>
<td>( c_3 )</td>
<td>3.5x10^9</td>
</tr>
<tr>
<td>( c_4 )</td>
<td>1.15</td>
</tr>
</tbody>
</table>
THERMOELECTRIC GENERATOR PACKAGE MODELING

A. Finite Element Analysis

The validated FEA damage model was used to predict performance of the proposed TEG package under thermal shock loading. The proposed TEG package design accommodates the p- and n-type semiconductors between two Direct Bonded Aluminum (DBA) substrates. As mentioned earlier, TEGs are subjected to fluctuating temperatures, thus the semiconductor materials are prone to oxidation and sublimation in the presence of air. To prevent these detrimental phenomena, a hermetic package was designed and manufactured to house the TEG assembly. The TEG assembly was analyzed using finite element simulations with ABAQUS. A peripheral window ring of Low Temperature Co-fired Ceramic (LTCC) was proposed to seal the TEG package. To ensure hermeticity, inert gas was inserted into the package.

A 3-D CAD model of the TEG package was generated in ABAQUS as shown in FIGURE 14. A cross-sectional view depicting the different layers of the TEG assembly is shown in FIGURE 15. Low cycle fatigue using the direct cyclic approach was used for analysis. Material coefficients obtained from the validation model were used for damage prediction.

In the finite element analysis only half of the geometrical model was considered due to symmetry. For the reliability testing, thermal shock testing is commonly recommended for the microelectronics devices, and it involves placing the device in an oven and varying the inside temperature over time. Another testing scenario is the power cycling, in which given
temperatures are applied to the hot and cold sides, and these temperatures are varied over time. In the present simulations, for the ambient temperature, the worst case scenario was considered by assuming a low temperature in the cycle of \(-40^\circ\text{C}\). Typically the hot side of the TEG is attached to the exhaust pipe of a vehicle, and the cold side of the TEG is attached to a cooler. The maximum hot side temperature (also the exhaust pipe temperature) was assumed to be 525 \(^\circ\text{C}\). And, the maximum cold side temperature (also the cooler temperature) was assumed to be 100 \(^\circ\text{C}\). At the beginning of each thermal shock cycle, both the hot and the cold sides of the TEG are at ambient temperature. When the engine starts, the temperature on both sides starts to increase. After a certain time period (5 min. for the hot side and 10 min. for the cold side), the temperatures of the hot side and the cold side become steady. When the engine stops, both the temperatures drop back to the ambient temperature. A 50-minute time period was considered for a single thermal cycle. The temperature fluctuations over time in a single cycle are shown in FIGURE 16, and was used in FEA as thermal boundary conditions.

Mechanical boundary conditions were applied by fixing the bottom surface of the TEG package model in \(y\)-direction. The symmetry plane was used to analyze only half of the model. A 100 N compressive load was applied in the top surface of the model to simulate a realistic mechanical load that the TEG device could experience in service.

B. Results

The finite element simulation was conducted for 3000 cycles. Damage initiation and evolution occurred in the braze layer at two locations: at the corner braze layer adjacent to the LTCC window wall (location 1), and at the braze layers adjacent to the SiGe and Al metallization (location 2). A damage contour plot demonstrating these locations is shown in FIGURE 16. Due to the presence of a large CTE mismatch, the maximum damage in model after 3000 cycles was found at location 2. The predicted damage was only 0.16% after 3000 cycles, which implies that the device will experience little damage under this loading condition.

CONCLUSIONS AND FUTURE WORK

Low cycle fatigue using a direct cyclic approach was successfully utilized to predicting damage in the aluminum braze for a thermoelectric generator package. A significant reduction of computational cost usually associated with fatigue simulations was achieved using this computational method embedded in the finite element method. A good agreement between the numerical and experimental results was obtained using the present model. The proposed die attach solution, i.e. aluminum alloy braze Al 718 (12% Si, 88% Al) provided an adequate mechanical behavior under fluctuating temperature conditions. The finite element results suggest that the damage in the braze material should not contribute to a major failure mode of the TEG package up to 3000 cycles of operation.

Future work will include a parametric study to determine the effect of different thicknesses of the TEG package on mechanical behavior and further optimize the TEG design. Different mechanical loading scenarios will also be investigated to determine the optimum loading for the proposed TEG package assembly for passenger vehicles.

ACKNOWLEDGMENTS

The authors would like to thank II-VI Foundation Inc. for funding this project under the Block-Gift Program.
REFERENCES


