Structural Analysis of a Thermoelectric Generator Element

James M. Newell
Fairchild Space Company

1. Background

Fairchild Space Company is currently assisting in a DOE program (under contract DE-AC01-81NE32090) to develop a nuclear-powered thermoelectric generator for long distance space voyages. Known as the Modular Isotopic Thermoelectric Generator (MITG), the device [1] differs from previous RTG designs in that it is built from identical generator sections or "slices", each producing the desired output voltage, which may be combined to meet the power requirements of any particular space mission. This paper outlines the structural analysis of the thermoelectric module or multicouple used in the MITG, as aided by the MSC/NASTRAN finite element code.

The multicouple is a cantilevered assembly consisting of a threaded stud and bolt head to which a matrix of semiconducting legs is bonded. These legs, being alternately n and p doped, are arranged to form 18 series connected thermocouples which, when supplied with a temperature difference from end to end, produce an electric current by the Seebeck effect. When bolted to the radiative generator housing, the threaded stud serves as the cold end of these thermocouples, while a thermally conductive plate at the opposite end serves as a heat collector for concentrating the heat provided by the decay of a radioisotope.

The required thermal conductors at each end of the thermopile were originally proposed to be made of tungsten, due to the closely related expansion characteristics of this material and the silicon-germanium alloy composing the legs. The first module design, however, incorporated a molybdenum stud at the cold end for ease of manufacture, with a layer of tungsten brazed on its face for compatibility with the semiconductor. The device is illustrated in Figure 1.

The module was designed for a hot junction temperature of 1000 C, with the cold junction operating at 300 C. This large temperature gradient indicates the reason for concern over material thermal expansion differences.

2. The Finite Element Model

A series of modules such as that shown in Figure 1 were constructed and subjected to thermal testing. During these tests however, a sudden increase in the internal resistance of the modules suggested the occurrence of a structural failure prior to attainment of the operating gradient. Subsequent inspection of the modules verified this, showing a dome-shaped breakage at the cold end of the multicouple, where the semiconducting thermopile is bonded to the cold stud. This led to the need of an analytical model which could predict not only the causes of failure but possible structural design solutions as well. NASTRAN was implemented for this purpose, with the model shown in Figure 2.

Generated using the PATRAN pre- and postprocessing software of PDA Engineering, the model contained 144 solid shell elements connecting 1290 grid points, for a total of 3000 static degrees of freedom. The elements used were the 20 noded HEXA and the 15 noded PENTA. As can be seen from Figure 2, the model represents a one-eighth segment of the generator element, with a symmetry argument invoked on its 2 sectioned faces. This constraint was imposed by specifying, under a cylindrical coordinate system, suppression of the theta degree of freedom on each face. The failure analysis was performed using Solution Sequence 24, with structural loads imposed solely by the temperature distribution within the device.

The MITG multicouple, being composed of a number of different materials, requires an involved manufacturing sequence. Under the original design, the first step was to manufacture the bimetallic cold stud by brazing the thin tungsten layer onto the molybdenum bolt head. The second process consisted of using a high-temperature glass to bond the tungsten heat collector onto the silicon-molybdenum hot shoes which were previously bonded to the silicon-germanium legs. Finally, the above assembly had to be glass-bonded to the tungsten layer of the cold stud. Since the temperatures at which these processes occur are very high, being 980 C, 1100 C and 680 C respectively, it was deemed necessary to account in the failure analysis for the thermal stress history which they induce. Another requirement of the analysis was that it account for the temperature dependence of the material coefficients of thermal expansion, since the temperature changes associated with the operating gradient are extreme.

Thus there existed four distinct thermal stress cases to be modeled via NASTRAN :

1. Bimetallic Cold Stud Braze (Tungsten to Molybdenum)
2. Hot Shoe Glass Bond (Tungsten to Silicon-Germanium)
3. Cold Stud Glass Bond (Silicon-Germanium to Tungsten)
4. Operating Gradient

3. The Modeling Process

Each of the three manufacturing processes described above is in turn composed of three sequential steps:

1. heat-up to temperature
2. connection
3. cool-down to room temperature

Processes such as these are very simple to perform in real life, but they do not readily lend themselves to computer modeling because they entail a cumulative stress history, and each NASTRAN subcase is restricted to start with an unstressed model. This constraint was overcome with linear superposition.

First, a subcase representing heat-up was created, consisting simply of thermal loads specified at grid points. The second case, representing connection and cool-down, was a bit more involved. MPC's at the interfaces between parts to be joined were activated in this subcase, with each part loaded to the connection temperature. The entire manufacturing process could then be simulated by combining the first subcase results with the negative of the second ... so that the cool-down was achieved mathematically as the negative of a heat-up. A diagram illustrating this concept is given in Figure 3.

This technique was utilized for each manufacturing process. It should be noted, however, that it was not strictly correct for the two glass bond cases. During cool-down, the flow of the glass will in reality allow slippage between the two connection planes and not produce the rigid attachment modeled. Since, however, the latter situation tends to introduce higher stresses than the actual process, it was deemed conservative and therefore acceptable for our purposes. The executive and case control decks for the model, indicating each process involved, are given in Figure 4.

4. Constraints On Thermal Expansion Coefficient

As stated previously, the large temperature variations involved with this problem indicated a need for temperature-dependent coefficients of thermal expansion. While this capability exists within MSC/NASTRAN via the TEMP(MATERIAL)=SID card, it is limited in that it may be used only once, and this one use must be above the subcase level.

This, however, was not sufficient for the MITG module problem, and so it was decided to simulate a temperature dependent alpha within each subcase by the specification of an altered temperature distribution.

From the definition of thermal strain, we know

$$\varepsilon(T) = \int_{T_1}^{T} \alpha(T)\, dT \qquad \text{------------------(1)}$$

and, in addition, we can approximate the temperature dependence of alpha for many materials with a linear model as

$$\alpha(T) = \alpha_1 + \frac{(\alpha_2 - \alpha_1)}{(T_2 - T_1)} T$$

$$= \alpha_1 + (\alpha_2 - \alpha_1) \frac{T}{T_2} \qquad \text{------------------(2)}$$

for an initial T_1 equal to zero degrees.

Substituting equation 2 into equation 1, we conclude

$$\varepsilon(T) = \int_0^T [\alpha_1 + (\alpha_2 - \alpha_1)\frac{T}{T_2}]\, dT$$

$$= \alpha_1 T + \frac{(\alpha_2 - \alpha_1)}{2T_2} T^2$$

What we want to do with our computer model, then, is to generate this true value of strain with a constant thermal expansion strain equation; that is, we want to force the result

$$\alpha_1 T + \frac{(\alpha_2 - \alpha_1)}{2T_2} T^2 = \bar{\alpha}\, T'$$

where $\bar{\alpha}$ is an average value of thermal expansion for the material in question over the specified temperature range, and T' is a fictitious value of temperature which satisfies the equation. Solving for T', we obtain

$$T' = \frac{\alpha_1 T + \frac{(\alpha_2 - \alpha_1)}{2T_2} T^2}{\bar{\alpha}}$$

$$= \frac{\alpha_1 T + \frac{(\alpha_2 - \alpha_1)}{2T_2} T^2}{\frac{1}{2}(\alpha_1 + \alpha_2)}$$

In summary, then, the linear change in thermal expansion coefficient was accounted for in our model by the specification of a non-linear temperature distribution. A list of fictitious temperatures is given in Table 1 along with their corresponding real values for the Silicon-Germanium leg assembly. This material region is particularly of interest because it was here that the linear change in temperature from

1000 to 300 C took place.

5. Results

The results provided by the solid element model proved extremely useful from an engineering standpoint. Immediately apparent was a grouping of high tensile stresses at the center of the cold end of the module, forming a pattern which closely resembled the domed failure region of the actual device. This comparison is given in Figure 5.

Another correlation between the model and element was discovered when the analytical results indicated tensile stresses in the hot end corner regions of the thermopile. While inspection had shown no failure as yet in these areas, a closer postmortem analysis indeed revealed small cracks here.

Once the predictive ability of the finite element model was verified, a parametric study was initiated to reduce the stresses in the critical regions. While the dominant cause of these stresses was not immediately obvious, some possibilities were:

* The bimetallic composition of the cold stud, causing bowing during cool-down
* Slight mismatch in expansion coefficient between tungsten and SiGe
* Bowing of the SiGe leg assembly due to the large temperature gradient
* The much higher expansion coefficient of the aluminum housing wall to which the multicouple is bolted

To identify which of these effects was dominant, the analytical model was used as a tool to isolate and examine them one at a time. This proved highly successful. The results indicated that the last effect, the high expansion of the aluminum wall, was the primary cause of thermal stress failure. This was corroborated by subsequent experiments.

The insight gained from the above analysis enabled the designers to devise a number of promising design solutions. One of these involved the use of a double headed stud, which is illustrated by the structural analysis model shown in Figure 6. The slot between the two cold-stud heads is designed to decouple the effect of the housing wall expansion from the SiGe leg assembly. Subsequent thermostructural analysis using this model confirmed the effectiveness of the design fix, as illustrated by the stress distribution plot shown in Figure 7. Thus, from the point of view of the stress analyst, this solution works magnificently, albeit at the price of increased thermal resistance. Other proposed design fixes are presently undergoing analysis, preparatory to experimental validation. The NASTRAN model continues to be a very useful tool in these analyses.

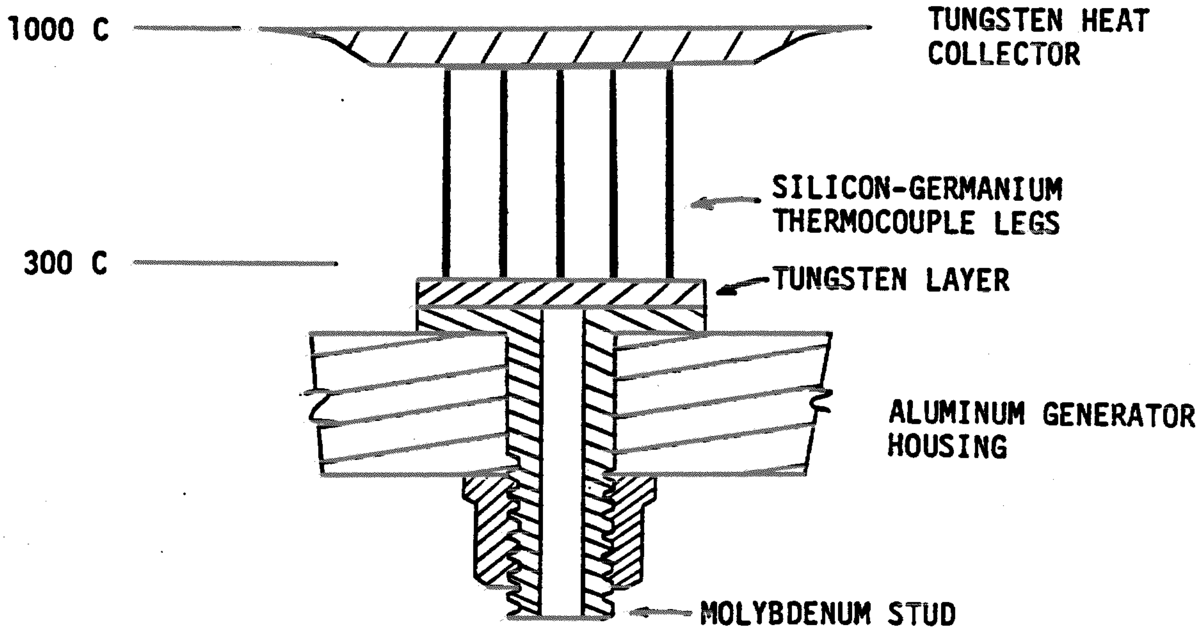
1000 C
TUNGSTEN HEAT COLLECTOR
SILICON-GERMANIUM THERMOCOUPLE LEGS
300 C
TUNGSTEN LAYER
ALUMINUM GENERATOR HOUSING
MOLYBDENUM STUD

FIGURE 1

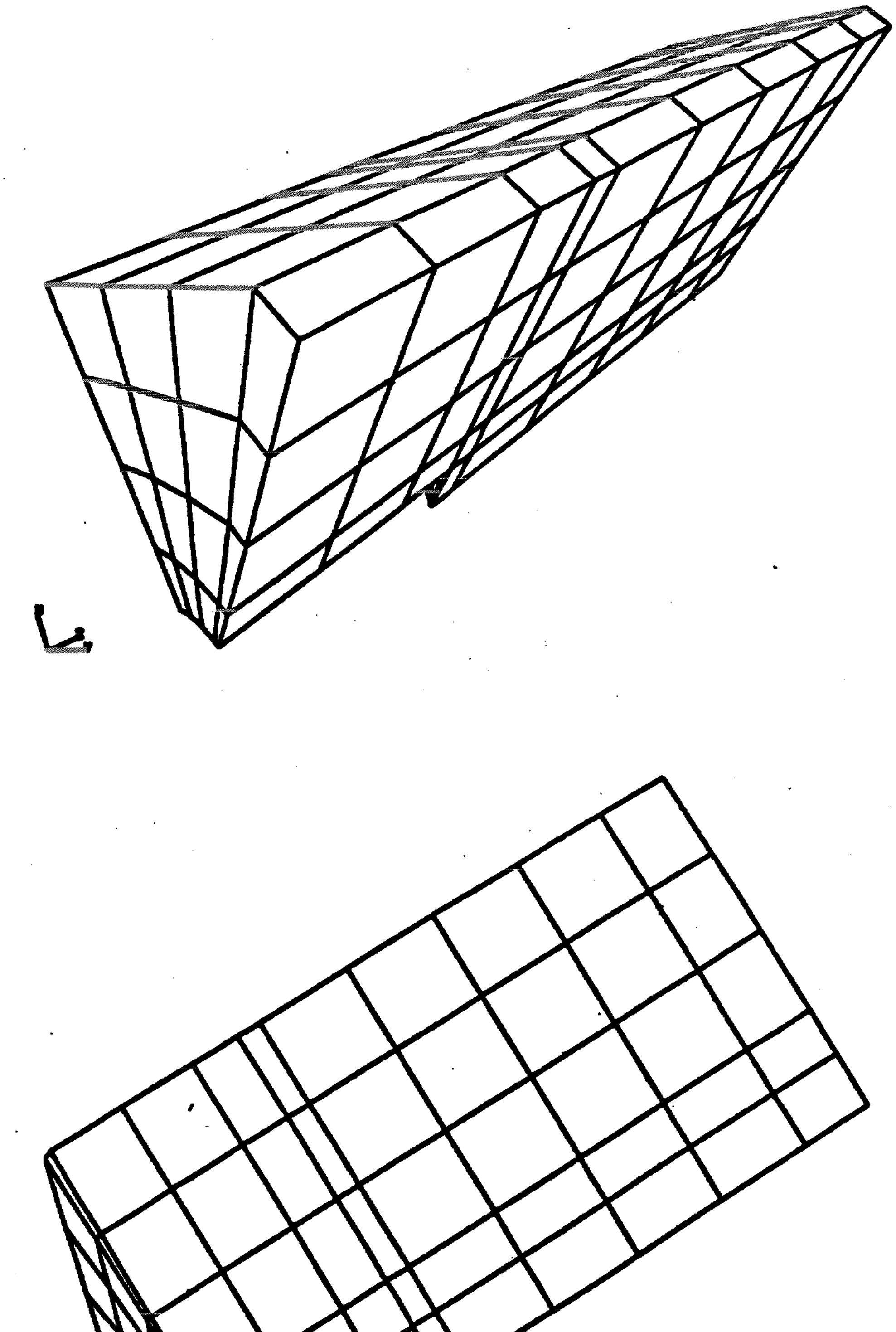

FIGURE 2

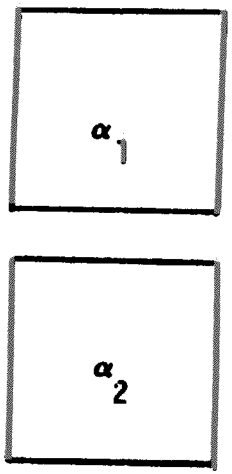

Figure 3a

Isolated Blocks of Material with $\alpha_1 > \alpha_2$

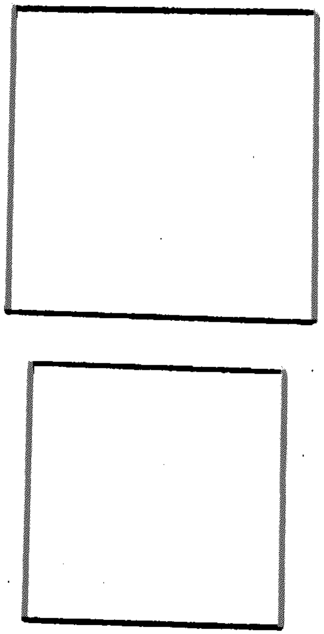

Figure 3b

Individual Heat-Up to a Uniform Temperature

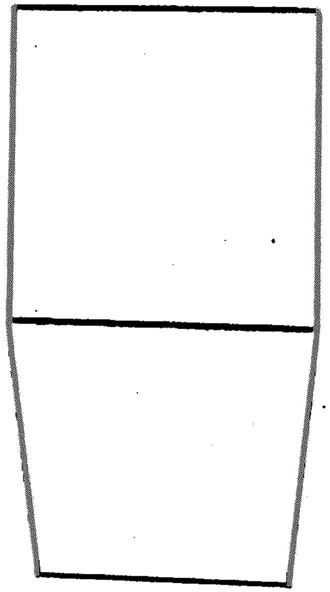

Figure 3c

The Same Heat-Up with the Blocks Connected

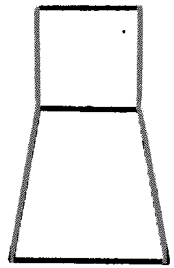

Figure 3d

Negative of a Connected Heat-Up

Superposition of Figures 3b and 3d yield room temperature strains due to a heat-up, connection, and cool-down.

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ID NEWELL,MITG THERMAL ANALYSIS
DIAG 5,6,8,13,19,20
SOL 24,0
TIME 600
CEND
$
TITLE=MITG THERMAL STRESS ANALYSIS
SUBTITLE=TUNGSTEN-MOLY STUD
LABEL=TEMPERATURE DISTRIBUTION SIMULATES TEMP DEPENDENT ALPHA
VECTOR=ALL
STRESS=ALL
SPCFORCES=ALL
SUBCASE 1
LABEL=HEAT-UP OF COLD SHOE AND HOT SHOE/SIGE ASSEMBLIES
TEMP(LOAD)=100
SPC=400 $HOLD BOTH HOT SHOE AND SIGE
SUBCASE 2
LABEL=CONNECTION OF THE HEATED HOT SHOE AND COLD SHOE PARTS
TEMP(LOAD)=100
SPC=300 $HOLD JUST SIGE (BECAUSE HOT SHOE IS BOLTED TO IT)
MPC=100 $BOLT HOT SHOE AND COLD SHOE PARTS TOGETHER
SUBCASE 3
LABEL=HEAT-UP FOR THE COLD SHOE BOND
TEMP(LOAD)=200
MPC=100 $KEEP HOT SHOE AND COLD SHOE PARTS BOLTED TOGETHER
SPC=300 $HOLD JUST SIGE (BECAUSE HOT SHOE IS BOLTED TO IT)
SUBCASE 4
LABEL=COLD SHOE TO SIGE BOND CONNECTION
TEMP(LOAD)=200
MPC=400 $CONNECT COLD SHOE PARTS;HOT SHOE PARTS;SIGE TO COLD SHOE
SPC=100 $SYMMETRY SPC RESTRICTIONS ONLY
SUBCASE 5
LABEL=CONNECTION TO PLATE AND START OF TEMPERATURE GRADIENT
TEMP(LOAD)=300
MPC=500 $CONNECT ALL PARTS, INCLUDING THE ALUMINUM PLATE
SPC=100 $SYMMETRY SPC RESTRICTIONS ONLY
SUBCOM 6
LABEL=ROOM TEMPERATURE STRESSES OF HOT AND COLD SHOES
SUBSEQ=1.0,-1.0,0.0,0.0,0.0
TEMP(LOAD)=500
SUBCOM 7
LABEL=ROOM TEMPERATURE STRESS AFTER COLD SHOE TO SIGE BOND
SUBSEQ=0.0,0.0,1.0,-1.0,0.0
TEMP(LOAD)=500
SUBCOM 8
LABEL=STRESS DISTRIBUTION DUE TO MANUFACTURE
SUBSEQ=1.0,-1.0,1.0,-1.0,0.0
TEMP(LOAD)=500
SUBCOM 9
LABEL=FINAL STRESS DISTRIBUTION IN OPERATION
SUBSEQ=1.0,-1.0,1.0,-1.0,1.0
TEMP(LOAD)=300
BEGIN BULK
```

Figure 4

TABLE 1 FICTITIOUS TEMPERATURE DISTRIBUTION FOR THE SiGe THERMOPILE

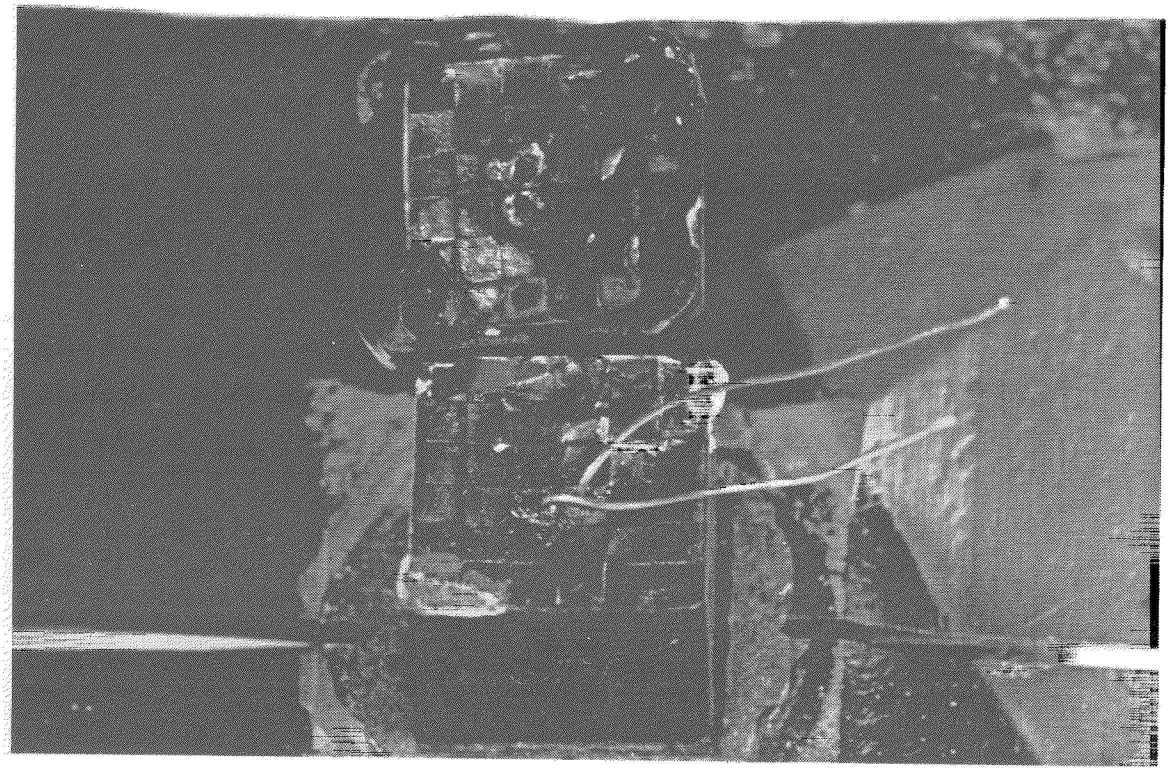
Values Based on the following data:

$T_1 = 0^{o}C, \quad \alpha_1 = 3.15 \times 10^{-6}\ C^{-1}$

$T_2 = 1000^{o}C, \quad \alpha_2 = 4.59 \times 10^{-6}\ C^{-1}$

$\bar{\alpha} = 3.87 \times 10^{-6}\ C^{-1}$

T, °C	T´, °C
0	0
100	83
200	170
300	261
400	355
500	453
600	555
700	661
800	770
900	883
1000	1000



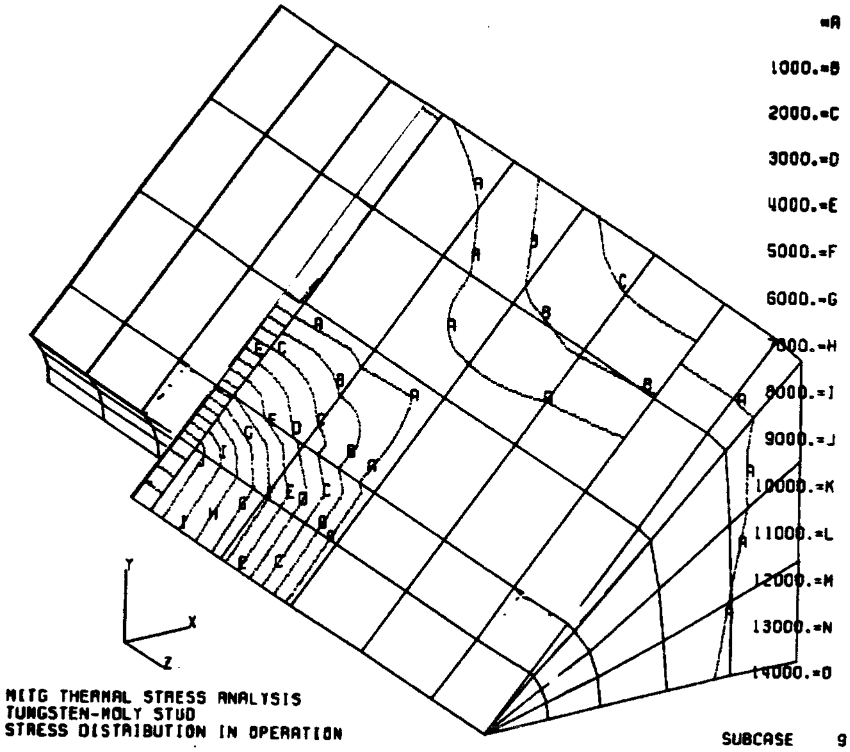
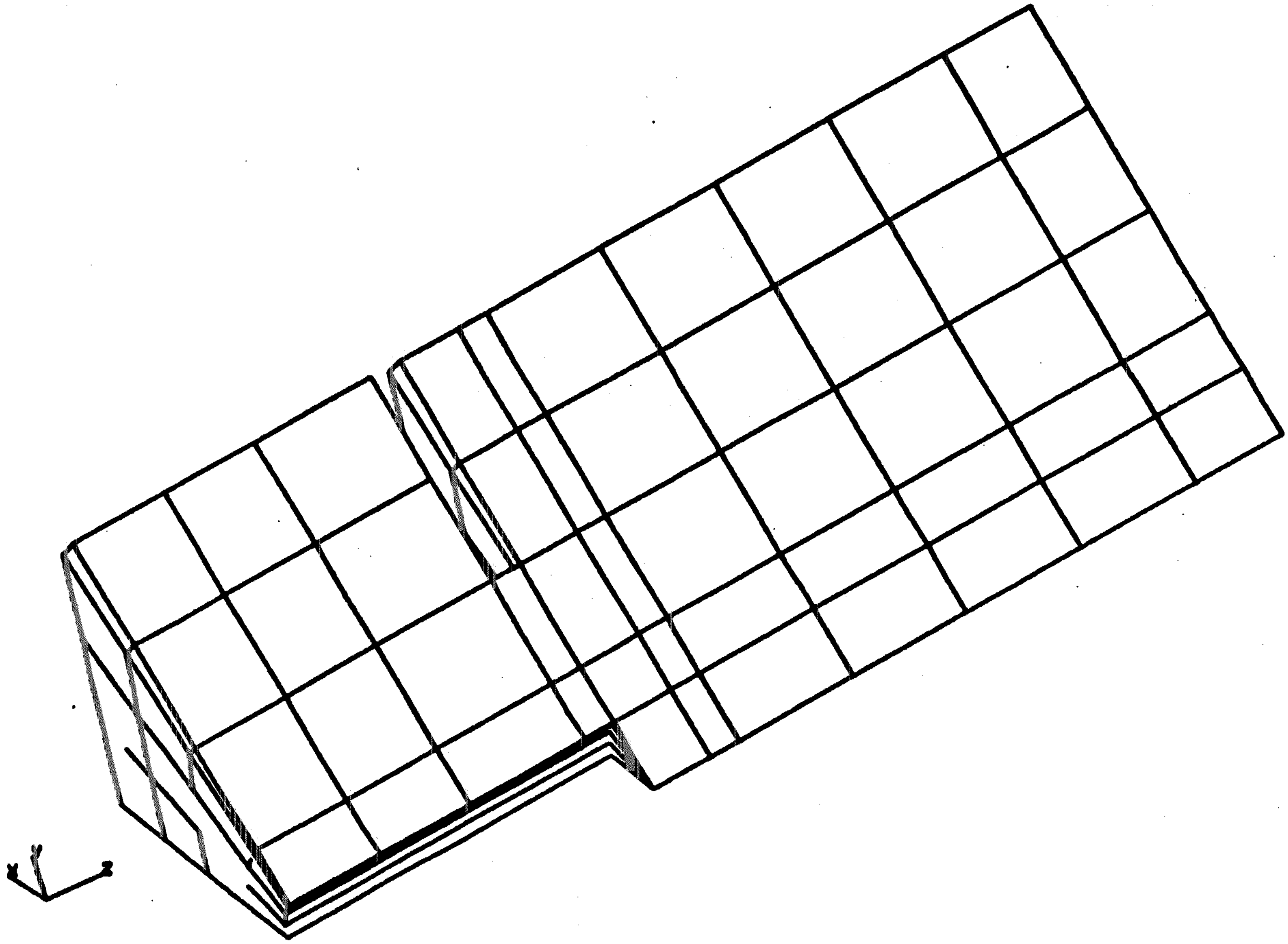

=A
1000.=B
2000.=C
3000.=D
4000.=E
5000.=F
6000.=G
7000.=H
8000.=I
9000.=J
10000.=K
11000.=L
12000.=M
13000.=N
14000.=O
Y
X
Z
MITG THERMAL STRESS ANALYSIS
TUNGSTEN-MOLY STUD
STRESS DISTRIBUTION IN OPERATION
SUBCASE 9

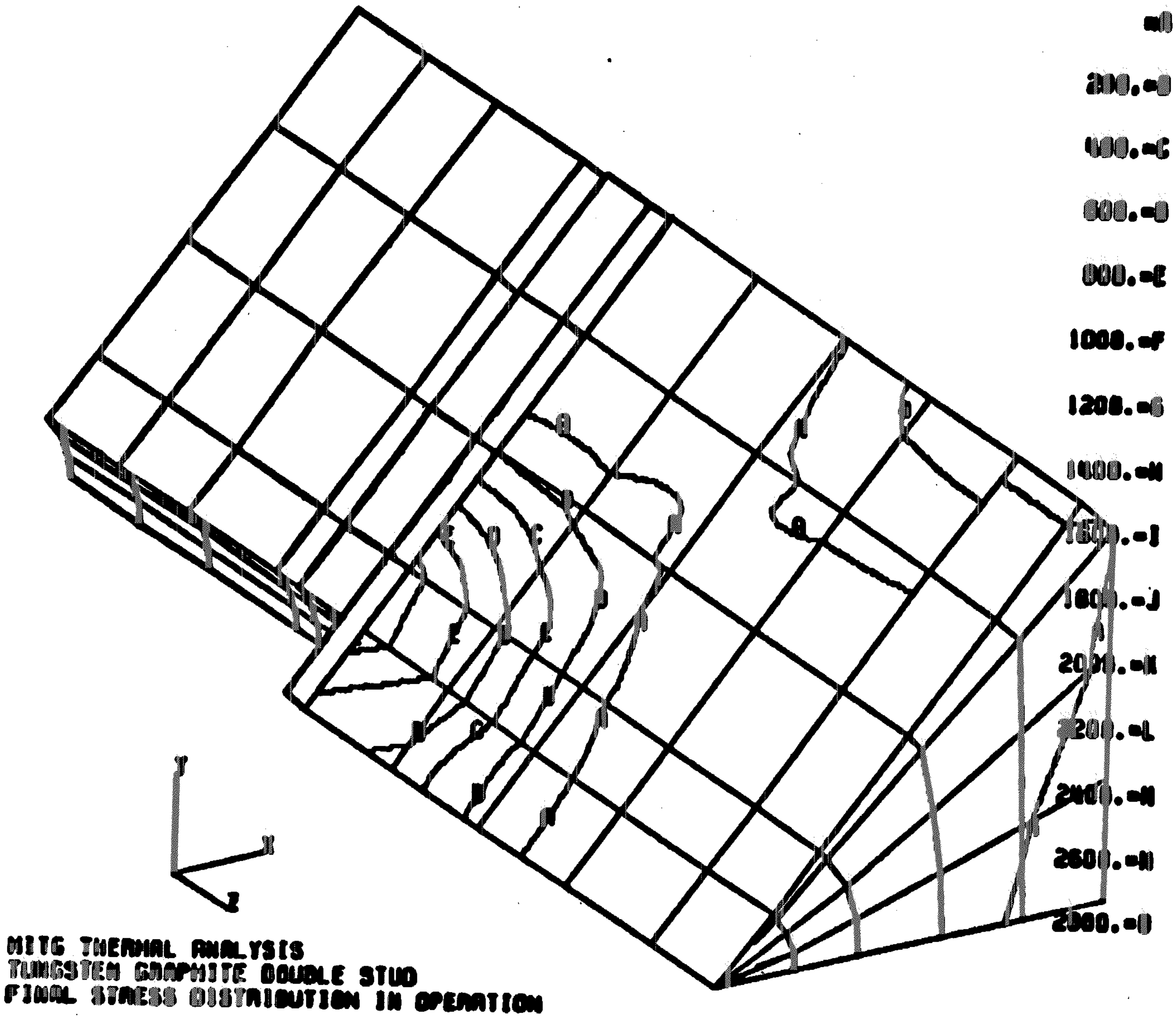
FIGURE 5

MITG THERMAL ANALYSIS

DOUBLE STUD (ALL TUNGSTEN)



Y-Z VIEW ELEMENTS: ALL
ALPHA = -30.0 BETA = 30.0 GAMMA = 40.0 MU = 0.0



200.=B
400.=C
600.=D
800.=E
1000.=F
1200.=G
1400.=H
1600.=I
1800.=J
2000.=K
2200.=L
2400.=M
2600.=N
2800.=O
Y
X
Z
MITG THERMAL ANALYSIS
TUNGSTEN GRAPHITE DOUBLE STUD
FINAL STRESS DISTRIBUTION IN OPERATION

FIGURE 7

REFERENCES

1. Schock, A., "Modular Isotopic Thermoelectric Generator", Fairchild Document FSEC-ESD-217-81/180B, April 1981

2. McCormick, C. W., et al, MSC/NASTRAN User's Manual, The MacNeal-Schwendler Corp., 1980

3. Joseph, J. A., et al, "Temperature Loads and Enforced Deformations in Subcase Combinations", MSC/NASTRAN Application Manual, The MacNeal-Schwendler Corp., April 1980

4. "Elements Subjected to Thermal Loads", MSC/NASTRAN Demonstration Problem Manual, The MacNeal-Schwendler Corp., November 1978