HIGHER ORDER THEORY - STRUCTURAL/MICRO ANALYSIS CODE (HOT-SMAC) SOFTWARE FOR THERMO-MECHANICAL ANALYSIS OF FGMS

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ABSTRACT

A new software package called Higher-Order Theory – Structural/Micro Analysis Code (HOT-SMAC), has been developed as an effective tool for design and analysis of functionally graded materials. The underlying analysis technology of the software is the well-established Higher-Order Theory for Functionally Graded Materials (HOTFGM), the accuracy and efficiency of which has been illustrated in the literature. The HOT-SMAC software is a self-contained package that includes pre- and post-processing through an intuitive graphical user interface, along with the HOTFGM thermo-mechanical analysis engine. Herein, the HOTFGM analysis approach and the features of the HOT-SMAC software are outlined. As an example application, the thermo-mechanical behavior of an internally-cooled, functionally graded silicon nitride plate with a thermal barrier coating is investigated.

INTRODUCTION

Functionally graded materials (FGMs) offer many advantages over monolithic materials and traditional composites. By spatially varying the microstructure, the material can be tailored for a particular application to yield optimal thermal and mechanical behavior [1]. Improved fatigue resistance, reduced thermo-mechanical property mismatch, interlaminar stress reduction, and more efficient joining techniques can be realized through the use of FGMs. Thus, FGMs are finding application in a wide range of structures, including aerospace engines, circuit boards, solar energy conversion devices, and dental implants [2].

The spatially varying nature of phase distribution within FGMs also makes design and analysis more challenging compared to traditional materials. Two commonly used methods for modeling FGMs are: 1) the uncoupled approach, in which spatially varying effective material properties are employed, and 2) the coupled approach in which the materials microstructure is explicitly taken into account. The uncoupled approach is popular due to its simplicity and efficiency. One example of this approach involves analyzing a functionally graded (FG) two-phase plate using classical lamination theory, wherein each through-thickness layer is given a different volume fraction. This analysis technique is uncoupled in that effective, or "smeared", properties are employed for each layer, and thus the actual distribution of the phases does not explicitly affect the structural solution for the plate. While the uncoupled technique can be accurate for FGMs with very fine phase distributions (thus justifying the smearing of the local properties), it has been shown that this approach is inaccurate (both globally and locally) when the phase microstructure is significant with respect to the characteristic structural dimensions [2-4]. FEA, on the other hand, while more complex and time consuming than the uncoupled approach, can be considerably more accurate. The availability of commercial FEA codes (e.g., ABAQUS, ANSYS, NASTRAN) also makes FEA attractive for design/analysis of FGMs.

The new FGM design and analysis tool described herein falls in between the less accurate uncoupled approach and the more cumbersome FEA approach. The Higher Order Theory - Structural/Micro Analysis Code (HOT-SMAC), is based on the analytical model known as the Higher Order Theory for Functionally Graded Materials (HOTFGM) [2-7]. Like FEA, HOTFGM explicitly couples the microstructural and macrostructural behavior of FGMs, which circumvents the inaccuracies associated with the use of the uncoupled approach. Further, HOTFGM is specially suited for analysis of FGMs, and for several reasons, it is an effective alternative to the finite element approach. First, HOTFGM employs a volume-average smoothing technique that renders it far less sensitive to mesh refinement than FEA [5]. Even with a coarse "mesh" representation of the FGM, HOTFGM is unconditionally convergent (in the sense that the governing conditions are satisfied). FEA, on the other hand, may require a relatively fine mesh in order to achieve convergence of the governing equations. However, like FEA, the HOTFGM mesh can be refined in regions of interest to yield high fidelity concentration solutions [2, 5]. In addition, HOTFGM is formulated to automatically solve coupled thermo-mechanical problems (wherein the unknown temperature distribution affects the mechanical solution). Not all commercial FEA packages have this capability, and those that do are often limited in some respects. Finally, the new HOT-SMAC software package has provided an intuitive and user friendly means for pre- and post-processing FGM problems, in addition to providing the HOTFGM analysis code itself. Thus, HOT-SMAC is far more efficient for FGM analysis compared to commercial FEA packages, which often require separate pre- and post-processors.

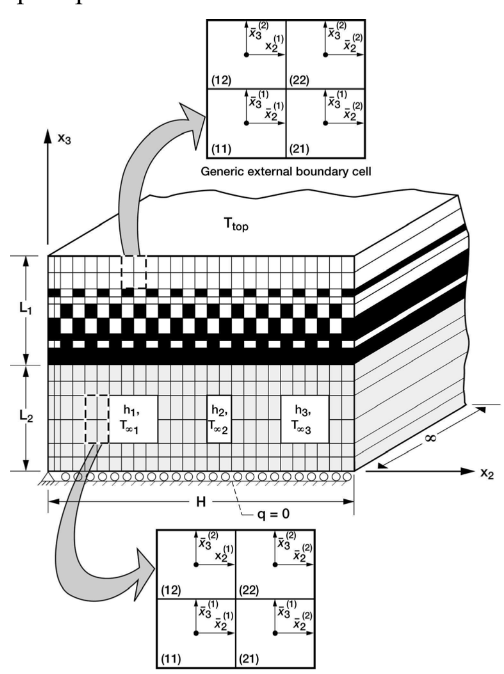

Figure 1: Example HOTFGM analysis geometry. The smoothing technique within the analytical formulation enables use of the rectangular subcell "mesh."

The version of HOTFGM currently implemented within the HOT-SMAC software is two-dimensional and based on Cartesian coordinates, Figure 1. The FGM is treated as a plate-like structure composed of "cells", each of which contains four rectangular "subcells". These subcells may each be a distinct material, which enables representation of the functionally graded (FG) geometry in two directions with a "mesh" of rectangular sub-cells. As Figure 1 indicates, boundaries exist in the two in-plane coordinate directions (x2 and x3), while the FGM is treated as infinite in the out-of-plane (x1) direction. The mechanical problem thus reduces to generalized plane strain, where the software user sets the average stress or strain in the x1-direction. In addition to the external boundaries of the FGM, HOTFGM admits internal boundaries as shown in Figure 1. This allows analysis of FGMs containing internal channels that may be used for cooling and requires additional thermal and mechanical boundary conditions to be provided for the internal boundaries.

Given the appropriate time-dependent (or time-independent) thermal and mechanical boundary conditions, HOTFGM first solves the thermal problem for the temperature distribution in the FGM and then solves the mechanical problem based on this temperature distribution. The currently implemented version of HOTFGM includes linear elasticity, history-dependent classical plasticity, and time-dependent power law creep of the FGM phases. In the presence of time- or history-dependence, the thermal and mechanical problems are solved at each increment of the applied boundary condition history.

As mentioned previously, while HOTFGM is in some ways similar to FEA, it is not a specialized (e.g., hybrid-mixed) finite element method. HOTFGM's analytical formulation employs a smoothing technique at the subcell boundaries, enabling satisfaction of the governing equations in a volume average sense regardless of subcell mesh density. This smoothing technique also enables HOTFGM to be accurate despite its rectangular subcells, which appear to have corners. The effect of the subcell corners is smoothed out, and thus, unlike FEA, the presence of a corner does not give rise to a significant concentration. However, if simulation of a concentration at an actual corner (or other location) within the analyzed geometry is desired, HOTFGM can capture the concentration by refining the subcell mesh in the region.

HOT-SMAC SOFTWARE FOR FGM DESIGN/ANALYSIS

The HOT-SMAC interface was developed to build on the well-established accuracy of the HOTFGM mechanics methodology, and make it available as a practical, commercial product. HOT-SMAC provides the graphical user interface allowing the user to specify the problem geometry and material distribution, thermal and mechanical boundary conditions, and analysis options defining a thermo-mechanical problem in a simple and intuitive manner. After the FGM problem is specified, the HOTFGM-based analysis can be executed from within HOT-SMAC, and the results are automatically loaded into the interface for viewing and post-processing.

HOT-SMAC is a Microsoft Windows native product providing all software options on a single multi-tabbed form. The user begins the analysis on a **Setup** tab by selecting the grading scheme (whether the domain is graded in one or two directions) and the local material constitutive models (Elastic, Plastic, Creep, etc.) to be employed in the problem. From the **Setup** tab, the user can also raise a Material Editor form, which allows temperature-dependent and temperature-independent material property entry, storage, and recall.

On the **Geometry** tab, shown in Figure 2, the problem's overall dimensions, number of analysis subcells in each direction, and local dimensions are specified in a variety of ways. The graphical control allows the user to select single subcells or ranges of subcells, as shown in Figure 2, and specify the height and width of the selected subcells or automatically grade the subcell dimensions using a "grading factor". This grading factor is the ratio of the first selected subcell height or width to the last. As a final fine-tuning control, pressing the "Enter Row Heights" and "Enter Column Widths" buttons allows the user to specify the dimensions for each row and column independently.

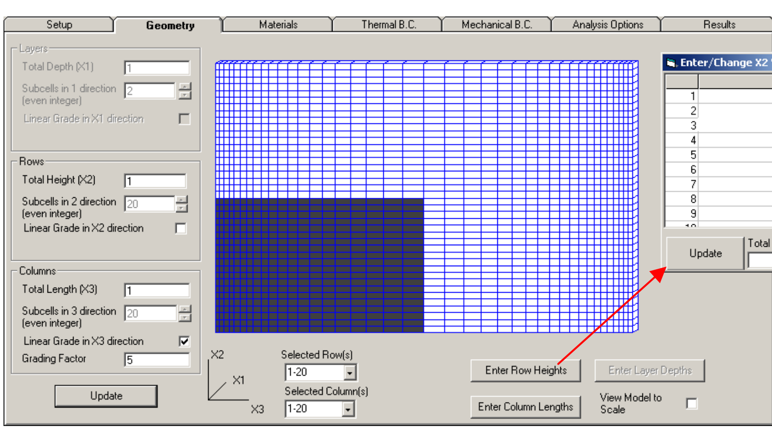

*Figure 2: The **Geometry** tab allows specification of the problem dimensions, number of subcells, and the row heights and column widths*

The **Materials** tab, shown in Figure 3, allows an arbitrary distribution of materials for each subcell in the problem domain. The user selects individual

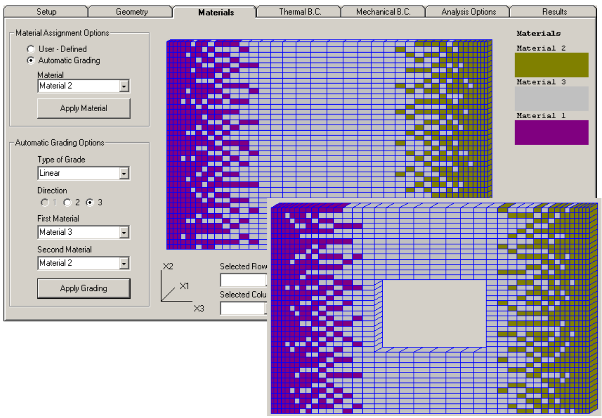

Figure 3: Material assignments for subcells are provided on the ***Materials*** *tab. This tab also allows automatic uniform, linear, quadratic, or uniform grading of the materials, and specification of voids (i.e. windows).*

subcells or ranges of subcells on the graphical control for material assignment. In addition to material assignment, the user can designate portions of the domain as "windows", or voids, to include features such as active cooling channels. The feature of the **Materials** tab that makes it especially suited for functionally graded materials is the ability to automatically functionally grade the material in a variety of ways (e.g., uniform, linear, quadratic, cubic) over any range of cells. In Figure 3, the presented domain is graded linearly in the x3-direction from "Material 1" at the left border to "Material 3", and then from "Material 3" to "Material 2" at the right border.

After specifying the dimensions and material assignment, the problem boundary conditions are entered on the **Thermal B.C.** and **Mechanical B.C.** tabs, see Figure 4. The boundary conditions are specified at the appropriate edge(s) of each border subcell, including external boundaries and the boundaries of any internal windows. The permissible thermal boundary conditions currently include specification of temperature, heat flux, or convective conditions for each border subcell individually, or over a range of subcells. The mechanical boundary conditions include three "pre-defined" boundary types, free (zero traction), pinned (zero displacement) and rollered. In addition, general mechanical boundary conditions can be input for any border subcell with options for specified traction, displacement, or gradients of these in either direction.

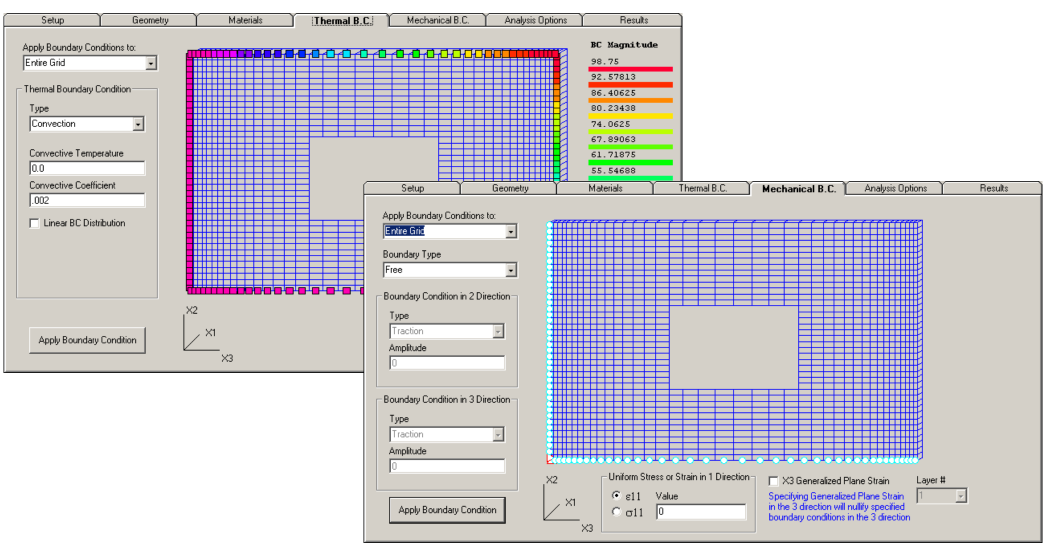

Figure 4: General or pre-defined thermal and mechanical boundary conditions are entered on the thermal B.C. and mechanical B.C. tabs, respectively.

After the problem is defined and the thermo-mechanical analysis is performed, HOT-SMAC automatically imports results and displays them on the **Results** tab. This tab presents the results in two ways. First, results can be plotted with color fringes, as shown in Figure 5. Available fringe plot quantities currently include temperature, stresses, mean stress, equivalent stress, inelastic strains, and displacements.

Second, the user may specify rows and/or columns in the problem domain for line plots of these same result quantities. The software will also export these line plots to a comma separated value (CSV) file for plotting in Microsoft Excel or any other post-processing software. A more detailed description of the HOT-SMAC software is available in reference [8].

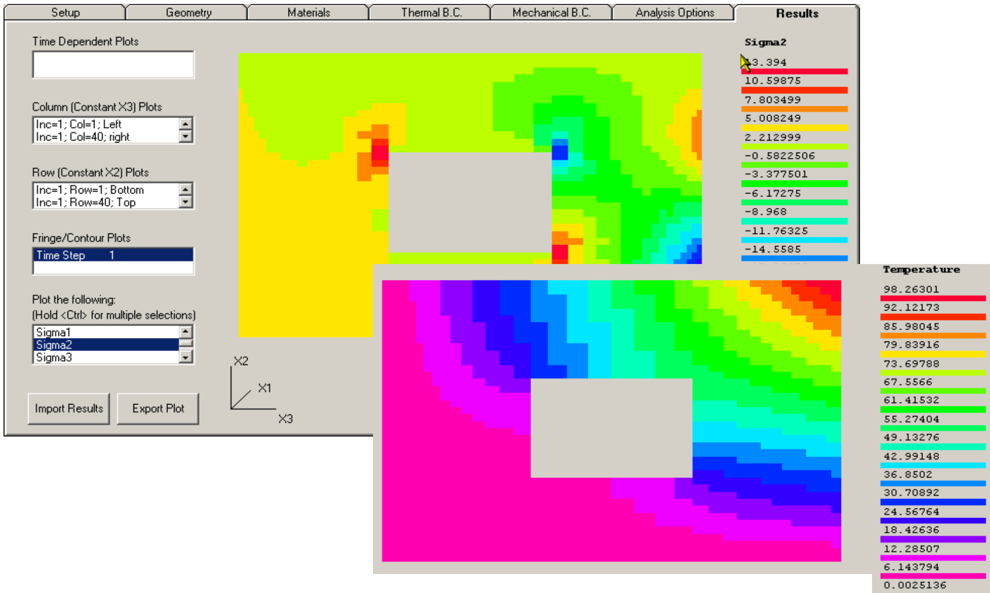

*Figure 5: Results of the HOT-SMAC analysis are plotted on the **Results** tab. Contour (fringe) results available include temperature, stress components, plastic strain components, and displacement components. The **Results** tab also allows line plots of the solution.*

EXAMPLE APPLICATION - COOLED SILICON NITRIDE PLATE

As an example of the HOT-SMAC software analysis capabilities, we consider a silicon nitride (Si_3N_4) plate with a thermal barrier coating (TBC) consisting of a mullite bond coat and a porous zirconia top coat. This system is under consideration for high-temperature engine applications by the NASA Glenn Research Center. In addition to the use of a TBC, the concept of including channels within Si_3N_4 through which air (or another fluid) could be forced is being evaluated to reduce the operating temperature of the material/structure. Reasonably small temperature reductions can significantly improve fatigue lives of ceramic components, such as those composed of Si_3N_4.

The simulated plate is 1.0 in. wide and 0.35 in. thick (0.25 in. substrate, 0.05 in. bond coat, 0.05 in. top coat). The thermal and mechanical boundary conditions imposed on the plate are shown in Figure 6. Over the middle 0.25 in. of the plate the imposition of a flame is modeled using a convective boundary condition. Three basic plate configurations are considered as shown in Figure 7. The first (Figure 7a) is a plate that lacks cooling channels. The second plate (Figure 7b) contains ten cooling channels within the monolithic Si_3N_4 substrate, while the third plate (Figure 7c) contains cooling channels within a functionally graded Si_3N_4

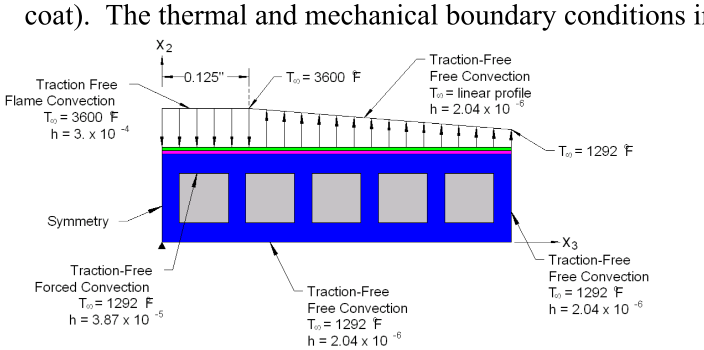

Figure 6: Cooled plate boundary conditions. Note: Symmetry is employed. Units for h are BTU/(in^2 s °F).

substrate. Convective boundary conditions within the cooling channels (and around the remainder of the plate) are intended to simulate engine air. The thermo-elastic properties of the plate materials are given in Table 1. While the TBC materials are fixed, two possible Si_3N_4 materials for use in the substrate are considered, HS-130 and SN-88.

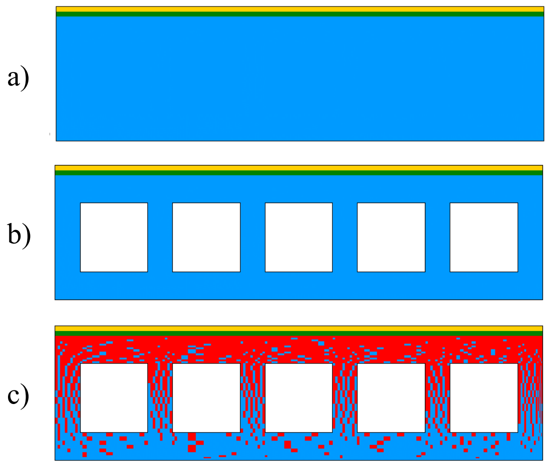

Figure 7: Panel configurations. a) no cooling channels, b) monolithic substrate, c) FG substrate

As the boundary conditions illustrated in Figure 6 indicate, the plate is free mechanically besides being pinned on the bottom at the midpoint (to eliminate rigid body motion). Thus, due to the through-thickness temperature gradient (as well as plate composition asymmetry), the plate will experience bending in response to the simulated loading. In order to maintain a tolerance in a particular application, it may be desirable to minimize the bending that the plate experiences. Towards that end, we consider five cases: 1) HS-130 substrate with no cooling channels, 2) HS-130 plate with cooling channels, 3) SN-88 substrate with cooling channels, 4) Linearly graded substrate with HS-130 on top with cooling channels, and 5) Linearly graded substrate with SN-88 on top with cooling channels.

Table 1. Material Properties [9]

Material	T (°F)	E (psi)	ν	a(10^{-6}/°F)	K (BTU/in·s·°F)
HS-130	**77**	**4.35×10^7**	**0.22**	**1.83**	**4.01×10^{-4}**
Silicon Nitride	**2552**	**3.63×10^7**	**0.19**	**1.83**	**1.61×10^{-4}**
SN-88 Silicon	**77**	**3.77×10^7**	**0.22**	**1.94**	**8.43×10^{-4}**
Nitride	**2552**	**3.37×10^7**	**0.19**	**1.94**	**3.37×10^{-4}**
Mullite	**77**	**2.10×10^7**	**0.20**	**2.94**	**7.84×10^{-5}**
	2552	**2.10×10^7**	**0.20**	**2.94**	**5.04×10^{-5}**
Porous	**77**	**3.63×10^2**	**0.25**	**6.25**	**2.68×10^{-6}**
Zirconia	**2552**	**3.63×10^2**	**0.25**	**6.25**	**6.69×10^{-6}**

Figure 8 plots the vertical displacement (u2) along the top and bottom of the plate as predicted by HOT-SMAC. The displacement along the bottom is a good indicator of the plate bending. Figure 8 shows that by adding cooling channels to the HS-130 substrate, the amount of bending is reduced significantly. Keeping the cooling channels and switching to a monolithic SN-88 substrate further reduces the bending slightly. Most important, however, is the effect of functionally grading the Si_3N_4 substrate (in the presence of the cooling channels). Linearly grading the substrate using the two types of Si_3N_4 with the HS-130 on top reduces the bending by approximately 50% compared to the monolithic substrate configurations. Conversely, linearly grading the substrate with the SN-88 on top increases the bending by approximately 50% compared to the monolithic substrate configurations. Clearly, the functionally graded design with HS-130 on top is superior in terms of plate bending, and it has been quickly and easily identified by the HOT-SMAC software.

Figures 9 and 10 show additional results for three of the plate configurations considered (cases 1, 2, and 4). The fringe plot of temperature in Figure 9 shows the dramatic reduction of the plate temperature due to the presence of the cooling channels predicted by HOT-SMAC. The functionally graded configuration (with HS-130 on top) tends to lower the temperature slightly in the region near the flame while increasing the temperature slightly away from the flame (as compared to the internally cooled monolithic HS-130 case). Figure 10 provides fringe plots of the I_1 stress invariant ($I_1 = \sigma_{11} + \sigma_{22} + \sigma_{33}$) for the three configurations. This invariant (which is proportional to hydrostatic stress) is an indicator of failure in brittle materials such as Si_3N_4. The HOT-SMAC results show that one can expect a significant reduction in the I_1 concentrations through the introduction of the cooling channels, and an additional reduction due to the functional grading of the substrate. For additional details on the cooled plate problem, see reference [9].

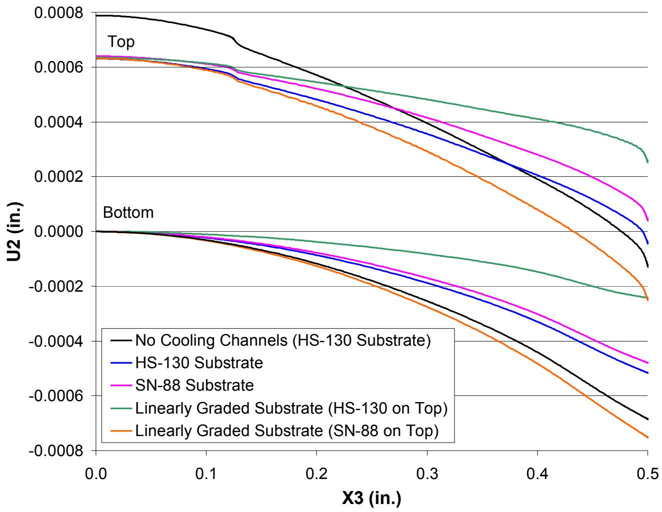

Figure 8: Vertical displacement along top and bottom of the plate predicted by HOT-SMAC.

CONCLUSION

The HOT-SMAC software is a new and important tool for design and analysis of functionally graded materials (FGMs). HOT-SMAC's ease of use and efficiency make it more attractive for modeling FGMs compared to the more computationally and user intensive commercial displacement-based finite element analysis packages with little, if any, loss in accuracy. Further, the analytical model underlying the HOT-SMAC software, HOTFGM, employs averaging to smooth the fields at the subcell edges, thus reducing mesh sensitivity while ensuring convergence. Yet, through mesh refinement, HOT-SMAC still possesses the ability to capture stress and strain concentrations that may occur within an FGM. In addition, HOT-SMAC, while less efficient than simple uncoupled methods for FGM analysis (which employ effective, or "smeared" properties), is considerably more accurate.

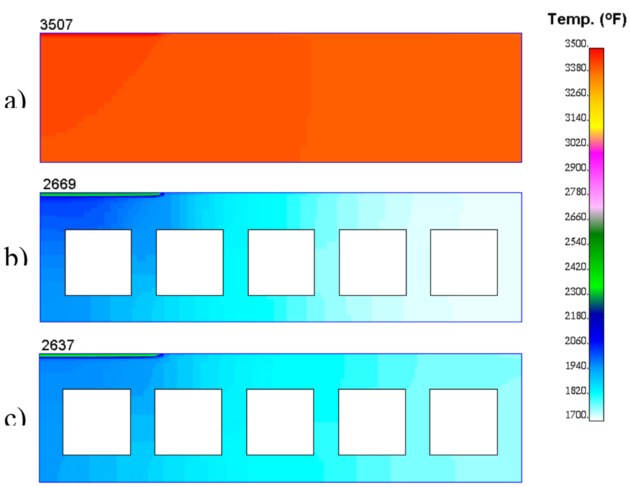

Figure 9: Temperature fields predicted in the plates predicted by HOT-SMAC.
a) case 1, b) case 2, c) case 4.

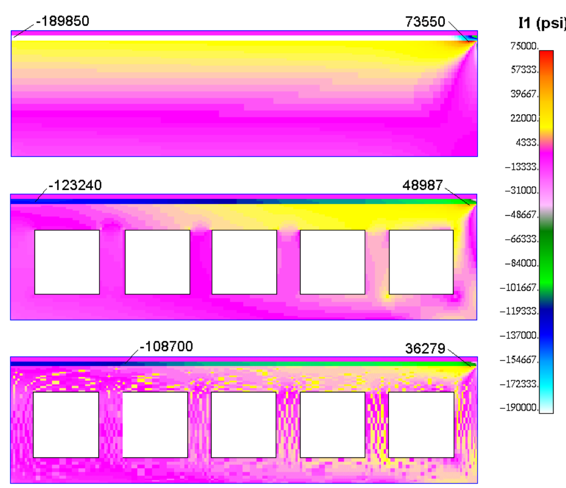

Figure 10: I_1 stress invariant fields in the plates predicted by HOT-SMAC. ($I_1 = \sigma_{11}+\sigma_{22}+\sigma_{33}$)
a) case 1, b) case 2, c) case 4.

The utility of HOT-SMAC was illustrated through a simple design/analysis problem involving a silicon nitride plate with a thermal barrier coating and internal cooling channels. HOT-SMAC was quickly and easily able to identify a functionally graded configuration that drastically reduced the bending of the plate. While this example illustrated the linearly elastic capabilities of HOT-SMAC, the software also admits time-dependent creeping phases and history-dependent plastic phases. Future improvements to the HOT-SMAC software will include incorporation of viscoelastic and viscoplastic constitutive models for the phases. Further, work is underway to surpass the current generalized plane strain formulation to enable analysis of fully three-dimensional functionally graded materials.

ACKNOWLEGEMENTS

The non-NASA authors gratefully acknowledge the financial support provided by the NASA Glenn Research Center through grants and contracts NCC3-650, NCC3-878, NAG3-2524, and NAS3-00159.

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