JTTEE5 6:29-34

A Software Tool to Design Thermal Barrier Coatings: A Technical Note

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This paper summarizes work completed for a NASA Phase I SBIR program that demonstrated the feasibility of developing a software tool to aid in the design of thermal barrier coating (TBC) systems. Toward this goal, three tasks were undertaken and completed. Task 1 involved the development of a database containing the pertinent thermal and mechanical property data for the top coat, bond coat, and substrate materials that constitute a TBC system. Task 2 involved the development of an automated setup program for generating two-dimensional finite-element analysis (FEA) models of TBC systems. Most importantly, task 3 involved the generation of a rule base to aid in the design of a TBC system. These rules were based on a factorial design of experiments involving FEA results and were generated using a Yates analysis. A previous study had indicated the suitability and benefit of applying FEA to perform computer-based experiments to decrease but not eliminate physical experiments on TBCs. This program expanded on these findings by developing a larger knowledge base and a procedure to extract rules to aid in the TBC design.

Keywords FEA, finite element, SBIR, TBC, thermal barrier coating

1. Introduction

APPLICATION of a thermal barrier coating (TBC) provides a method for improving turbine efficiency by allowing the engine to operate at higher temperatures. By coating the surface of a turbine blade with a ceramic material (top coat) having a low thermal conductivity, such as yttria-stabilized zirconia (YSZ), the maximum temperature in the blade can be maintained below a critical level as the combustion temperature is increased. However, direct application of a ceramic to a metallic substrate by plasma spraying does not produce acceptable performance due to mismatch between the coefficients of thermal expansion (CTEs) of the substrate and ceramic, and because the ceramic does not sufficiently protect the substrate from oxidation. Both conditions lead to large stress at the ceramic/substrate interface, resulting in delamination and failure due to spalling. The addition of a compliant bond coat between the substrate and the ceramic top coat has been found to improve greatly the operating life of a TBC system (Ref 1). The properties of the bond coat relative to those of the substrate and the top coat, along with the interface roughness that provides mechanical bonding sites for the plasma-sprayed top coat, determine TBC system performance.

At this time, the nature of the relative effects of system variables and the interrelations between these variables has not been quantified. Thermal barrier coating system design, therefore, has progressed by judicious experimentation. Previous studies have investigated the effects of properties and surface geometry on a limited scale by applying finite-element analysis (FEA) (Ref 2). More recently, a study by Ferguson et al. (Ref 3) has shown that the CTE, cooling rate, the creep rate of the TBC constituents, and the roughness of the bond coat significantly affect the stresses generated at the bond coat/top coat interface of the TBC. The trends derived from these FEA simulations of a burner rig cycle have agreed with trends observed from burner rig tests (Ref 4).

Based on the qualitative agreement between FEA results and experimental results from these prior studies, it seems reasonable that computer-based experiments could be performed to examine the effects of TBC variables in greater detail. Furthermore, the use of a designed set of experiments coupled with a method of interpreting the results should allow derivation of quantitative relationships of the effects of TBC variables on performance criteria. On these assumptions, a plan for the development of a software tool to aid in the design of TBC systems was formulated, with the purpose of Phase I being to demonstrate feasibility.

Three main technical tasks were identified to demonstrate the feasibility of this approach to TBC design. First, a material property database was developed to incorporate the properties of selected substrate, bond coat, and ceramic materials. Second, an automated setup program was built to generate two-dimensional (2-D) models for FEA evaluation. This setup program would access the database to extract material properties, and it would create a command file used for actual FEA model generation by the FEA preprocessor. Third, a set of rules was constructed based on the results of a designed set of computer simulations.

2. Methodology

2.1 *Task 1: Material Properties Database Development*

The functional form and framework of a database needed to support finite-element simulation of TBCs was developed. The database structure allows for addition, modification, and deletion of material property data. The database was sparsely populated with several known materials to demonstrate that it functions as required. Written in the C-language, most programmers can easily modify the program if necessary. The program stores and retrieves various properties for substrates, bond coats, and top coats. The program outputs the data in the correct form

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so that the property data can be directly included in the input file for computer simulation.

2.2 *Task 2: Development of a FEA Setup Utility*

Since the finite-element method will be used extensively for computer-based experiments, the user will need an easy method of generating model geometry and building analysis input files. Since the analysis code to be used in this study has a preprocessor, MAZE, that generates input files, the function of the setup utility was defined to generate MAZE command files (Ref 4). A set of generic geometries commonly used for TBC tests was defined. These configurations included a cylinder and a flat, circular disk. These shapes can be defined by a dimensional set—namely, radius, length, bond coat thickness, top coat thickness, and interface roughness. Materials can be linked to each TBC component to add the necessary material property data to the command file.

Using the programming language Pascal, a PC-based setup program for 2-D model development was written. The user selects the geometry type (cylinder or disk in this limited case) and then enters the radius, length, bond coat thickness, top coat thickness, and interface roughness. After these selections have been made, the setup program writes the proper MAZE command file and terminates.

The MAZE command file is an ASCII text file of a list of commands that drives the preprocessor MAZE, which is then used to generate a complete NIKE2D input file (Ref 5). The MAZE command file defines the model geometry, the mesh for each component, the nature of the interface between components, the material properties, and the model boundary conditions. Once the input files have been written, they are ready for execution by NIKE2D without modification. While NIKE2D was the finite-element code of choice for this program, this setup tool can be expanded to include other codes. As in task 1, the setup utility is a feature to speed model development.

2.3 *Task 3: Rule Base Methodology and Development*

A burner rig test is commonly used to evaluate the performance of turbine engine components and has been widely used to examine TBC behavior (Ref 6, 7). Because of the large experience base for this test, it also provides a sound framework for developing a methodology for rule base development. Therefore, the burner rig cycle test was chosen for all the simulation work completed in this study.

Figure 1 shows the burner rig cycle that was used as the basis for a set of computer simulations of TBC response. Also shown in Fig. 1 is a modified cycle with a more rapid cooling rate that was also simulated. The burner rig cycle time can be divided into three regions: heatup, steady state (at operating temperature), and cooldown. In performing these simulations, a factorial experimental design was followed to allow examination of the effects of several material properties and TBC system features. Details of the computer model, the experimental design, and the variables follow.

2.3.1 Model Geometry

Modeling was performed on a 486-class PC using a steady-state creep model to examine the time-dependent effects of the thermal cycle on stress and deformation in the TBC system. A thin, axisymmetric slice of a typical burner rig test bar was selected as the geometry to model. The bond coat and ceramic outer coat were applied to the outer surface of the bar. Since axisymmetry was assumed by this geometry, a single radial cross section was used to develop the finite-element mesh. The basic radial dimensions for the various cross sections were:

- Superalloy bar radius: 0.0127 m (0.5 in.)
- Average bond coat thickness: 130 μm (5.1 mils)
- Average ceramic coat thickness: 250 μm (9.8 mils)

The coating thicknesses correspond to typical TBC system thicknesses.

The geometry of the bond coat/ceramic interface was modeled as a sine wave to simulate surface roughness axially along the test bar. In simulating roughness, the effect of increasing the amplitude is to increase the surface roughness. The effect of decreasing the wavelength (increasing the frequency) is to reduce the roughness spacing. The model geometry is shown in Fig. 2 and 3 for low- and high-roughness materials, respectively. These figures indicate the elements corresponding to the peak, the valley, and the midheight of the sine waves. The stresses at these elements as a function of burner rig cycle time were used to develop functional relationships. In this geometry, a peak is defined to be a peak in the bond coat.

2.3.2 Model Boundary Conditions

The thermal profiles of Fig. 1 were imposed uniformly on the entire body for the models in this study. Future transient heat-transfer models will be implemented, and actual time-temperature histories for each node will be computed.

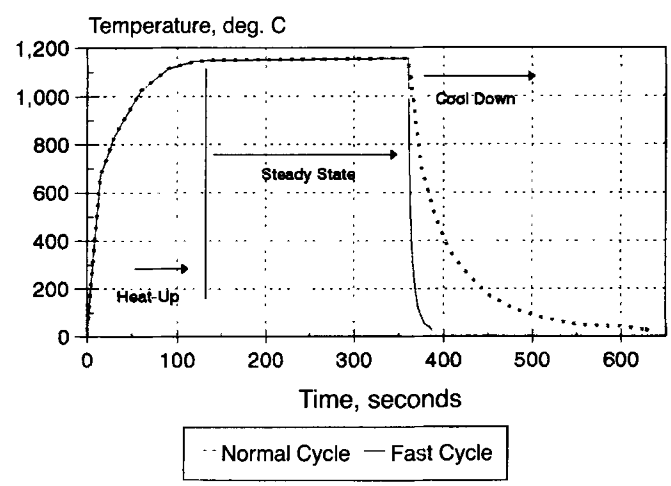


Fig. 1 Burner rig test cycle

2.3.3 Steady-State Creep Model

A power-law creep model resident in the NIKE2D code was used. The basic relationship in this creep model is summarized by:

$$\varepsilon = A \cdot (\sigma_{effective})^B$$

where A is the creep coefficient and B is the power-law creep exponent. As implemented, A and B are functions of temperature. This model is discussed in more detail in Ref 3 and 8.

2.3.4 2^5 Factorial Experiment

A factorial analysis is a means of designing experiments whose factors or variables can be discretely separated into a high value and a low value, a middle value, or even a multiple set of values. This type of experimental design provides an opportunity to determine the effects of each of the factors or variables, as well as the interactions between them on a desired property or performance indicator. In addition, an analysis of variance (ANOVA) table can be constructed to rank the significance of the factors and their interactions. In this task, a two-level, five-variable factorial experiment was conducted, resulting in the execution of 32 finite-element models. The maximum and minimum stresses in the three regions of the burner rig cycle were documented.

2.3.5 Parameters for the Factorial Experiment

The parameters used in this experiment are presented in Ref 9 and are too detailed to include here. The tables in Ref 9 contain all of the material property data used in the various simulations. The ceramic top coat material data were for YSZ (ZrO_2-8Y_2O_3). Bond coat properties were similar to those of Ni-35Cr-6Al-0.95Y bond coat materials. The superalloy base material properties were those of a typical nickel-base superalloy. The low and high values were somewhat arbitrarily selected to demonstrate the feasibility of rule development.

2.3.5.1 *Bond Coat Creep*

Bond coat creep resistance was studied primarily because the TBC will be subjected to high temperatures at the operating regime of turbines. It has been reported in previous studies that the bond coat creep rate or the bond coat creep strength is a significant variable in TBC failures (Ref 3, 7). The values used for "low" and "high" refer to resistance to creep, so the numerical values for the power-law creep coefficient A are higher for low creep resistance than for high creep resistance. The creep coefficient values in the "low" creep resistance bond coat are for a Ni-35Cr-6Al-0.95Y bond coat material; this material is known to have low resistance to creep. The numerical values in the "high" column of creep coefficient were taken as an order of magnitude less than those in the "low" column.

2.3.5.2 *Bond Coat CTE*

The functional correlation between CTE and temperature was assumed to be a linear relationship. The CTEs used in this experiment have the same intercept at 0 °C (12.0E–6/°C), but different slopes. The slopes for the high-CTE material and the low-CTE material are 8.0E–9/°C^2 and 2.0E–9/°C^2, respectively. The graph of the two CTE lines is shown in Fig. 4.

2.3.5.3 *Bond Coat Roughness*

A certain degree of roughness is necessary to promote a mechanical bond between the top coat and the bond coat because chemical bonding between the two materials is minimal. However, a rough interface provides stress concentration sites at the interface between materials. A smooth interface would have no stress concentration sites, but bonding of the top coat to the bond coat would be poor due to lack of mechanical bonding sites and very weak chemical bonding. It is desirable to define an optimum roughness that minimizes interfacial stress while adequately providing for mechanical bonding.

The interface is assumed to be a sine wave that has a defined amplitude and wavelength. In this experiment, the low- and high-roughness geometries are taken as one-half and two times the normal roughness, where the normal roughness is defined as that having an amplitude of 10 μm and a wavelength of 50 μm. Thus, the low roughness would have an amplitude and wavelength of 5 and 25 μm, respectively, while the high roughness would have an amplitude and wavelength of 20 and 100 μm, respectively. Refer to Fig. 2 and 3 to compare the profiles for the low- and high-roughness configurations. Roughness was arbitrarily represented as a single factor by (Ref 9):

$$\text{Roughness} = \frac{\text{Amplitude}^{1.5}}{\text{Wavelength}}$$

2.3.5.4 *Top Coat Creep*

In the previous report by Ferguson et al. (Ref 3), it was observed that the top coat stress decreases slightly during the operating temperature regime, whereas the bond coat stress is nearly zero. This indicates that the top coat creeps during the operating temperature regime. In this case, the creep of the top coat can relieve stresses due to CTE mismatch at higher temperatures, thus prolonging or preventing failure. On the other hand, creep can

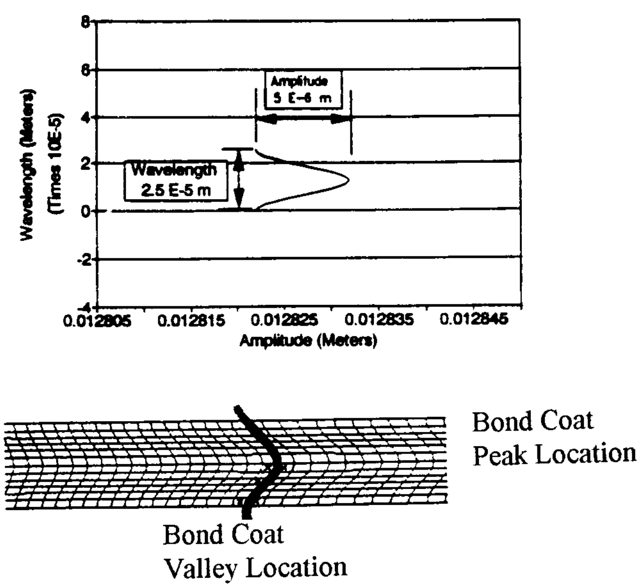
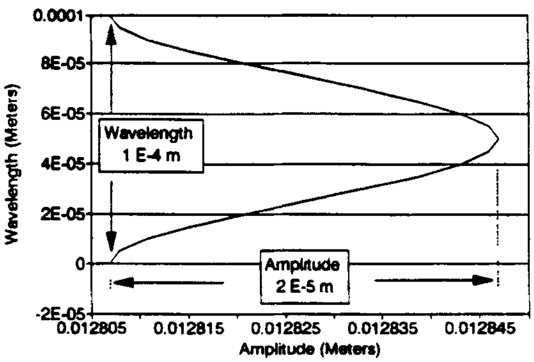


Fig. 2 Low-roughness profile of bond coat



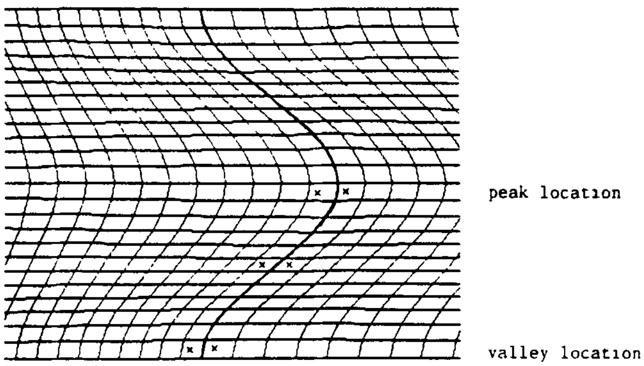


Fig. 3 High-roughness profile of bond coat

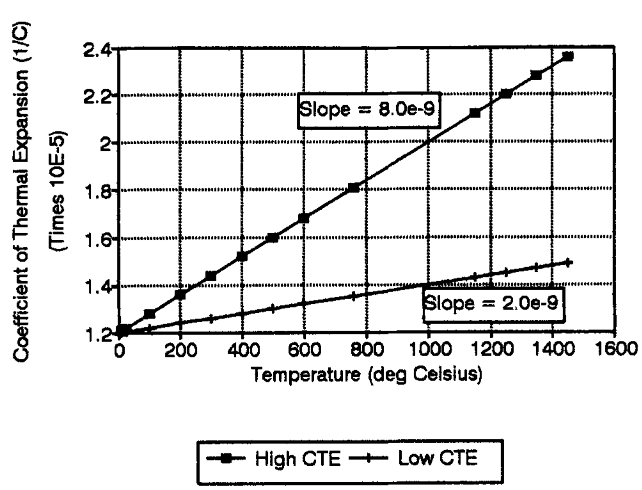


Fig. 4 Bond coat CTE

also weaken the top coat to such an extent that failure occurs. In this experiment, a knowledge of the degree to which creep strength affects the failure characteristics of TBCs will aid in the design and materials choice for a top coat.

2.3.5.5 *Burner Rig Test Cooling Rate*

The cooldown portion of the burner rig cycle has been shown to promote TBC failure (Ref 9). A rapid cooling rate promotes a high thermal stress rate due to CTE mismatch and the differential cooling rate in materials. A slow cooling rate results in the development of stress at a lower rate, and this could allow rate-sensitive relaxation mechanisms to be active, depending on the time at elevated temperatures. A finite-element simulation that includes creep behavior, as this one does, can predict stress development during the cooldown region of the burner rig cycle. Figure 1 shows the different cooling rates used in these models.

3. Yates Analysis

Yates analysis is a means of computing the effects of the independent variables used in a factorial analysis on the dependent variables. This analysis method also determines the amount of interaction between the variables. The result is a response surface that amounts to a mathematical curve fit of the five independent variables and any output of choice from the simulations (e.g., radial stress in the top coat at the interface peak). In addition, from the response surface, an ANOVA table can also be constructed. This table can be used to examine the main effects to determine the significance of a factor and its interaction with other factors.

The response surface (equation) generated by the Yates analysis can be used to determine how much each of the factors should be changed to reach the maximum stress as quickly as possible, or, conversely, how to maintain minimum stress. The method used to analyze the response surface is called the path of steepest ascent.

4. Results and Discussion

The superalloy substrate controls the global stress state of these models due to its mass dominance. The roughness of the interface between the bond coat and top coat, however, plays a dominant role in establishing the local stress state. Failure of TBC systems has been associated with the interface region, and for this reason the interface has been a focal point of attention. The direct effect of bond coat mechanical behavior on TBC performance can be seen by examining the stresses at the bond coat/top coat interface.

A typical simulation result is shown in Fig. 5 for radial stress as a function of time at bond coat and top coat peak and valley interface locations. Figure 5 represents simulation results using a regular cooling cycle, with low roughness. The three regions of the burner rig cycle are indicated in Fig. 1. Notice that during heating, radial stress builds in both the top coat and bond coat, but in opposite senses. Before heating is completed, relaxation occurs and stresses drop toward zero. During the operating or steady-state region, the bond coat radial stress is nearly zero, and the top coat stress continues to decrease toward zero. Creep of the top coat is most likely responsible for this radial stress reduction. Upon entering the cooldown region, radial stress builds very quickly. Interestingly, the interface roughness effect can be seen by the difference in the sign of the stress at the peak and valley in the top coat.

During the operating-temperature regime, where the temperature is held constant, the bond coat creeps and stresses relax to nearly zero, whereas the top coat shows a stress decreasing more slowly with time. During cooldown, both the bond coat and the top coat experience a stress opposite in sign to that experienced during heatup. The stresses at the end of cooldown are generally larger on the cooldown portion of the cycle than on the heatup portion. The creep mechanism in the materials is responsible for this. Upon heatup, stresses are induced due to CTE mismatch between materials. However, as temperature rises, creep mechanisms are activated to relax the stresses induced by the CTE mismatch. Thus, at the end of heatup, a large portion of the thermally induced stress may be relieved, depending on the magnitude of the CTE mismatch and the creep resistance of the bond coat and top coat materials.

After a sustained time at operating temperature, the TBC system (except for the top coat peak) nearly settles to a new equilibrium stress state due to relaxation at the high-temperature hold. Upon cooldown, the CTE mismatch and increasing creep resistance work to build the stress state back up to high levels, and thermal stresses (opposite in sign now) begin to again be imposed. In this case, the temperature is decreasing and, as the thermal stresses increase, creep (or stress relaxation) mechanisms are no longer active due to the cooler temperatures. Compounding this difference between heatup and cooldown is the level of stress in the TBC while the material is at temperatures where creep is active. During cooling, the stresses in the TBC are low while creep is active. The bulk of the cooling regime occurs when creep is not active, and as a result stress can only be relieved by plasticity or by fracture. During heating, the stresses are high when creep becomes activated due to the large temperature change from ambient to the operating temperature. The combination of high stress and high temperature drives stress relaxation.

The top coat radial stress generally shows an initial compressive stress at the peak of the interface, whereas the valley has a tensile stress during the heatup cycle. During the end of heatup, where bond coat stress relaxation begins, and during operating temperature, where bond coat stress moves toward zero, the top coat stresses tend to reverse. Once the stress in the bond coat is nearly relaxed, the top coat stresses slowly move to zero due to creep, although more slowly than the bond coat. At the cooldown, the stresses reverse themselves from the heating cycle and end up in tension for the peak and in compression for the valley. This may be a significant factor as the top coat is relatively weak in tension.

Increased roughness results in higher stresses during heating and cooling, and was shown to be the second most significant factor by ANOVA. It is also interesting to note that there is a relatively high level of radial tension in the top coat at the end of the cooldown period caused by stress concentrations of the rough interface in some of the simulations. Radial tension is thought to contribute significantly to cracking near the interface.

By using Yates analysis, the relative dominance or importance of each of the five parameters tested in this experiment could be determined. In the analysis, the variable values are normalized between –1 (low) and +1 (high), and the resulting coefficients are for the normalized values. The Yates analysis shows that bond coat CTE is the largest contributor in generating stress and is the most significant factor. This is evident in the majority of the experimental simulations, where CTE ranked first and second. Interface roughness was the second most significant factor.

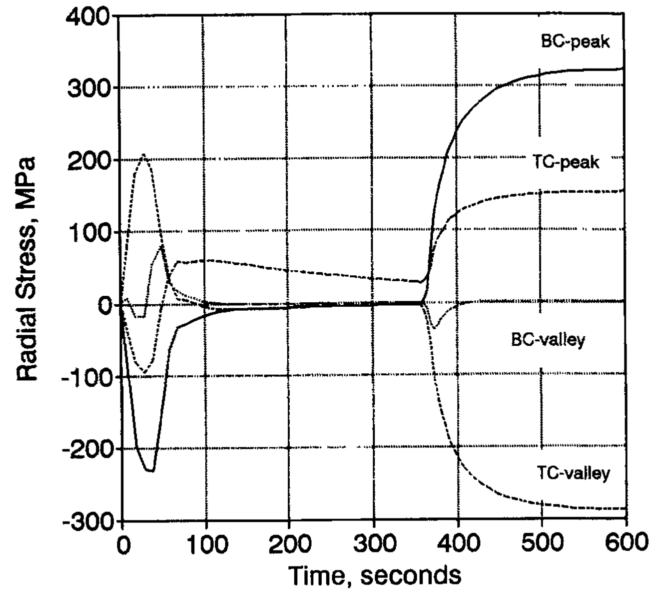


Fig. 5 Typical stress versus burner rig time plot. BC, bond coat; TC, top coat

Bond coat and top coat creep strength are of roughly equal significance and rank third for these simulations, but at a much lower level of significance than CTE or roughness. From previous work, the bond coat creep strength was shown to be significant, especially during cooling (Ref 3). A purely elastic response of the TBC system (no creep effects) to the burner rig cycle would be to return to the initial stress-free state upon cooling. The fact that a different stress state results after burner rig cycling for simulations that include creep effects indicates the significant effect that creep does have on TBC response. The significance of this effect was discernible from these simulations: Creep during the operating hold time relaxed stress to nearly a zero level for both high and low bond coat creep levels. In other words, the presence of creep for both high and low values showed nearly full effects, thus statistically indicating a lower significance. If some of the simulations had not had creep behavior, as opposed to high and low creep materials, the significance of the creep effect would have been more prominent.

To determine the conditions that result in the desired maxima or minima in the resulting stress equations, an analysis to determine the change in variable values can be performed. For efficiency, the path of steepest ascent or descent offers the fastest method of determining conditions that generate maxima or minima.

Finite-element simulations, such as those described in this paper, provide an excellent means by which results can be generated in a cost-effective manner in the least amount of time. In addition, newly developed materials for TBCs can be tested immediately and quickly, and without the significant expenditure of generating and testing actual TBC systems. The complexity of the response surface equations can be increased as more variables are included or as higher-order effects are included. The assumptions used in these analyses included linearity of response. Additional FEA simulations can be performed to augment the results, and nonlinear effects can be investigated. Also, sensitivity studies can be conducted to identify the variables that have the most significant effect on TBC life. As in all successful design engineered systems, knowledge of the process-property relationships can be used to produce TBCs with improved life.

5. Summary and Conclusions

This Phase I SBIR effort has demonstrated the feasibility of developing a software system to aid in the design of TBC systems. Of primary significance was the development of a set of equations that form a rule set that can be used to avoid aggravating stress conditions through specification of bond coat/top coat interface roughness, bond coat CTE, bond coat creep strength, and top coat creep strength. This development relied on the use of the FEA method to perform computer simulations in place of or to complement physical experiments. By following an experimental design such as a full or fractional factorial design, standard statistical methods can be applied to determine these equation sets. In this case, Yates analysis was successfully used on a 2^5 factorial design to generate a response surface to the five dependent variables investigated. For more complex analysis, other statistical models can be used to describe the response surface if needed. The results of the Yates analysis used in this study represent a portion of the framework that is needed to build complex relationships among the process used to produce the TBC system, the materials that make up the TBC, and the predicted life.

These developments demonstrate the feasibility of this approach to TBC design. The methodology will be extended in Phase II by expanding and enhancing the rule base through further finite-element simulations. These will include: the transient effects of thermal gradients generated during heating, operation, and cooling; the effects of multiple burner rig cycles; the use of a wider range of system variables to examine nonlinear effects as well as other possible critical variables; the incorporation of top coat fracture and crushing; and additional harmful stress at the interface due to bond coat oxidation. Thus, the simulations will account for more factors that would force the simulation to more closely approximate actual conditions to which TBCs are exposed.

Acknowledgments

This work was sponsored by NASA under SBIR contract no. NAS3-27281. The authors also wish to acknowledge Dr. William Brindley and Dr. Robert Miller at NASA Lewis Research Center for their input and insight on this project, and Mr. Rex Ordillas, now at Brush Wellman Inc., for his contribution to the Yates analysis.

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