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OPTIMIZING FUNCTIONALLY GRADED NICKEL-ZIRCONIA COATING PROFILES FOR THERMAL STRESS RELAXATION

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Abstract:

The investigations on optimization of composite composition of Nickel-Zirconia for the functionally graded layered thermal barrier coating for the lowest but uniform stress field under thermal loading is presented. The procedure for obtaining temperature- and composition-dependent thermal and mechanical properties of various coating compositions is discussed. These material parameters were used in thermo-mechanical finite element stress analyses of a nickel substrate with the coating. The results showed that the Von Mises stresses in the substrate and the interfaces were the lowest with the coating profile that followed a concave power law relationship with the index $n \approx 2.65$.

Keywords: *Finite element analysis; Power law; Optimization; Functionally graded coating; Thermal stress.*

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1. Introduction

In aerospace industry, achieving higher efficiency for gas turbines and aircraft engines has always been an important research area. Higher efficiency requires the gas turbines to operate at higher temperatures. Such high heat input, however, weakens the metallic, mostly super-alloys, structure of the gas turbine. Ceramic thermal barrier coatings (TBC) are, therefore, widely used as insulation protecting the underlying metallic structure of a gas turbine blade. It is claimed that each 0.001-inch of TBC thickness reduces the temperature of the blades by 17 to 33°C [1]. Advanced engines, in the foreseeable future, may be expected to rely even more heavily on these coatings [2].

Despite unique advantages, cracks and interfacial de-bonding of the ceramics coatings are the undesirable problems associated with TBCs. This is primarily due to the fact that ceramics and metal have very different properties. The high degree of brittleness combined with low thermal expansion and thermal conductivity render TBCs highly susceptible to the generation of thermal stresses of high magnitude.

The functionally graded coatings (FGCs) are expected to improve the disparity as the FGCs consist of several intermediate layers whose structure and composition changes gradually at the micron level from substrate metal to ceramic coating, as shown in Figure 1. The composition profiles of FGC microstructure can have either a discrete step change or continuous variation in material properties through the thickness. A resultant temperature gradient over the coating generates less thermal mismatch between any two adjacent layers due to small local changes in thermo-mechanical properties. The FGC could possess several coating layers of graded properties to

withstand severe heat environment and steep temperature gradients across their thickness with the lesser risk of interfacial failure [3]. Note that one such popular technique used for FGC applications is plasma spraying [4].

----- Insert Figure 1 here -----

In order to exploit the potential of FGC, two problems have to be overcome. Firstly, the gradient of layer composition through the coating thickness or the distribution of metal-ceramic mixture has to be controlled and optimized for minimizing the thermal stresses. Secondly, to achieve the first objective, the effective mechanical and thermal properties of each of the locally graded layers have to be determined a priori. Many studies have been proposed to derive the local properties as functions of the local volume fractions primarily using the linear rule of mixtures. For the plasma sprayed materials, the mixture consists of randomly distributed concentrations of the two constituent materials, namely metallic and ceramic phase normally produced by co-spraying the two materials.

In the field of FGC design and characterization, different techniques from analytical, numerical to experimental analysis have been demonstrated. Among them, Finite Element (FE) method is the most popular numerical method [5] used to characterize FGCs. In this paper, details of the investigations carried out to obtain an optimized composition of Nickel/Zirconia (Ni/ZrO_2) FGC for nickel substrate that would result in the lowest and more uniform stress field in the coating interface structure under thermal loading are discussed. Temperature- and composition-dependent thermal and mechanical properties of the various coating mixtures were used in the thermo-mechanical FE analyses in order to achieve a better simulation of the real life situation.

The studies shows that among the various configurations, the configuration where the FGC profile that follows a concave power law relationship has lower peak stress, and for the power law relationship with the parameter $n \approx 2.65$, the peak stress is the lowest amongst all.

2. Finite Element Modelling

2.1 Geometric and FE details

A circular disk shaped substrate with 10 layers of Ni/ZrO_2 FGC is taken as the candidate geometry in the present investigation. However, in view of the symmetry of the configuration, the geometry was reduced to an axially symmetric two-dimensional rectangular model as shown in Figure 2 for stress analysis.

----- Insert Figure 2 here -----

A nickel-based super-alloy is used as the metal substrate and Zirconia is used as the ceramic material to form the FGC. Ten layers of FGC with graded composition of Ni/ZrO_2 were formed. It was assumed that there was perfect bonding between the applied coating and the substrate. The bonding between layers was also considered defects-free. In addition, friction in any form as well as presence of residual stresses was not considered. Although, the presence of residual stresses is an important issue, it will require a complex FE modeling and reliable material properties data. Any conductance of experiments to address this will need elaborate experimentation. It may be noted that the metal particles are likely to reach and exceed their plastic limits during the process of high temperature plasma spraying. However, it is extremely

difficult to account for changes in material properties due to these plasticity effects in want of reliable data. It is therefore assumed that both, the substrate and the coating, materials have little effect of plasticity on their properties. The aim of the simulation presented in this paper is to find the conditions leading to the highest elastically calculated stresses within the coating.

LUSAS (version 13), a general-purpose FE software [6], was used to analyze the FGC for stress distribution due to the thermal loading. The following elements in *LUSAS* were used to create the thermo-mechanical analysis model:

- for thermal analysis: - 2D axially-symmetric field elements (QXF4), and,
- for mechanical analysis: - 2D axially-symmetric solid continuum elements with enhanced strains (QAX4M).

The disc is subjected to a nodal temperature of 500K on the top surface of the coating while the bottom of the substrate is maintained at 300K. For the structure analysis, the displacement in X-direction was constrained at the nodes along the line of symmetry. The Y- displacement of the nodes defining the bottom of the substrate was also set to zero. The physical properties of the substrate and the ceramic coating are shown in Table 1.

----- Insert Table 1 [7, 8] here -----

2.2 Sensitivity to mesh density

After the FE model is created, a sensitivity study is carried out to determine the optimum mesh density. The optimum mesh density is determined by comparing the

highest Von-Mises stress for various FE models with different element sizes obtained using the material properties listed in Table 1; the analysis results are presented in Figure 3.

----- Insert Figure 3 here -----

Figure 3 shows that, the Von Mises stress does not change much for FE models with 1235 and more elements. Thus to minimize computing time, and at the same time to ensure the accuracy of the results, the FE model with 2231 elements was chosen for the subsequent analysis.

2.3 Temperature and composition dependent material properties

The properties of *Ni* and *ZrO₂* vary with temperature, and also the properties of *Ni/ZrO₂* mixture depend on the mixture composition. Although previous researchers attempted the use of either temperature-dependent or composition-dependent material properties of *Ni/ZrO₂* mixture for their FE analysis, the temperature and compositional effects on to the material properties of the TBC were not incorporated together and applied simultaneously. One of the features of the current investigation was to incorporate both, the temperature and the compositional, effects into the material properties for FE to achieve a more realistic simulation.

----- Insert Table 2 [8] here -----

The temperature-dependent properties of *Ni* and *ZrO₂* based on the review of articles from literature [9,10] are summarized in the form of equations in Table 2 and Table 3 respectively.

----- Insert Table 3 [10] here -----

The polynomial relationships for the effective properties of randomly distributed mixtures of Ni/ZrO_2 as a function of volume fraction “C” of ZrO_2 are required to model the local properties within the layers. To obtain these relationships, the authors conducted a series of finite element analysis to determine the effective thermo-physical properties i.e. elastic modulus, thermal expansion coefficient, thermal conductivity and heat capacity, which are essential for heat transfer and thermal stress analyses of FGCs. The methodology enabled the derivation of properties of a FGC having a random distribution ranging from 0 to 100% by volume of two solid phase materials with known bulk properties. The resulting effective thermo-physical properties are shown in Table 4. For the sake of completeness, a brief description of the approach is presented in section 2.4.

----- Insert Table 4 here -----

The properties of the Ni/ZrO_2 FGC at temperatures other than 300K are not known. These values were estimated using the trends depicted by the equations listed in Tables 2 and 3. The resulting curves for different material properties are presented in Figures 4 (a) to 4 (d).

----- Insert Figure 4 here -----

2.4 Modelling of effective properties of random mixtures of two materials

The objective of this section is to explain the method and its application to predict the properties of the resulting mixture having different composition of the pure substances.

A two-dimensional model was constructed to represent the cross section of the sprayed layer. The lengthwise and depth wise dimensions of the model are 5mm by 1 mm as shown in Figure 5. The model is meshed into 100 by 20 elements respectively, giving a total of 2000 elements. Further assumptions inherent to the method are that there are no chemical interactions or diffusion between the materials to form a material different from the original constituents.

----- Insert Figure 5 here -----

In order to represent the mixture of the two materials, a method is required to distribute the two materials randomly over the FE mesh with a high level of homogeneity and randomness. An Excel spreadsheet program with the uniform probability distribution random number generator is used as the material selection algorithm. The core of this randomizing program lies in formulating conditional probabilities for assigning the two materials: metallic and ceramic. Figure 6 shows the complete set of randomized models representing varying percentage by volume of metallic and ceramic materials, from 0%, to 100% in increments of 10% by volume of ceramic.

----- Insert Figure 6 here -----

To extract the effective properties, the FE models are provided with the appropriate loading, boundary conditions. The bulk properties of the constituents assigned to various elements in random manner are listed in Table 1. The effective properties to be found namely: Young's modulus, thermal conductivity, heat capacity, thermal expansion coefficient were generated in accordance to the testing methodology of the ASTM (American Society of Testing and Materials) standards [11-14].

The results of the numerical simulations were curve fitted with polynomial functions presented in Table 4. The plots of the functions can also be seen in Figure 4 (a-d) at 300K. It is noted that the effective properties deviate from the linear rule of mixture, most significantly in the transition zone where the mixture is composed of almost equal percentage of both solid materials. The accuracy of the results depended on the care taken in designing of the FE mesh, a mesh sensitivity study was conducted to ensure that the numerical model closely represents the continuum, i.e. a sufficient element density required to increase the resolution of particle mixture. Three attempts in randomizing the materials distribution were performed to reduce the statistical scatter in the effective properties and obtain a statistically reliable mean value.

2.5 Modelling of different FGC compositions

To begin with, a single layer coating of 1mm thick ZrO_2 was considered for the analysis. Subsequently, a linear and three non-linear coating configurations as depicted graphically in Figure 7 are evaluated. The effective thermal and mechanical properties of the coating layers of different composition are estimated using polynomial relationship derived by FE analysis described in section 2.4. The suitability and effectiveness of the different coating profiles is assessed based on the Von-Mises stresses in the coating layers. The Von-Mises stresses for these configurations are compared and the peak Von-Mises stresses identified. The profile that provides the lowest peak Von-Mises stress is considered as the most suitable coating profile. As described in Table 5, each FGC configuration can be represented by a power law series.

After the most suitable coating profile is identified, the FGC profile is further optimized by varying the power index so as to achieve the lowest possible peak Von-Mises stress.

----- Insert Table 5 here -----

----- Insert Figure 7 here -----

3. Results and Discussion

3.1 Selection of the FGC Composition

The temperature variations along the thickness of the coated substrate for all the six FGC profiles are presented in Figure 8.

----- Insert Figure 8 here -----

From Figure 8, it is observed that the temperature profile for the simplex or single layer of 100% ZrO_2 coating (Case-0) has a sharp transition at the interface between the substrate and coating at which the slope of the temperature increases sharply. This sharp transition in temperature is one of the main factors contributing to the cracking or interfacial debonding of the thermal barrier coating.

The other four curves representing different ZrO_2 coating composition profiles at which the temperature gradient at the interface is significantly reduced as compared to the simplex ceramic coating configuration. However, it may be noted that, from the 7th to 10th coating layer, the temperature gradient is somewhat similar to each other for the various FGC configurations. Based on this finding, it is concluded that different coating profile does not have significant impact on the insulation properties of the top layers of

the FGC. The Von-Mises stress profiles for the simplex ZrO_2 coating, linear, quadratic and cubic FGC configurations are presented in Figure 9.

For the simplex ZrO_2 coating (Case-0), most of the stresses are concentrated in the Ni/ZrO_2 interface. The peak stress of 115MPa occurred at the edge of the Ni/ZrO_2 interface region. From the stress contours for the linear profile (Case-1) FGC, it is observed that the stresses decreased, especially at the interface area. The peak stress of 105MPa occurred at the edge of the Ni/ZrO_2 interface region.

It was observed that for quadratic profile (Case-2), the peak stress is 100MPa whereas for cubic profile (Case-3) the peak stress is 111MPa. For reversed cubic profile (Case-4) the peak stress also occurred at the edge of the interface region; its magnitude is 106MPa.

Relating the results of the temperature profiles (Figure 8) with the associated Von-Mises stress profiles (Figure 9), it is observed that the temperature gradient is directly related to the peak Von-Mises stress of the structure. Amongst the various configurations, the cubic profile (Case-2) leads to a gradual temperature gradient transition deep into the coating profile and has the lowest peak Von-Mises stress. On the other hand, the simplex ZrO_2 coating that exhibits a sharp temperature gradient transition starting at the Ni/ZrO_2 interface and has the higher peak Von-Mises stress.

----- Insert Figure 9 here -----

It may be noted that the aim of this study is to minimize stress and not the substrate temperature. It can be observed in Figure 8 that the temperature at the interface between the substrate and coating increased with the application of FGC. The lowest temperature at the interface is achieved with a simplex i.e. single coat of Zirconia which has the highest stress of all the cases. This is because the insulating property of the FGCs due to its metallic content is less than pure coat of Zirconia given the same thickness of coating. There is a tradeoff between stress and temperature, in minimizing the stress, a small increase in the substrate temperature is expected.

Since the peak stresses are concentrated along the outer edge, a closer look at the magnitude of the stresses in that region is needed (see Figure 10).

----- Insert Figure 10 here -----

Along the x-axis of Figure 10, the distance from 0 to 0.004m represents the Nickel substrate and the distance from 0.004 to 0.005m represents the FGM coating.

It was observed that the stresses in the Nickel substrate at a distance far away from the FGC were similar regardless of the coating profiles. The variations in the stresses among different configurations are noticeable near to the coating interface. Among the configurations, the stress level for the single ZrO_2 coating increases rapidly reaching its peak at a distance of 3.86mm whereas the increase in the stress level for Case-2 is much gradual and reaches its peak at 4.1mm.

In the coating region, the stress varies significantly within the different configurations. All configurations have the peak stress around the Ni/ZrO_2 interface area. This phenomenon is expected due to material discontinuity at the interface. Among the various configurations, the quadratic profile (Case-2) has the lowest peak stress of 100MPa, and therefore, was chosen to be the most suitable composition profile for further analysis.

3.2 Optimization of the power law series for FGC Composition

After establishing that the power law series with $n \sim 2$ provides a low peak stress, the effect of various values of index n on the stress distribution in the coated substrate is studied. Figure 11 shows the distribution of Zirconia in FGC for different indices n .

----- Insert Figure 11 here -----

The resulting temperature distribution obtained from the FE heat transfer analysis for these coating profiles are presented in Figure 12.

----- Insert Figure 12 here -----

From Figure 12, it is observed that the temperature profile is directly related to the n in the power law equation. In the Nickel substrate, the temperature gradient increased as n increased. In the coating region, as n increased, the transition in the temperature gradient shifted deeper into the coating region. This is because as n increased, the rate of increase in the proportion of ZrO_2 in the first few layers (i.e. 1st to 4th) decreased significantly. Since ZrO_2 is a good thermal insulation material, a small proportion of it has a slower transition in the temperature gradient.

The corresponding Von-Mises stress profiles across the thickness of the coated substrate obtained at the outer edge and at the centre of the specimen are shown in Figure 13.

----- Insert Figure 13 here -----

Figure 13 (a) shows that, as n increased from 0 to 2, the peak stress at the edge decreased from 115MPa to 100MPa. However for $n \geq 2.5$, the peak stress at the outer edge section stabilized around 100MPa. Besides, as n increased, the peak stress shifted from the Nickel substrate into the coating region. This is because as n increased, the amount of ZrO_2 in the coating also increased, but at a slower rate, hence the stress due to the mismatch of the material properties in the FGC did not show any drastic increase.

Figure 13(b) shows that unlike in the edge region, at the centre of the specimen higher stresses occurred near the top surface of the coating, at around 4.9mm from the bottom of the substrate. For larger values of n , the amount of ZrO_2 in the coating increased at a faster rate in the region near to the top surface whereby causing the material properties to change drastically over the few top layers leading to higher stresses in that region.

----- Insert Figure 14 here -----

Figure 14 shows how the magnitude of the peak Von Mises stresses along the outer edge and at the centre of the Ni substrate vary with n and eventually cross-over at $n \sim 2.65$. Thus, it may be concluded that if the FGC profile follows a power law $X^{2.65}$ for % volume of ZrO_2 in the coating, the thermal stresses will be more evenly distributed

within the coating layers with the lowest peak stress among all. This can be confirmed from the thermal stress distribution shown in Figure 15. The highest stress is approximately 90 MPa.

----- Insert Figure 15 here -----

The results of the present studies are comparable with the results obtained by a few other researchers. Based on experimental studies, Kawasaki [15] reported a concave profile with $n=3$ as the optimized plasma sprayed Zirconia/stainless steel FGC coating. Tanigawa [16] used numerical approach for the optimization of $Al-Al_2O_3$ FGC. His results show that FGC described by a power law with $n=1.895$ provides optimum performance. This substantiates the validity of the present investigations, which is more comprehensive and hence, realistic.

Figures 16 (a) and 16 (b) show the resultant optimized composition profile and its temperature distribution respectively. The composition profile show an exponential trend in the ceramic content having a gentle increase near the interface followed by rapid rise at the surface. The gentle increase in ceramic content near the substrate is effective in reducing high shearing stresses at the interface. The temperature distribution reflects the same trend as the composition profile, having lower gradient at the interface leading to lower stress and high gradients at the surface with increasing stress.

----- Insert Figure 16 here -----

It may be noted that the effect of plasticity will be examined in future work using the following approach starting from the mixture composition models. The yield stress of the metallic and ceramic particles will be included in the mixture models. A loading scheme such as a tensile test will be applied and the load versus displacement curve derived. It is expected that the sign of first yield will coincide with the yielding of metal particles which has lower yield stress irrespective of the composition of the mixture. The post yielding behavior of the mixture models will be however dependent on the mixture composition. At a high ceramic composition, the post yield stress strain curve will be higher than at a lower ceramic composition. The finite elements models will be much finely discretised in order to accurately simulate the yielding behavior of the metal particles. As such, each particle will have to be discretised into finely divided elements, increasing the size of the FE model considerably along with correspondingly high computation time.

4. Conclusions

The results of the numerical simulations for the effective properties of the $Ni-ZrO_2$ mixture were obtained by means of finite element analysis in combination with a random number generator to homogeneously distribute the two materials in pre-defined proportion in an FGC. The effective properties thus obtained were described by polynomial functions against % volume of the ceramic component. Using the effective properties, a number of FGC distribution profiles through the coating thickness were attempted. Initially, thermal stress analysis of simple distributions profiles, such as; simplex, linear, quadratic, cubic and reversed cubic were performed. Among all, the quadratic profile offered the largest decrease in thermal stress; the peak stress dropped

from 115 MPa to 100 MPa. Based on this finding, subsequent thermal stress analysis focused on the power law with different index n . By optimizing on a number of thermal stress analysis with different power law indices, $n = 2.65$ was found to achieve the greatest reduction (to 90 MPa) in the thermal stress and thus provide an optimum solution.

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Figure 1: Schematic of functional graded thermal barrier coating showing high ceramic content at the exposed surface (top) and pure metallic interface next to the substrate and a graded composition in between.

(a) FE model used for the analysis

(b) schematic of the substrate with coating

Figure 2: Geometric and FE details of the axi-symmetric substrate.

Figure 3: Variation in the highest Von Mises stress with mesh density.

(a)

(b)

(c)

(d)

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(a) at the outer edge section

(b) at the centre

Figure 13: Von Mises stress distribution with various FGC profiles defined by a power law series with variable power index n .

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Figure 15: Contour plot of Von-Mises stress [Pa] for the coating profile defined by $X^{2.65}$.

(a)

(b)

Figure 16: Composition profile and temperature distribution for the optimized FGC defined by $X^{2.65}$.

Table 1: Bulk material properties for Nickel [7] and Zirconia [8] at 300K .

Material Properties	Nickel based superalloy [7]	Ceramic coating ($ZrO_2 - 8\% Y_2O_3$) [8]
Young's Modulus, E (Pa)	2.2×10^{11}	5.00×10^{10}
Poisson's ratio, ν	0.3	0.25
Thermal Expansion Coefficient, α (K^{-1})	1.3×10^{-5}	9.0×10^{-6}
Density ρ , (kgm^{-3})	8900	4400
Thermal conductivity, K ($Wm^{-1}K^{-1}$)	91.2	2.94
Specific Heat, C_p ($Jkg^{-1}K^{-1}$)	461	504

Table 2: Temperature-dependent properties of Nickel [8] (300K – 500K)

Young's Modulus, E (GPa)	$-1.508946 \times 10^{-5} T^2 - 4.161243 \times 10^{-2} T + 234.8317$	(1)
Heat Capacity, C_p (J/kgK)	$0.5023 T + 310.522$	(2)
Thermal Conductivity, K (W/mK)	$1.876168 \times 10^{-7} T^3 - 2.126458 \times 10^{-4} T^2 + 2.717507 \times 10^{-2} T + 97.62$	(3)
Thermal expansion coefficient, α (K^{-1})	$1.143460 \times 10^{-8} T + 9.5696 \times 10^{-6}$	(4)

Table 3: Temperature-dependent properties of ZrO_2 [10] (300K – 500K)

Young's Modulus, E (GPa)	$- 8.1 \times 10^{-6} T^2 - 50.3 \times 10^{-3} T + 65.819$	(5)
Heat Capacity, C_p (J/kgK)	$1.71 \times 10^{-7} T^3 - 6.19 \times 10^{-4} T^2 + 7.95 \times 10^{-1} T + 3.16593$ $\times 10^2$	(6)
Thermal Conductivity, K (W/mK)	$0.116 \times 10^{-6} T^2 + 0.21 \times 10^{-3} T + 2.8936$	(7)
Thermal expansion coefficient, α (K^{-1})	$12.7 \times 10^{-12} T^2 - 18.9 \times 10^{-9} T + 13.527 \times 10^{-6}$	(8)

Table 4: Composition-dependent properties of Ni/ZrO_2 mixture at 300K where “C” ranges from 0.0 (pure nickel alloy) to 1.0 (pure Zirconia)

Young's Modulus, E (GPa)	$46.9C^5 - 204C^4 + 280.8C^3 - 35.8C^2 - 257.8C + 219.7$	(9)
Heat Capacity, C_p (J/kgK)	$2.536C^5 + 7.676C^4 - 1.985C^3 + 13.87C^2 + 20.88C + 461$	(10)
Thermal Conductivity, K (W/mK)	$-189.2C^5 + 327.9C^4 - 78.8C^3 - 5.1C^2 - 143.1C + 91.2$	(11)
Thermal expansion α (K^{-1}) $\times 10^{-5}$	$-0.662C^5 + 1.58C^4 - 1.328C^3 + 0.186C^2 - 0.176C + 1.3$	(12)

Table 5: Polynomial representation of the coating profiles in Figure 7.

Polynomial id	Description of profile	Polynomial equations ⁺
Case 0	Simplex	$C = k^n \ (n = 0)$
Case 1	Linear	$C = \kappa^n \ (n = 1)$
Case 2	Quadratic	$C = \kappa^n \ (n = 2)$
Case 3	Cubic	$C = 0.0031\kappa^3 - 0.0566\kappa^2 + 0.3629\kappa - 0.3182$
Case 4	Reversed cubic	$C = -0.0034\kappa^3 + 0.0609\kappa^2 - 0.1842\kappa + 0.1385$

C = vol % ZrO_2 in the coating layer; k = normalized coating thickness