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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 $n \approx 2.65$.

1. Introduction

In the 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-in. of TBC thickness reduces the temperature of the blades by 17–33 °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 Fig. 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].

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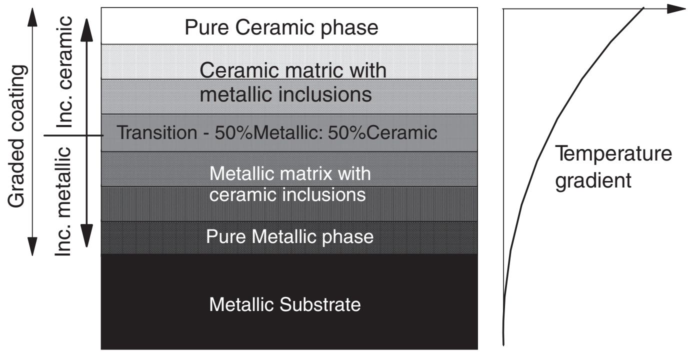

Fig. 1. Schematic of functional graded thermal barrier coating showing high ceramic content at the exposed surface (top) and pure metallic interface next to the substrate and a graded composition in between.

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 Fig. 2 for stress analysis.

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 modelling 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 (QAX4 M).

The disc is subjected to a nodal temperature of 500 K on the top surface of the coating while the bottom of the substrate is maintained at 300 K. 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.