



## Numerical Simulation of Stress in Conventional and Functionally Graded Thermal Barrier Coating YSZ/ NiCrAlY and Comparison with Results of the Nano-Indentation Stress Measurement Method

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**ABSTRACT:** Thermal barrier coatings (TBCs) are one of the most conventionally- used protective materials which are employed as insulation media to save underlying metallic substrate from harmful effects at high temperature services. In this study, a finite element-based numerical method was developed to simulate stress distribution in conventional and functionally graded thermal barrier coatings applied on the Hastelloy-x. Comparisons of simulation model results with experimental results of nano-indentation stress measurement method showed good agreement. The results of simulation showed that in samples after thermal shock without oxidation time (without Thermally Grown Oxide layer-TGO), the average value of the maximum stress is 29 MPa in duplex TBC (interface of top coat /bondcoat), 3.15 MPa in three-layer FG-TBC system (interface of 50% NiCrAlY - 50% YSZ / YSZ) and 1.8 MPa in five-layer FG-TBC system (interface of 25% NiCrAlY- 75% YSZ / YSZ). Also, the stress distribution is more uniform in five-layer FG-TBC system that helps to increase the performance and extend the life time of thermal barrier system.

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### 1- Introduction

In aerospace and turbine industry, achieving higher efficiency for aircraft engines working in high temperatures has always been an important issue to engineers. Higher efficiency means tolerating quite higher elevated temperatures in sensitive components and parts of internal combustion engines. Thermal Barrier Coatings (TBCs) are one of the advantageous materials widely used as insulation materials to protect the underlying metallic structure of a gas turbine blade from thermal damages and to increase its lifetime. The typical TBC is composed of double layers including the bond coat and top coat. The bond coat is MCrAlY (where M=Ni and/or Co) and the ceramic-based topcoat is often made of Yttria-Stabilized Zirconia (YSZ).

Some of the main threats to durability these coatings are as follow: residual stresses stemmed from the technical process, the mismatch between different materials in layers and finally compound and rough character of the TBC/bond-coat boundary. Residual stresses can occur in three places in real conditions of application which are stresses induced during phase transformation, solidification and further contraction of splat droplets from spraying temperature to the room

temperature and the origin of such stress is the difference between the linear Coefficient of Thermal Expansion of two materials at two sides of interfaces in substrate / bond-coat or bond-coat / top-coat. This matter is worse and more hazardous when the coating system is cooling down from high temperatures to ambient temperatures, drastically decreasing the lifetime of the protective layer.

The existing residual stress field in thermal barrier coatings has a strong effect on their performance and plays a vital role in their failure behavior. Thus, the determination of the residual stress field is very important in both scientific and technological perspectives. Various methods have been developed to measure the residual stresses in materials, such as neutron and X-ray tilt, beam bending, hole drilling, layer removal, indentation crack and methods using nano-indentation technique. Among all these methods, the methodologies based on nano-indentation technique have recently attracted extensive research attention. Generally, there are two ways that nano-indentation technique can be used to determine the surface residual stresses. One is by making an indentation in a residual stress field that generates radial cracks at the corner of the indent. The lengths of these cracks are sensitive to the magnitude and sign of the residual

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stress state where the indent is made. By measuring the crack lengths of indentations on stressed surfaces and comparing them with the crack length of indentations on the unstressed surface, the residual stress can be estimated. This approach is usually known as “indentation fracture technique”. The other way is based on the influence of residual stress on the P-h curve of nano-indentation. Residual stresses are found to have significant effects on the contact area, the loading curve and unloading curve of nano-indentation, which may be used for the determination of residual stress. There are many studies about fracture mechanic approach, stress state evolution and failure mechanism of thermal barrier coatings using both analytical and numerical methods.

In this study, a finite element-based numerical method was developed to simulate stress distribution in conventional and functionally graded thermal barrier coatings YSZ/NiCrAlY plasma sprayed on the Hastelloy-x.

### 2- Methodology

Finite element numerical method was used in this study to investigate residual stress in duplex and graded thermal barrier coating. The composition and thickness for the layers are schematically shown in Fig. 1. The selected functionally graded 3-layer TBC system used in this research possess the following layers: Hastelloy-x substrate, a NiCoCrAlY bond-coat (BC), 50% BC + 50% YSZ, Ytria Stabilized Zirconia (YSZ) top-coat. The capability of making accurate and repeated measurements in localized areas at small loads makes a nanoindentation system an ideal tool for fracture toughness study on small samples. In this paper, the indentation fracture technique for measuring residual stress is used. The indentation fracture technique for measuring residual stress is based on the classical fracture mechanics. When a brittle material is indented using a moderate force, a permanent impression is often formed with radially oriented cracks at the indent corner.

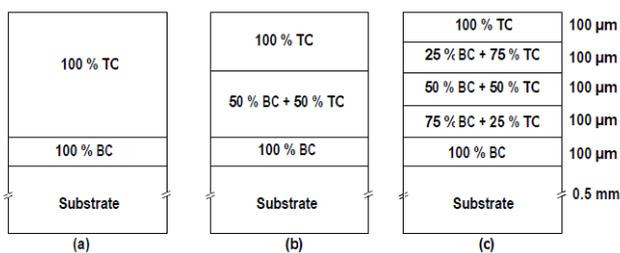


Fig 1: Composition profiles of three types of coatings: (a) duplex, (b) 3-layers, (c) 5-layers

### 3- Discussion and Results

Thermal shock results show that conventional thermal barrier coating is less thermal shock resistant than a functionally graded coating.

Fig. 2 shows the stress distribution contours in (a) conventional TBC, 3-layer Functionally Graded Thermal Barrier Coating (FG-TBC) and 5-layer FG-TBC system after cooling step. Because of the higher value of thermal expansion in a bond coat with respect to the ceramic layer, compressive strength is induced in peak regions and tensile strength in the valley and a slow transition is seen while approaching from peak to valley. In FGM coating, more similarities in thermal expansion of FGM layers lead to better adhesion between layers and less

stress concentration in interfaces which are feeble regions of the coating. This may cause a delay of crack initiation and fatigue crack growth rate in the interface.

As a fabulous point in FGM material, it can be mentioned that the utmost stress in the structure is just about half of conventional TBC structure and for that; it can be recommended as an innovative proposition of elevated temperature material. As a comparison of this work with related studies mentioned in the references, the usage of FG-TBC has been mentioned as a factor for improving corrosion and environmental damages. Also in some of them, the formation of the thermally grown oxide layer was considered as a deteriorating parameter that reduces the lifetime of coating. However, in FGM, this oxide layer was not formed in a specific concentrated place and improve lifetime.

Some investigations focus on the crack growth and fracture mechanism of the interfaces that influence the stress relaxation and also spallation. In this study, the zones with the maximum stress values take account as crack initiation places both in low cycle fatigue and first and second fracture modes.

According to the nano indentation result, Residual stresses play an important role in the determination of fracture toughness by the indentation method. Comparisons of simulation model results with experimental results of nano-indentation stress measurement method showed good agreement.

The results of the simulation showed that in samples after thermal shock without oxidation time (without Thermally Grown Oxide layer-TGO), the average value of the maximum stress is 29 MPa in duplex TBC (interface of top coat / bondcoat), 3.15 MPa in three-layer FG-TBC system (interface of 50% NiCrAlY - 50% YSZ / YSZ) and 1.8 MPa in five-layer FG-TBC system (interface of 25% NiCrAlY- 75% YSZ / YSZ). Also, the stress distribution is more uniform in the five-layer FG-TBC system that helps to increase the performance and extend the lifetime of the thermal barrier system.

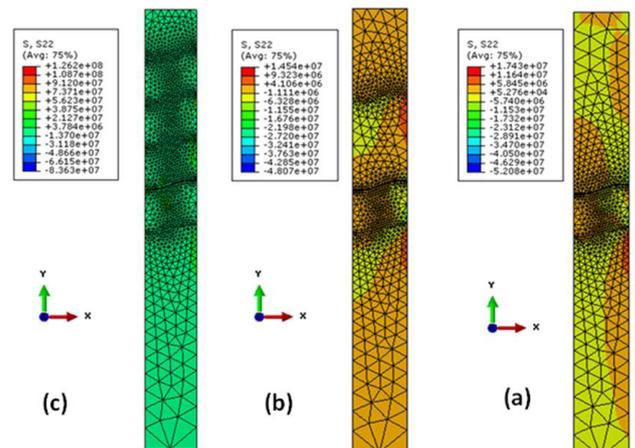


Fig 2. Stress distribution in (a) conventional TBC, (b) 3-layer FG-TBC and (c) 5-layer FG-TBC.

### 4- Conclusion

In this study, a finite element-based numerical method was developed to simulate stress distribution in conventional and functionally graded thermal barrier coatings YSZ/NiCrAlY plasma sprayed on the Hastelloy-x. Comparisons of simulation model results with experimental results of nano-indentation stress measurement method showed good agreement. Thermal

shock results show that conventional thermal barrier coating is less thermal shock resistant than the functionally graded coating. The results of the simulation showed that in samples after thermal shock without oxidation time (without Thermally Grown Oxide layer-TGO), the average value of the maximum stress is 29 MPa in duplex TBC (interface of top coat / bondcoat), 3.15 MPa in three-layer FG-TBC system (interface of 50% NiCrAlY - 50% YSZ / YSZ) and 1.8 MPa in five-layer FG-TBC system (interface of 25% NiCrAlY- 75% YSZ / YSZ). Also, the stress distribution is more uniform in the five-layer FG-TBC system that helps to increase the performance and extend the lifetime of thermal barrier system.

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