

Thermo-Mechanical Analysis of Thermal Barrier Coating System Using Finite Element Method

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Abstract— Currently in the aerospace and other industries it is not very common to use computational analysis to analyze the effects of temperatures on the stresses in thermal barrier coatings, nor are there many life prediction methods for use during a design phase. The effectiveness of TBCs is often determined by trial and error and based on experience. Industry and research would be interested in the thermo-mechanical behavior of high temperature coatings for a variety of reasons. Life prediction modeling methods for coatings would allow for more efficient design of new coatings and develop comprehensive coating selection and design optimization of operating systems with coatings. Today, coatings are often omitted from system structural analysis. Thicknesses and layers of coating systems could be evaluated without as much expensive and time consuming trial and error prototyping and testing. Better analytic tools are essential to design and manufacturing of thermal barrier coatings. The study describes the investigation of the thermo-mechanical effect of varying initial temperature and varying bond coat, top coat and substrate thicknesses of thermal barrier coating system using the finite element method and also the various cases of varying coating thickness are evaluated and the effect of this on residual stresses are analyzed.

Index Terms— Thermal barrier coatings, Residual stress, thickness ratio, and effect of temperatures.

I. INTRODUCTION

A thermal barrier coating is material adhered to a parent material or substrate, most often a metal, to protect the parent metal, increase temperature capability and lengthen the longevity of the parent metal, allowing a part to function in a more challenging environment, perhaps increasing system efficiency or allowing more powerful operation. Thermal barrier coatings are used in aerospace and many industrial applications as a barrier to protect and insulate metal from high temperatures, mechanical wear and corrosive environments in jet engines components and other uses. Today, thermal barrier coatings are typically a two-layer or bi-layer metallic or ceramic system but they can also be applied as a single layer or tri-layer to date. Some materials used in coatings are nickel, aluminum, cobalt, yttrium, platinum and zirconium, just to name a few. Coating systems are designed to best suit the system requirements and be effective while being cost effective. TBC's are also used to perform important functions in mechanical systems such as retaining or recovering structural properties and mass (for rebuilding and repairing parts), eliminating thermal-mechanical fatigue, reducing oxidation, reducing

creep and reducing transient effects in many industries including but not limited to the aerospace, automotive and industrial turbine industries. Over the last century, several different types of coatings have been developed, including dipped, electroplated, vapor deposited and plasma spray coatings. Some of the first thermal barrier coatings were used to allow aircraft engines components to fly higher and faster. Today, advanced thermal barrier coating systems push operating envelopes further and further by reducing component temperatures by over 200°C, further increasing the high temperature capability of current state of the art alloys. In gas turbine engines this allows for engine efficiency improvements, since cooling air that would be supplied to cool components can be reduced and re-routed for propulsion purposes, not to mention higher thrust capability. In diesel engines, the use of thermal barrier coatings on pistons and cylinder heads allows for higher temperature and increased efficiency, which directly translates to higher fuel economy. In a most recent publication, finite element analysis was used to evaluate the cyclic loading and creep within a substrate in evaluating the stress distribution close to the asperity of the TGO/bond coat interface and to examine if only elastic substrate behavior can be assumed during thermal loading. This finite element analysis study showed that the development of early interfacial cracks at bond coat peaks allow for micro-crack formation within the thermal barrier coating and that subsequent TGO growth to a critical thickness results in a tensional zone within the oxide layer. Subsequent TGO thickening increased the area under tension within the TBC and promoted cracking through the coating. There have been many manufacturing methods developed to apply thermal barrier coatings. They can be broken down into two basic types, overlay coatings and diffusion coatings. An overlay coating is a type of coating in which a coating layer (or layers) is physically laid on top of the substrate and adhered often through the use of heat. In a diffusion coating, a coating material is chemically or physically diffused onto the substrate. There are advantages and disadvantages to all methods. Examples of overlay coatings are air plasma spray (APS) coatings, high velocity oxygen fuel (HVOF) coatings, low pressure plasma spray (LPPS) and electroplating and of diffusion coatings are electron beam physical vapor deposition (EB-PVD), physical vapor deposition (PVD) and chemical vapor deposition (CVD). High temperature coatings are used in various industrial applications for increased life from mechanical wear, thermal barrier protection, increased engine performance and low radar observe ability. Today's metallic and plastic coatings have evolved to multilayered gradient coatings better capable of performing as a system together than a single layer or material coating. Surface temperature of metallic components working at high temperatures can be reduced by 100-300°C by using TBCs. This temperature drop is significant considering the

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mechanical properties of the structural materials, such as cobalt or nickel based super alloys. In practice TBCs can extend the maintenance interval and component lifetime. On the other hand TBCs make it possible to improve the process efficiency by increasing the combustion temperature. Continually increasing process temperatures set high requirements for TBC development too. Fig-1 illustrates the effect of TBC on the temperature gradient of a diesel engine piston head.

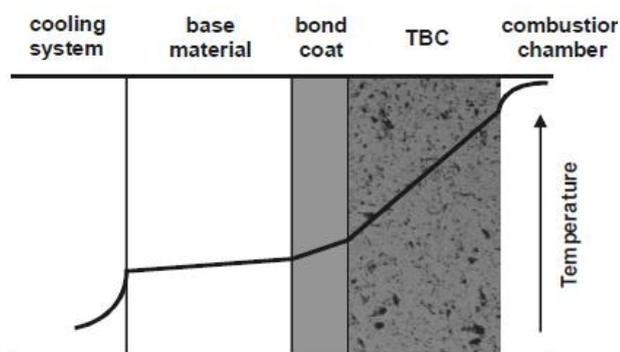


Fig -1: Effect of TBC on temperature gradient of a diesel engine piston head

Thermal barrier coatings (TBCs) have been used since the 60's in thermal protection of gas turbine hot section components. From the early 1980s, many investigators have applied TBCs to the combustion chambers of diesel engines as well to lower heat losses. As a TBC material, most investigators have used zirconia (ZrO_2), partially stabilized by magnesia (MgO), calcia (CaO) or yttria (Y_2O_3), because of its low thermal conductivity, high temperature stability and relatively high coefficient of thermal expansion (CTE) compared to other ceramic materials. Traditional TBCs have been manufactured by atmospheric plasma spraying (APS) using the partially stabilized zirconia in powder form. Recently there has been a good amount of research in studying the residual stresses, thermal stresses and the stress state of certain defined coating applications.

A. Thermal Barrier Coating

Thermal barrier coatings (TBCs) provide thermal resistance to the metallic substrate and reduce the substrate surface temperatures in many power generation systems such as diesel engines, gas turbines and aircraft engines, and hence increase the service life of the components in the systems [1]. Thermal barrier coatings also permit the components in above systems to operate at higher temperatures. Thermal spray is a micro-solidification consolidation process for metals, intermetallic, ceramics, polymers and composites. Thermal spray processing has become an important powder consolidation technique and represents a group of widely used techniques for the production of various overlay protective coatings, which find application as thermal barrier, wear resistant, and corrosion-resistant surface layers, as well as restoration of worn parts [2]. A thermal spray deposit is composed of millions of individually solidified micron-sized particles. Formation of the layers results in due to the fact that accumulation from multitude of individual droplets leads to

characteristic lamellar microstructure which gives rise to unique properties of the deposits [3]. Increasing turbine inlet temperatures while maintaining constant cooling conditions improves gas turbine efficiency. In order to operate at these higher temperatures, the hot gas path components, e.g. the nickel alloy turbine blades, have to be protected by thermal barrier coatings (TBC) [4]. TBC material should have low thermal conductivity and a Co-efficient of thermal expansion close to those of the metallic bond coatings and substrates. It should also have long-term phase stability at whole service temperature range and adequate corrosion resistance against impurities present in the process (such as Na, S, and V). TBC material should have a low sintering tendency to maintain the strain tolerant microstructure. Sufficient mechanical properties are also needed (bond strength, erosion resistance). Various materials, mostly oxide ceramics, have been studied as TBC candidates. Partially stabilized zirconia is the most used TBC material, and $8Y_2O_3-ZrO_2$ has been the industrial standard composition for years.

B. Structure of TBC

The thermal barrier coating system consists of a thermal insulation layer and bond coating. The typical thickness of a TBC layer is 150-500 μm and 150-250 μm for bond coating as shown in Fig-2. The properties required from a TBC layer are low thermal conductivity, high stain tolerance, and long-term stability at high temperatures, good erosion and hot corrosion resistance. The lamellar and porous microstructure of plasma sprayed coating is advantageous if considering low thermal conductivity and strain tolerance, but erosion and hot corrosion properties can be moderate. APS TBC is mechanically bonded to the bond coat, whereas chemical bonding is formed in EB-PVD coating (due to thermally grown oxide (TGO)). The columnar microstructure of EB-PVD coating is extremely strain tolerant, but its thermal conductivity is higher than that of plasma sprayed coating [6].

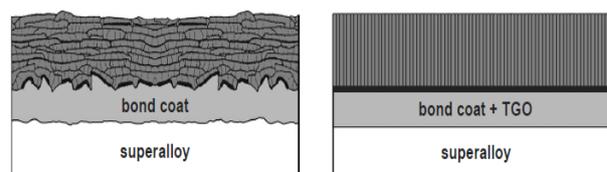


Fig -2: TBC Structure

C. Applications of TBC

Efficiency and performance of advanced gas turbines for aircraft and land-based applications can be increased considerably if the gas temperatures in the high-pressure turbine are raised. Application of thermal barrier coatings on super alloy turbine blades allows such an increase of gas temperature owing to their thermal insulation properties and correspondingly lowered temperature of the metal components [7]. In the last decades the efficiency of gas turbines has improved greatly. State-of-the-art gas turbines are reaching 40% efficiency and combined cycle efficiencies as high as 60% are now achievable. This improved efficiency has been made possible by the increase of combustion temperatures mainly achieved through using various cooling techniques, TBCs and modern super alloy materials. Turbine inlet temperatures in stationary gas turbines are normally over 1100°C, in modern turbines close to 1500°C and in aero engines even higher. TBCs are widely used in gas turbine hot section components such as burners, transition ducts, shrouds,

blades and vanes. Mean component surface temperatures in diesel engines are much lower than in gas turbines. However, in a diesel engine almost 30 % of the fuel energy is wasted due to heat losses through combustion chamber components. For that reason, lots of research activity has focused on applying TBCs to diesel engines.

D. Drawbacks of TBC

Several studies have shown that, as the thickness of plasma sprayed TBCs increases, their reliability deteriorates, especially when exposed to thermal cycling. So only increasing the coating thickness, without modifying the coating microstructure, will not produce strain tolerant thick thermal barrier coatings. With thicker coatings the problem is with residual stresses, originating in the coating manufacturing, are emphasized. When the coating thickness is increased by introducing more spray passes, the substrate and coating temperature rises step by step unless adequate cooling is used. This temperature increase and reduces the cooling rate of individual splats and leads to better contact of lamellae and decreased number of vertical micro cracks in lamellae. These are the mechanisms through which the tensile (quenching) stresses impact the coating. After the spraying, when the component cools down, compressive (thermal) stress is induced to TBC ($CTETBC < CTESUBSTRATE$). The final residual stress state of the coating is a sum of all the stress components, in this case mainly the quenching and thermal stresses. The formation of residual stresses (or strains) in plasma sprayed coatings and TBCs has been widely studied [8]. It has been reported that residual stresses in plasma sprayed TBCs can be tensile or compressive and can be affected by controlling the substrate temperature during spraying [9]. In the same studies it was also reported that the stress state change in high temperature exposure is towards compression. Considering the combined effect of residual stresses and the stresses caused by thermal cycling loads on TBCs, the residual stresses, as low as possible, should be beneficial. The bond strength or the intrinsic cohesion of the coating is also lowered in thicker coatings [10]. All these drawbacks of traditionally prepared TTBCs, residual stresses, low bond strength and low strain tolerance, combine to lower the reliability of the coating. With increased coating thickness the temperature drop through the coating increases at service temperatures and at the same time the dimensional mismatch of the coating surface and bond coat interface becomes higher, due to low strain tolerance. This dynamic induces more stresses into the structure and increases total strain energy available for crack initiation. Typically with TTBCs the crack is initiated near the bond coat interface leading to macroscopic coating delamination. In practice the coating failure mechanism is not so simple: varying thermal loads due to thermal cycling, thermal shocks and local hot spots make the situation even more difficult.

II. ANSYS AN OVERVIEW

The problem consists of calculating temperatures and stresses in coating-substrate systems. Although FEA was originally developed for and used in automotive, aerospace and nuclear industries, today it is also used for a wide range of subjects such as oceanic wave analysis and weather prediction models and can be used in any physical mathematic model use. In this case we will build a model of the coating system using a simplified cylindrical and plate structure to represent a piece

of metal with a coating and assign material properties and physical and thermal and mechanical boundary conditions. In our model using the finite element method, the final thermal stresses of the system are determined by Hooke's Law, $\sigma = E\varepsilon$. The thermal stress in the coating is determined by the following equation, $\sigma_c = E_c(\alpha_s - \alpha_c)\Delta T$. The goal of the study is to investigate how residual stresses are affected with varying physical parameters. We will analyze the effect of varying coating thicknesses and substrate thicknesses of two material coating systems. Coating thickness to substrate thickness ratios will vary from 2% to 10%, in 2% increments, along with variation in initial and final temperatures. The effect due to cooling residual stresses will be studied and compared.

A. Element Plane42 Description Used In Analysis

PLANE42 is used for 2-D modeling of solid structures. The element can be used either as a plane element (plane stress or plane strain) or as an axisymmetric element. The element is defined by four nodes having two degrees of freedom at each node: translations in the nodal x and y directions. The element has plasticity, creep, swelling, stress stiffening, large deflection, and large strain capabilities.

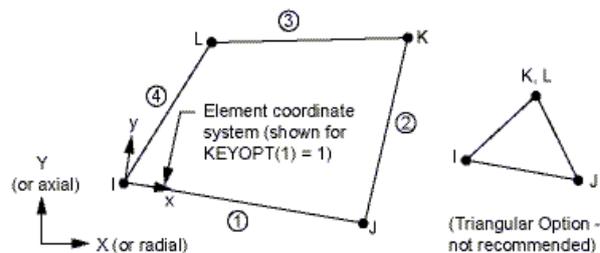


Fig -3: PLANE42 Geometry

The geometry, node locations, and the coordinate system for this element are shown in Fig-3 PLANE42 Geometry. The element input data includes four nodes, a thickness (for the plane stress option only) and the orthotropic material properties. Orthotropic material directions correspond to the element coordinate directions. The element coordinate system orientation is as described in Coordinate Systems. Element loads are described in Node and Element Loads. Pressures may be input as surface loads on the element faces as shown by the circled numbers on Fig-3 PLANE42 Geometry. Positive pressures act into the element. Temperatures and fluencies may be input as element body loads at the nodes. The node I temperature T (I) defaults to TUNIF. If all other temperatures are unspecified, they default to T (I). For any other input pattern, unspecified temperatures default to

TUNIF. Similar defaults occurs for influence except that zero is used instead of TUNIF.

B. Materials and their Properties

The material properties of the two layered ANSYS model vary with temperature.

Table -1: Axis-symmetric material properties

	T (°C)	E (GPa)	α (e-6 / K)	k (W/mK)
Top coat: ZrO2	25	53	7.2	1.5
	400	42	9.4	1.2
	800	46	16	1.2
Bond coat: NiCoCrAlY	25	225	14	4.3
	400	186	24	6.4
	800	147	47	10.2
Substrate: Ni-alloy	25	200	14.4	11.5
	400	179	14.4	17.5
	800	149	14.4	23.8

T- Temperature, α - CTE (Coefficient of thermal expansion), E- elastic modulus, k- thermal conductivity.

C. Thermal Barrier Coating Analysis

The FEA model consists of varying thicknesses of a two dimensional axis-symmetric model with three materials such as substrate, the bond coat and the top coat as shown in figure. Altogether represents a thin cylindrical test piece and the thickness of the substrate is modeled to be 0.001 meters thick, that may perhaps represent a coated heat shield in an aerospace application. The two layered coating is made to represent 2 to 10% in total thickness with incremental of 2%. Figure 4 and 5 shows a typical meshed model with elements and boundary conditions.

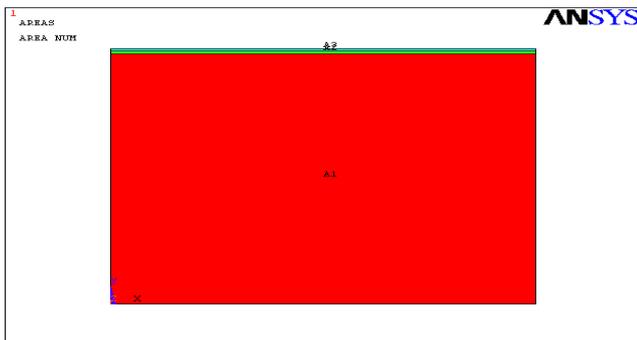


Fig. 4: FEA model displaying the different areas

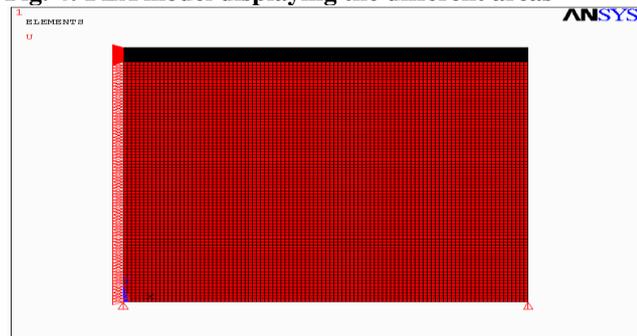


Fig. 5 FEA model with mesh and boundary conditions

D. Two Layer Comparison

The model is assumed to be a perfect elastic body without plastic deformation during analysis. A two-dimensional axis-symmetric model is used and the area at the coating/substrate interface was refined manually to improve accuracy of calculation. Fig-6 shows a nickel-alloy substrate of 0.010 m thickness, with a NiCoCrAlY bond coat of 0.002m and a ZrO₂ top coat of 0.004 m. These coating thicknesses are fairly consistent to thickness of coatings applied to parts in industry. The two layered coating is made to represent 2% to

10% in total thickness with incremental of 2%.The bond thickness is kept to a maximum of 0.002 m, which is close to nominal values used in actual bond coat thickness applications. So to all analyzed systems, the final residual stresses are only generated due to the cooling of the coating specimens from higher temperature to room temperature (i.e., 25°C). Fig-6 shows a typical FEA areas representing substrate, bond coat and top coat and meshed model with elements.

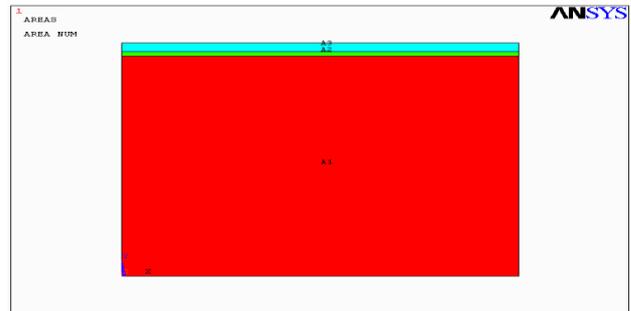


Fig -6: FEA areas representing substrate, bond coat and top coat

III. RESULTS AND DISCUSSIONS

A. FEM Model

Due to symmetry boundary conditions, the functional representation is a thin cylinder, as noted in Figure 7. A 12.5 mm radius specimen was modeled with a substrate thickness of 0.010 m. The coating thickness of this model was set to be 10% of the substrate thickness. The coating material properties were set to initial temperature of 1020° C to 20° C. Upon running the model with the set boundary conditions, radial, axial and shear stresses throughout the specimen are plotted below in Figures 7 to 9.

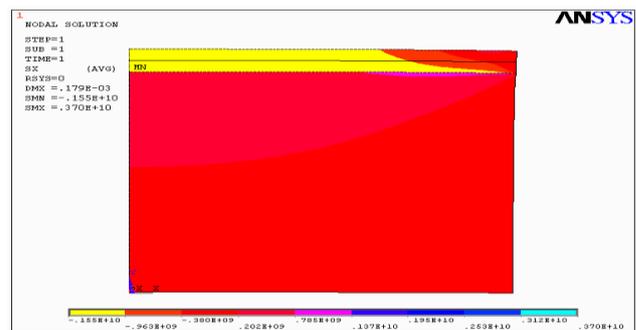


Fig.7: Radial stress of 12.5 mm radius piece with 0.010 m thick substrate

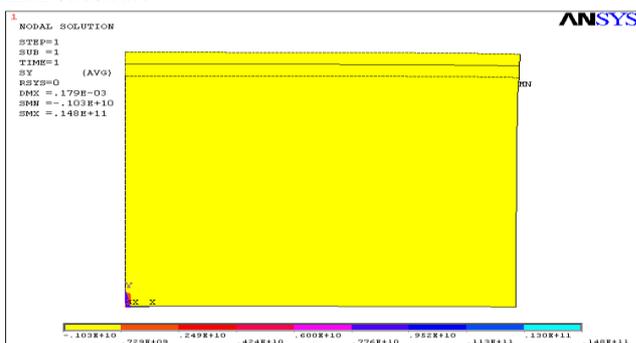


Fig- 8: Axial Stress of 12.5 mm radius piece with 0.010 m thick substrate

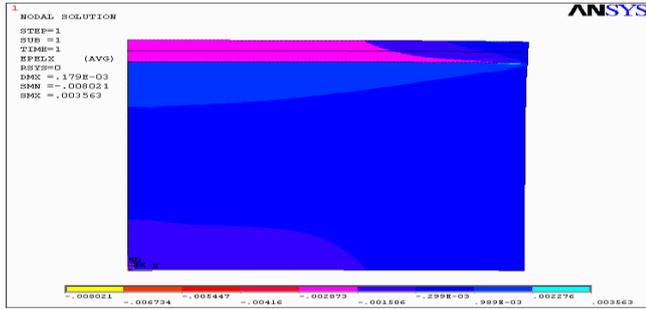


Fig- 9: Shear stress of 12.5 mm radius piece with 0.010 m thick substrate

In Figures 10 and 11 the radial (x-direction) and axial (y-direction) displacements due to thermal growths are plotted. Due to the difference in thermal expansion coefficients, visually it can be seen that the coating is growing or expanding less (or contracting less) due to thermal mismatch.

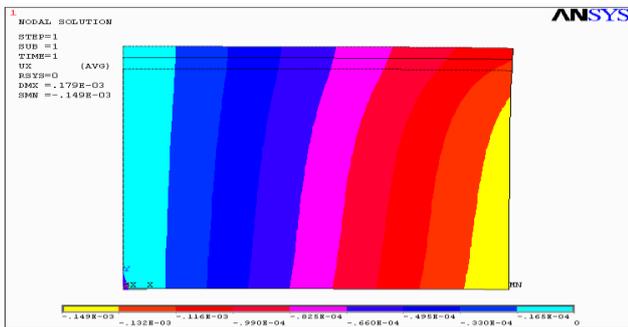


Fig- 10: Radial displacement of 12.5 mm radius piece with 0.010 m thick substrate

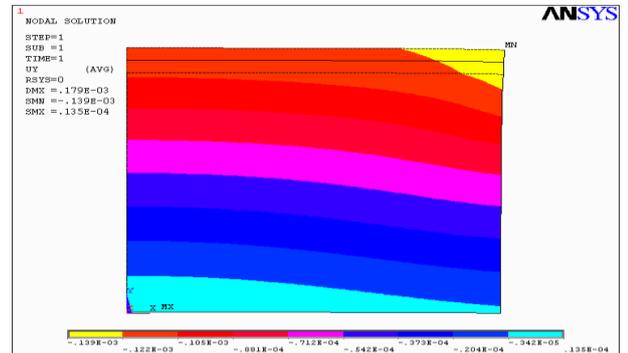


Fig- 11: Axial Displacement of 12.5 mm radius piece with 0.010 m thick substrate

By defining a path in ANSYS we are able to plot the stresses through the centerline of the cylindrical FEM, for example Radial stress through a 12.5 mm radius model with 0.010 m thick substrate which is plotted below in Figure 12.

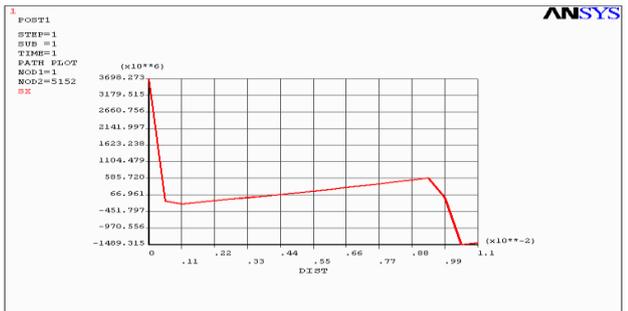


Fig-12: Radial stress through 12.5 mm radius model with 0.010 m thick substrate

B. Two Layer Coating with Varying Temperatures

In the following section, a two layer coating modeled using FEA with material properties from Table 1 is made to represent 2 to 10% in total thickness with incremental of 2%. The bond thickness is kept to a maximum of 0.002 m, which is close to nominal values used in actual bond coat thickness applications. All of the following cases are run with residual stresses from 1000° C to 25° C to represent Air Plasma Spray coating temperatures for example, cooled to room temperatures. So to all analyzed systems, the final residual stresses are only generated due to the cooling of the coating specimens from higher temperature to room temperature (i.e., 25°C).

C. 2% Coating Thickness

The following are the two percent coating thickness with varying temperature of 1000° C to 25° C. With the thinnest of the coatings analyzed here, we observed the smallest local stress concentration area in which the radial stress is dispersed throughout the coating and the substrate in the upper right hand corner shown below in figure. Note that the majority of the substrate has positive stress in tension, while the coating exhibits negative stress in compression.

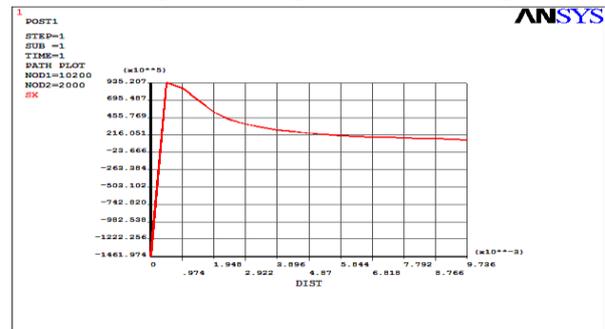


Fig- 13: Radial Stress through center of 2% t_c/t_s specimen, from 1000°C-25°C

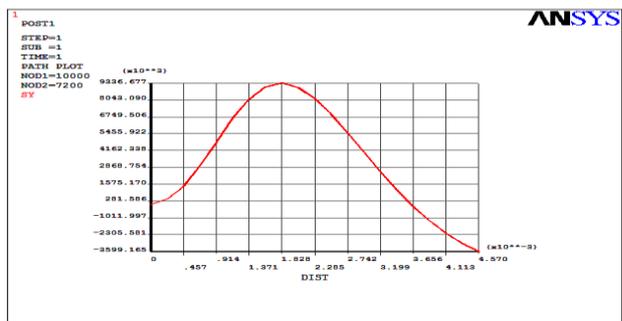


Fig- 14: Axial Stress through center of 2% t_c/t_s specimen, from 1000°C-25°C

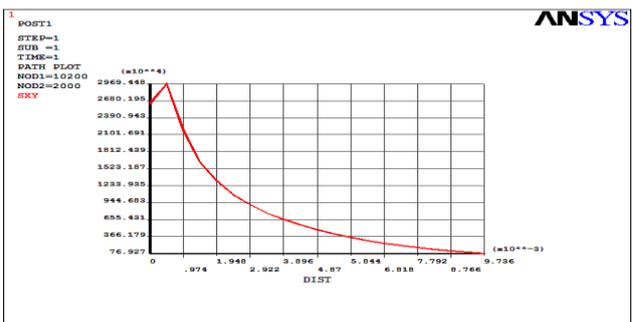


Fig-15: Shear Stress through center of 2% t_c/t_s specimen, from 1000°C-25°C

D. 10% Coating Thickness

The following are the 10% coating thickness with varying temperature of 1000 °C to 25 °C. The areas under stress concentrations in the radial, axial and shear directions are all increased with the increase in coating thickness. This pattern is seen increasing proportionately in this study as the coating thickness increase up to 10% from 2% coating thickness. The maximum residual radial stress, axial stress, shear stress in the substrate has doubled as compared to previous coating thickness.

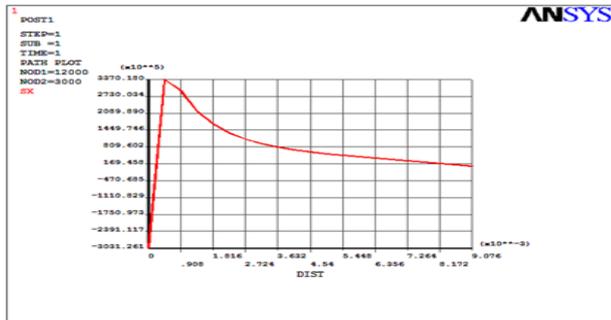


Fig- 16: Radial Stress through center of 10% t_c/t_s specimen, from 1000°C-25°C

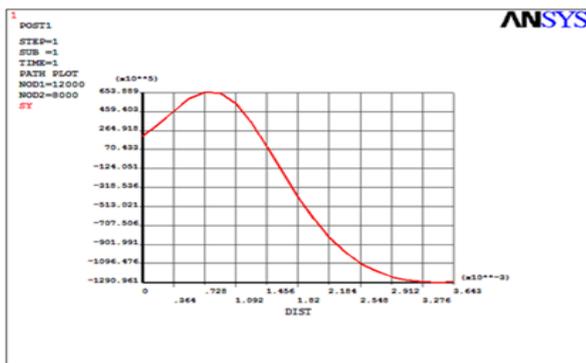


Fig-17: Axial Stress through center of 10% t_c/t_s specimen, from 1000°C-25°C

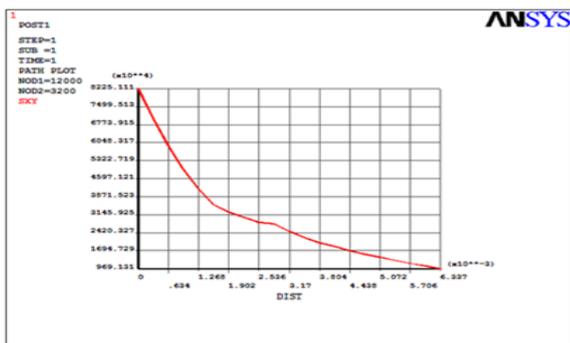


Fig- 18: Shear Stress through center of 10% t_c/t_s specimen, from 1000°C-25°C

From the above graphs from 2% to 10% coating thickness, we observed that as the coating thickness increases the compressive radial stress decreases and tensile radial stress increases gradually with the increase of radius and in the axial stress, the tensile stress is decreased abruptly and compressive stress increases with the increase of specimen radius, whereas shear stress will always tends to be tensile.

E. Effect of Varying Initial Temperature in a Two Layer Coating

The effect of increasing the difference in initial and final temperature results in higher tensile stresses in the substrate and higher compressive stresses in the coating which would lead to a shorter life of the coating, if it was able to adhere and remain coated at all. While the substrate, bond coat are the same in all above analyses and the initial temperature varies in approximately 300°C increments, from 427°C to 1000°C because the used coating specimens in the present investigation are relatively small, all specimens are assumed to be stress free at the temperature 427°C (i.e., reference temperature), at which the spraying process is assumed to be end. So to all analyzed systems, the final residual stresses are only generated due to the cooling of the coating specimens from reference temperature to room temperature (i.e., 25°C). The concluding results are summarized in following section. This relationship is to be expected as a simple estimation of stresses due to thermal growth can be estimated

$$\sigma = E\alpha (T_f - T_i)$$

by a variation of Hooke's Law:

The compressive radial stress decreased and changed to tensile stress gradually with the increase of radius. The largest tensile stress, occurred near the edge of the interface. Because of the large tensile stress, the interfacial cracks can initiate at the free edge and propagate radially toward the center region causing a progressive delamination.

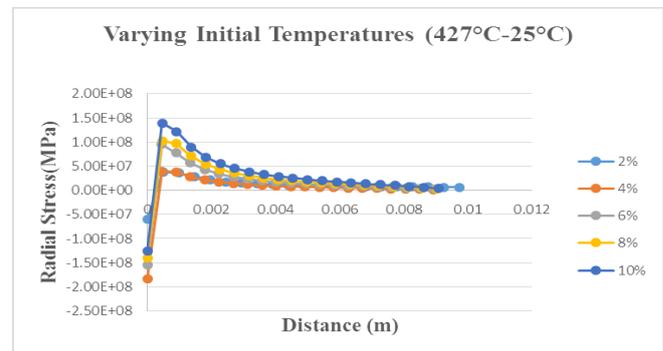


Fig -19: Effect of Radial Stresses varying with initial temperature, 427°C-25°C

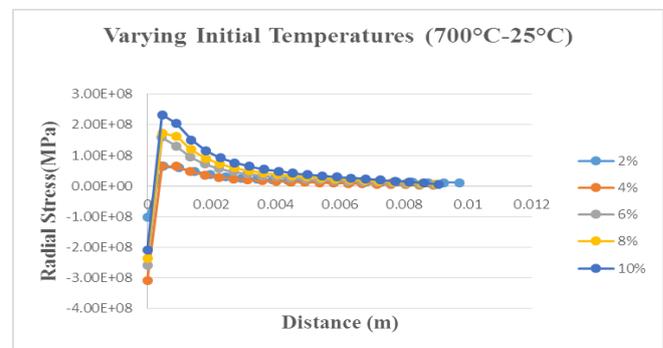


Fig -20: Effect of Radial Stresses varying with initial temperature, 700°C-25°C

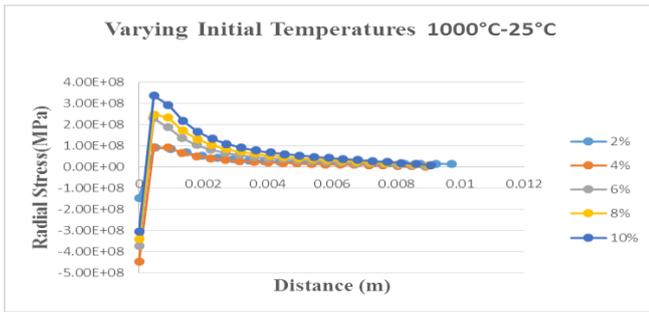


Fig -21: Effect of Radial Stresses varying with initial temperature, 1000°C-25°C

To the axial stress, the tensile stress occurred near the edge of the specimen and it decreased abruptly and changed to compressive stress with the increase of specimen radius. The largest compressive stress, occurred at the edge of the interface. Generally, the large stress concentration near the edge of interface and this large compressive stress at the edge of the interface may cause the spallation and the buckling of the coating.

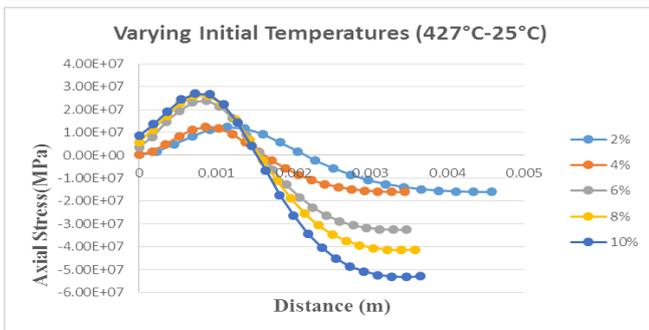


Fig -22: Effect of Axial Stresses varying with initial temperature, 427°C-25°C

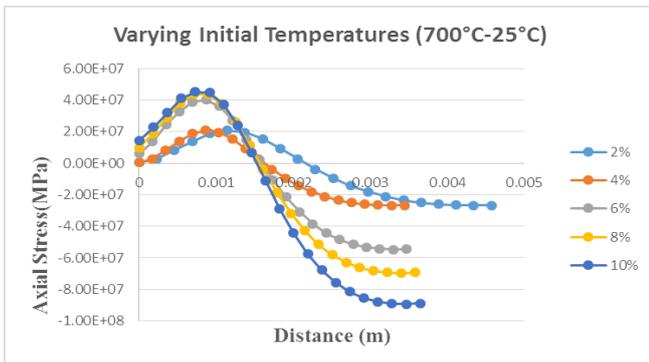


Fig -23: Effect of Axial Stresses varying with initial temperature, 700°C-25°C

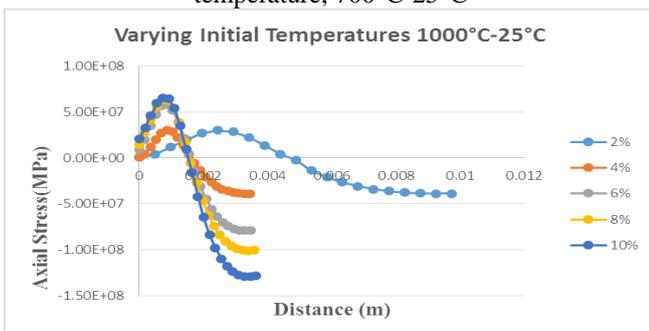


Fig -24: Effect of Axial Stresses varying with initial temperature, 1000°C-25°C

The shear stress is always tensile and the largest stress, occurred at the edge of the interface. This large tensile stress can contribute either shear or mixed modes of failure of coating. It also can be seen that the ratio t_c/t_s can only changed the stress level and cannot change the pattern of stress distribution.

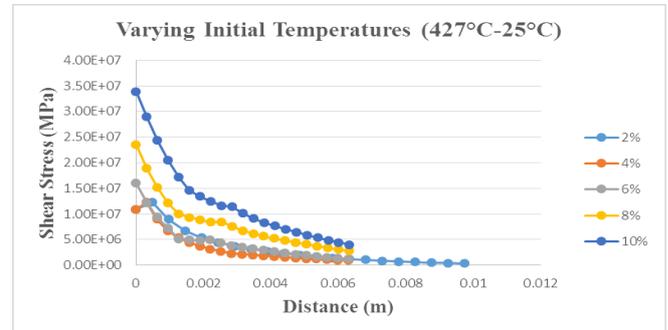


Fig -25: Effect of Shear Stresses varying with initial temperature, 427°C-25°C

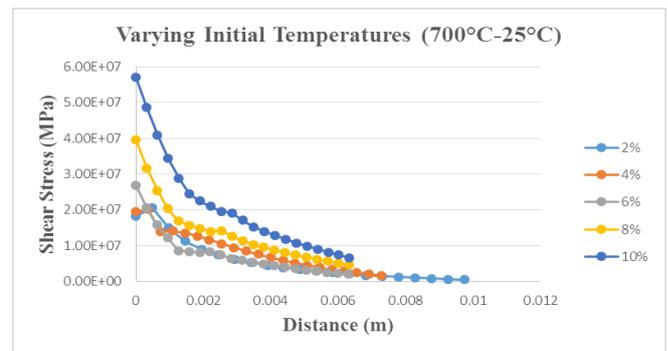


Fig -26: Effect of Shear Stresses varying with initial temperature, 700°C-25°C

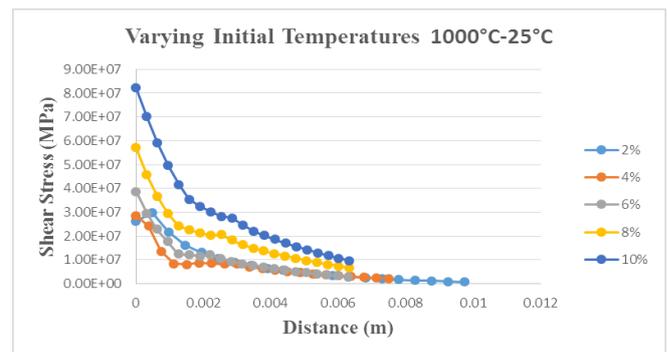


Fig -27: Effect of Shear Stresses varying with initial temperature, 1000°C-25°C.

IV. ONCLUSION

Using the FEM, we explored several parameters, such as variances in coating thickness and temperature, while keeping certain other parameters constant. In both cases of these, we kept the substrate thickness and geometric boundary conditions constant while varying initial temperature in one study and coating thickness in another study. This allowed us to understand the affect of changing these parameters on the

coating and substrate system. Increasing the difference in initial and final cooled temperatures resulted in an increase in the residual stresses in the coating and substrate. Therefore, many of today's methods of coating, such as plasma spray coating which allow for metal to be adhered to metal of any shape and form in effect create the residual stresses. Some work could be done to evaluate if there are ways of layering coatings at lower temperatures or decreasing the final temperature at the point of contact with the substrate to perhaps lower residual stresses and allow for thicker coatings to be applied. We found that while increasing coating thickness with varying initial temperature, the residual tensile stress in the substrate material increased proportionately while the residual compressive stress in the coating actually decrease slightly, towards the top surface of the coating. These stresses are local high stress concentrations that occur during the cooling phase due to differences in elasticity and coefficients of thermal expansion, which if not accounted for, worked around and designed properly could lead to lack of adherence of a coating, early spallation of a coating and decreased coating life. Short of new materials being introduced and metal cooling techniques that can be used, thermal barrier coatings are the next step in furthering the life and operating range of metals and materials, including but not limited to ceramic coatings in combustion engines and any operating system that involves heat or mechanical wear. The computational modeling of coatings for stress, life and wear will be next step in increasing productivity in realm of thermal barrier coating design, manufacturing and use.

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