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Residual Stresses in Thermal Barrier Coatings for a Cu-8Cr-4Nb Substrate System

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RESIDUAL STRESSES IN THERMAL BARRIER COATINGS FOR A Cu-8Cr-4Nb SUBSTRATE SYSTEM

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ABSTRACT

Analytical calculations were conducted to determine the thermal stresses developed in a coated copper-based alloy, Cu-8(at.%)Cr-4%Nb (designated as GRCop-84), after plasma spraying and during heat-up in a simulated rocket engine environment. Finite element analyses were conducted for two coating systems consisting of a metallic top coat, a pure copper bond coat and the GRCop-84. The through thickness temperature variations were determined as a function of coating thickness for two metallic coatings, a Ni-17(wt%)Cr-6%Al-0.5%Y alloy and a Ni-50(at.%)Al alloy. The residual stresses after low-pressure plasma spraying of the NiCrAlY and NiAl coatings on GRCop-84 substrate were also evaluated. These analyses took into consideration a 50.8 μm copper bond coat and the effects of an interface coating roughness. The through the thickness thermal stresses developed in coated liners were also calculated after 15 minutes of exposure in a rocket environment with and without an interfacial roughness.

INTRODUCTION

Since 1998, various studies have been conducted to significantly improve the performance of rocket engines and to reduce the weight of specific engine components under NASA's third generation Reusable Launch Vehicle (RLV) program [1]. Efforts have focused on reducing the weight of the thrust chamber as well as improving the component life at higher operating gas temperatures. One candidate material under consideration for the thrust chamber component is a NASA-developed copper-based alloy known as GRCop-84 (Cu-8(at.%)Cr-4Nb) [2] that is being considered as a replacement for the NARloy-Z alloy currently used in various thrust chambers [3]. Table I compares the material properties of extruded GRCop-84 with those for NARloy-Z at 538 °C [2–3]. As shown in Table I, the GRCop-84 has a lower density than the NARloy-Z, higher strength at elevated temperatures, and longer fatigue and creep life. These properties suggest the advantages of GRCop-84 as a liner material to achieve longer component life.

Although, GRCop-84 shows an improvement in its high temperature properties compared to the current liner material, a coating is still desirable to further increase the operating temperature by protecting the substrate hot-wall from oxidation and blanching. Various metallic and ceramic coatings are being considered as coating materials for the GRCop-84 liner. Two metallic top overlay coatings will be considered in this paper: a nickel-based alloy with Ni-17(wt.%) Cr-6Al-0.5%Y used primarily as a bond coat for ceramic thermal barrier coatings on superalloys [4] and a Ni50(at.%)-Al alloy. Furthermore, a 50.8 μm copper bond coat layer is also applied between the two top coats and the GRCop-84 substrate to promote bonding. The NiCrAlY coating has been successfully used with NARloy-Z liners and was applied to the GRCop-84 substrate for comparison. The NiAl intermetallic alloy is of interest as a coating due to its ability to form a protective Al_2O_3 scale on the surface while maintaining the mechanical properties of the underlying substrate [5]. Table II summarizes key material properties for the two coating systems at 900 °C. The NiCrAlY has a lower thermal conductivity but a higher coefficient of thermal expansion (CTE) compared to NiAl. The NiAl shows higher yield and tensile strengths, but lower creep resistance, compared to NiCrAlY.

Table I. Comparison of the 538 °C Material Properties of GRCop-84 and NARloy-Z.

Material	Density (kg/m^3)	Thermal Conductivity (W/m °C)	Yield Strength (MPa)	Tensile Strength (MPa)	CTE $\times 10^{-6}$ (1/°C)	Fatigue Life at 0.7%$\Delta\varepsilon_{total}$ (Cycles)	Creep Life at 500 °C σ = 84 MPa (h)
NARloy-Z (wrought)	9130	351	90	117	22	3,601	12
GRCop-84 (extruded)	8756	290	120	155	20	10,990	250

Table II. Material Properties of NiAl and NiCrAlY at 900 °C

Material	Density (kg/m^3)	Thermal Conductivity (W/m °C)	Yield Strength (MPa)	Tensile Strength (MPa)	Elastic Modulus (GPa)	CTE $\times 10^{-6}$ (1/°C)	Time to 1% Strain at 900 °C σ = 40 MPa (h)
NiCrAlY	5500	13	49	69	135	18	32
NiAl	5900	80	78	141	157	15	0.3

For the combustor liner design, the variation of the substrate temperature with coating thickness is first determined using the finite element method for the two top coats, under typical steady-state thermal conditions expected in the rocket chamber liner. Furthermore, the residual stresses built up after cool down from the plasma spraying conditions are determined in the coatings and the substrate. A precise determination of these residual stresses after processing is key to understanding the behavior of these coatings after cool down from the processing temperature, as well as the response to subsequent thermo-mechanical loads. The effect of the surface roughness of the interfaces on the residual stresses is also determined for the two coatings. The surfaces of the substrate materials are usually grit blasted prior to the application of the coating in order to improve the coating adherence through a mechanical interlock. The presence of this surface roughness was shown to introduce a complex stress field that can lead to cracking along the coating-substrate interface and ultimately to the spallation of the coating [6–9]. Hence, the perturbations of the residual stress distribution with the presence of interfacial asperities are also delineated for the two coatings in this investigation. Finally, the thermal stresses developed in a simulated engine environment are determined with and without interfacial roughness.

HEAT-TRANSFER ANALYSIS

The steady-state temperature distributions through the thickness of coated GRCop-84 substrates were determined as a function of the coating thickness using the finite element method. The applied thermal boundary conditions simulating the gas temperature conditions in the rocket chamber are shown in Fig. 1(a). The hot gases are estimated to reach temperatures as high as 3,277 °C. The liquid hydrogen fuel provides the back face cooling for the liner. The variations of the temperatures along the various interfaces as well as the hot and cold outer walls at steady-state conditions are shown in Figs. 2(a) and (b) for the NiCrAlY and NiAl coatings, respectively. It is noted that similar thermal analyses were conducted by Holmes and co-workers on a copper alloy

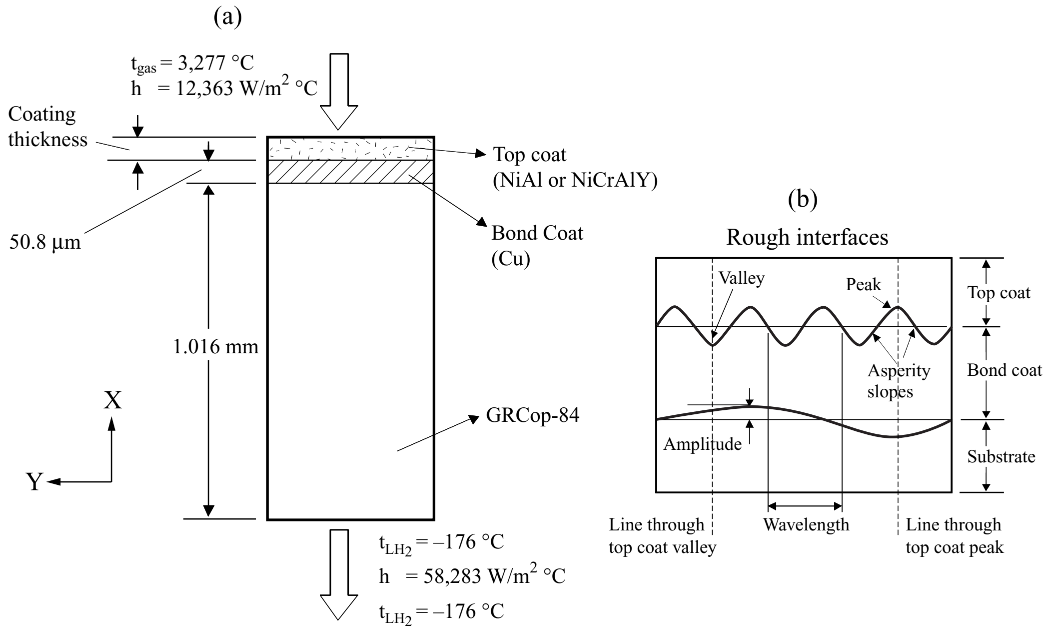

Fig. 1.—(a) Geometry and convective heat transfer boundary conditions, (b) rough interfaces.

coated only with NiCrAlY at lower hot gas temperatures [10]. The bond coat material for both coatings is a 50.8 µm pure Cu. The hot outer surface temperature of the NiCrAlY top coat increases rapidly for higher thicknesses, starting at 593 °C for a 25.4 µm coating thickness to 993 °C for a 228.6 µm coating thickness. The temperature of the GRCop-84 along the GRCop/Cu interface decreases from 513 to 411 °C for coating thicknesses of 25.4 µm and 228.6 µm, respectively. The resulting temperature difference observed through the thickness of the coating increases from 50 to 444 °C for a coating thickness of 25.4 and 228.6 µm, respectively. The variation in temperature of the GRCop-84 with the NiAl top coat is not as pronounced as the NiCrAlY top coat due to its higher thermal conductivity. The effect of the high NiAl thermal conductivity is to reduce the hot wall coating temperature with a corresponding reduction in the temperature difference through the thickness of the coating. Furthermore, the NiAl top coat increases slightly the temperature along the GRCop-84/Cu interface as well as the GRCop cold wall temperature, as shown in Fig. 2(b), compared to the NiCrAlY top coat. For example, at a coating thickness of 101.6 µm, the overall temperature difference through the thickness for the NiAl coating is 164 °C compared to 400 °C for the NiCrAlY, (a factor of 2). In addition, the NiAl hot surface coating temperature reaches only 564 °C compared to the 758 °C for the NiCrAlY coating. The temperature difference through the coating is only 43 °C for the NiAl compared to 283 °C for the NiCrAlY, for the same coating thickness of 101.6 µm.

COOL DOWN RESIDUAL STRESSES

The residual stresses developed in the coated GRCop-84 play an important role in the production and performance of the coatings. Their precise determination is essential to study the coating behavior upon cool down from the processing temperatures and its subsequent behavior under the thermo-mechanical loading observed in the rocket chamber environment. The residual stresses were determined upon cool down from plasma spraying using the finite element method. As the temperature of the coated substrate is dropped to room temperature, thermal residual stresses are developed in the various layers. Two-dimensional eight-node quadratic finite element meshes were generated for flat interfaces as well as for rough interfaces to model the various layers shown in Fig. 1(b). It should be noted that edge effects are not considered in the present

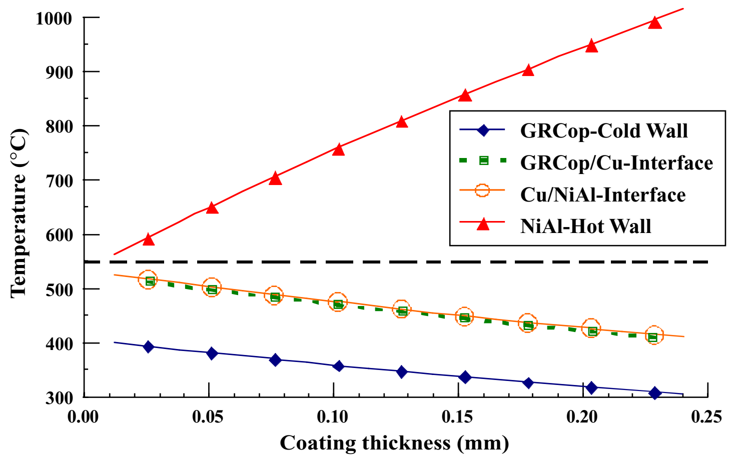

Fig. 2. (a)—Temperatures at the various interfaces as a function of the NiCrAlY top coat thickness.

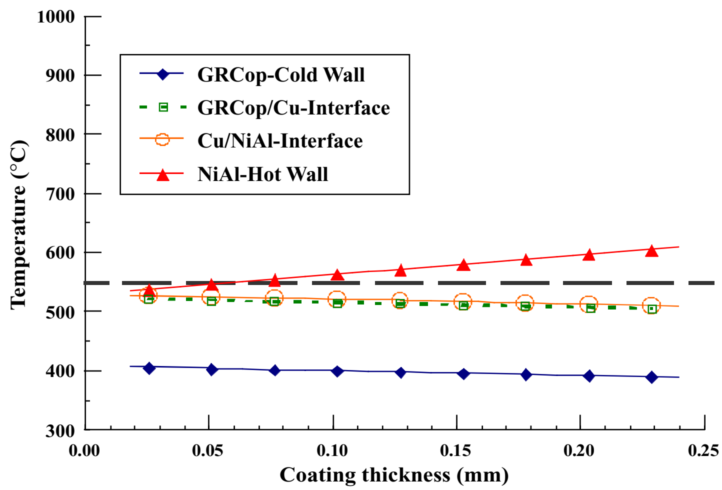

Fig. 2. (b)—Temperatures at the various interfaces as a function of the NiAl top coat thickness.

analysis for simplicity. The assumed bond coat/top coat wavelength is 48 µm with a 10 µm amplitude, and the substrate/bond coat roughness is assumed to have a 152 µm wavelength and a 6 µm amplitude. These values were estimated from microstructures of coated substrates. The stresses in each layer in the Y-direction, corresponding to Fig. 1(a) are shown in Table III assuming flat interfaces for three top coat thicknesses of 25.4, 101.6, and 228.6 µm, for both alloy top coats. The assumed bond coat thickness for both top coats was 50.8 µm thick pure copper deposited on a 1.016 mm thick GRCop-84 substrate. The stress distribution is constant in each layer. The stresses in the coating in the Y-direction are compressive and decrease with increasing coating thickness. The Y-stresses in the substrate are tensile and increase with increasing coating thickness. The stress in the copper bond coat is almost independent of the top coat composition and thickness. The magnitude of the stresses in the NiCrAlY is about a factor of 2~3 times the stress magnitude in the NiAl. For flat interfaces, the stresses in the X-direction are zero.

Table III. Variation of the Y-direction stress with coating thickness for flat interfaces.

Coating Thickness (μm)	NiAl Coating Substrate Stress σ_{yy} (MPa)	NiAl Coating Bond Coat Stress σ_{yy} (MPa)	NiAl Coating Top Coat Stress σ_{yy} (MPa)	NiCrAlY Coating Substrate Stress σ_{yy} (MPa)	NiCrAlY Coating Bond Coat Stress σ_{yy} (MPa)	NiCrAlY Coating Top Coat Stress σ_{yy} (MPa)
25.4	0.2	30	–53	2	31	–148
101.6	3	29	–47	11	32	–121
228.6	7	29	–39	19	32	–93

When the interface roughness is taken into consideration, the stresses near the interfaces are perturbed as shown in Figs. 3 and 4 for the NiAl and NiCrAlY top coats, respectively where the coating thickness was assumed to be 101.6 μm. The stress distributions along the thickness through a valley and a peak corresponding to Fig. 1(b), of the bond coat/top coat interface are shown as a function of the normalized distance, x/t, where t is the total substrate and coatings thickness, i.e., t = 1.1684 mm. Due to the shallowness of the interface roughness of substrate/bond coat, no appreciable stress perturbation was calculated. Along the valley of the bond coat/top coat, the stress perturbation is also minimal. But along the peak, there is a sharp decrease in the stress in the top coat associated with a corresponding increase in stress in the bond coat, but limited to a small region of less than 25 μm. The presence of the roughness also introduces X-direction stresses, but of relatively small magnitude on the order of ±5 and ±15 MPa for the NiAl and the NiCrAlY coatings, respectively. The tensile stresses occur in the valley of the top coat and the compressive stresses occur at the peak of the top coat. Furthermore, the presence of the rough interfaces also introduces a shear stress along the slopes of the asperities with magnitudes of ±38 and ±77 MPa along the bond coat/top coat interfaces for the NiAl and NiCrAlY coatings, respectively, (see Fig. 1(b)).

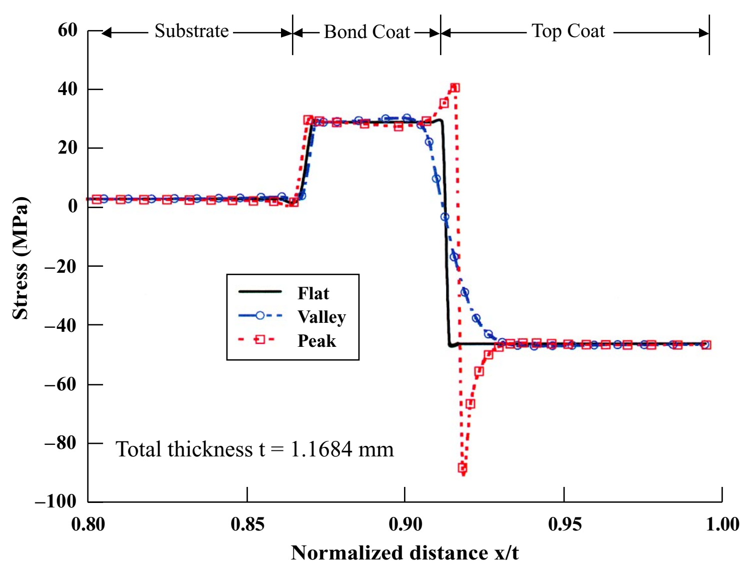

Fig. 3. Y-direction post processing stress variation for a 101.6 μm rough interfaces.

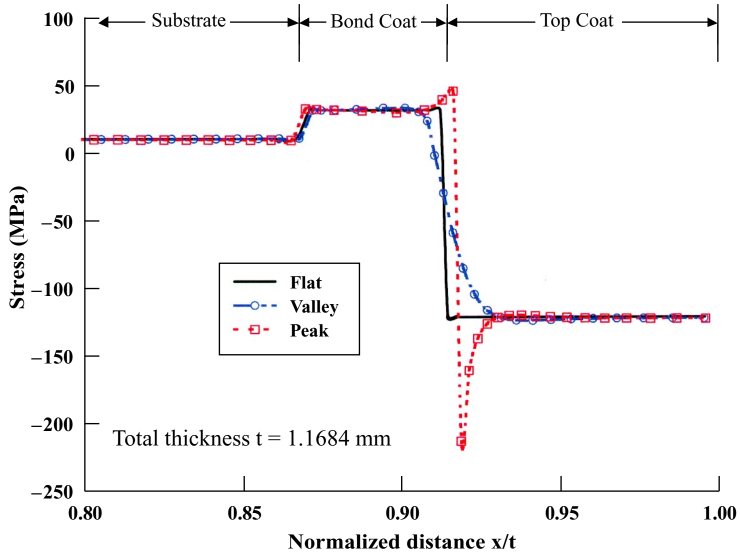

Fig. 4. Y-direction post processing stress variation for a 101.6 µm NiCrAlY top coat with flat and rough interfaces.

HEAT-UP THERMAL STRESSES

The steady-state stresses developed after exposing the coated GRCop-84 to a simulated rocket combustion chamber environment and subjected to the convective heat transfer boundary conditions shown in Fig. 1(a) were calculated subsequent to the build-up of the residual stress after plasma spraying for only a 101.6 µm thick top coating. It is considered that these simulations assume that the liner surfaces are flat. Realistic simulations would require curvature effects and thickness variation be considered in the analyses. The Y-direction stresses after 15 minutes of exposure time are shown in Figs. 5 and 6 for the NiAl and NiCrAlY top coats, respectively. After exposure, the coated GRCop-84 reached the steady state temperatures shown in Fig. 2. The overall temperature difference is only 164 °C as seen in Fig. 2(b), for the NiAl top coat. Hence, the resulting stress distribution in the GRCop-84 substrate (Fig. 5) reveals a bending stress due to the effects of the thermal gradient producing tensile stresses at the cooled surface and compressive stresses towards the bond coat hotter region. The stresses in the bond coat are almost zero, showing a reduction of the stresses from the cool down conditions after processing (Fig. 3). The stresses in the NiAl top coat are now tensile (Fig. 5) compared to the compressive post-processing stresses (Fig. 3) and have a slight gradient. Nevertheless, the tensile stresses in the NiAl coating are much smaller than the room temperature fracture stress of about 300 MPa [11]. The presence of the rough surface results in a sharp increase of the top coat tensile stresses along the bond coat interface at the peak of the asperity, while through the valley no appreciable stress perturbation is observed.

For the NiCrAlY coating, with the larger temperature difference shown in Fig. 2(a) and lower yield stress (Table I), plastic deformation occurred in the coating outer region causing an unloading of the stress along the outer surface. The stress variation in the NiCrAlY coating is tensile at the bond coat/NiCrAlY interface, which decreases to a high compressive stress of –390 MPa before increasing slightly to reach –150 MPa at the outer surface (Fig. 6). The stresses through the bond coat are again close to zero, and the stress distribution in the substrate follows a similar trend as the NiAl coating, (Fig. 5).

Again, the presence of the interfacial asperities introduces X-direction stresses along the valley and the peak path with tensile stresses along the peak and compressive stresses along the valley with a magnitude of 5 and 20 MPa, for the NiAl and NiCrAlY coatings, respectively. The introduction of interfacial roughness leads to shear stresses along the slopes of the asperities. The

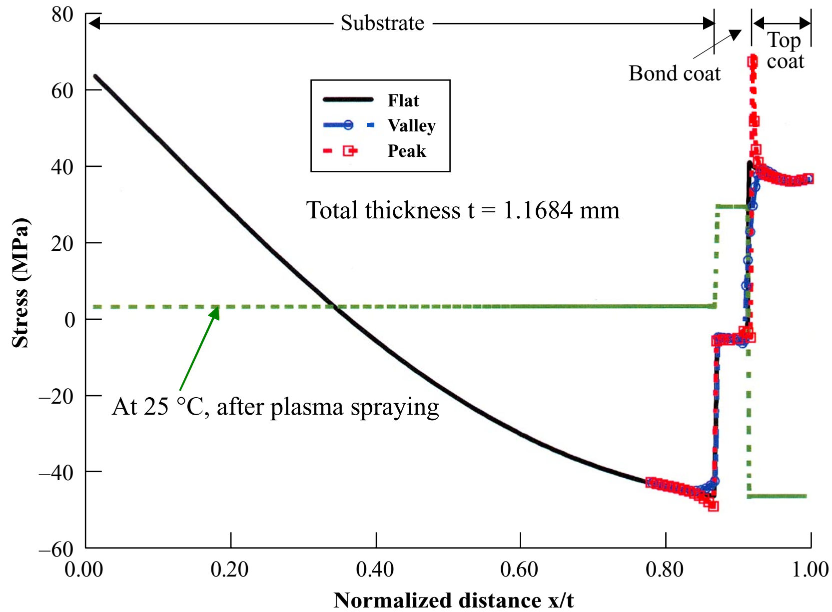

Fig. 5. Y-direction stress as a function of the normalized distance for a NiAl top coat with flat andrough interfaces.

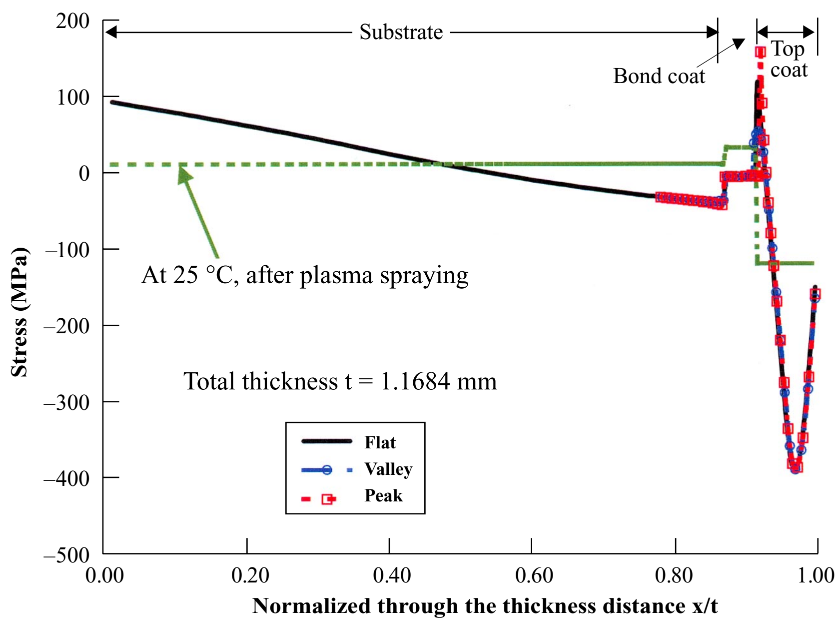

Fig. 6. Y-direction stress as a function of the normalized distance for a NiCrAlY top coat with flat and rough interfaces.

shear stress magnitudes are 22 and 61 MPa for the NiAl and NiCrAlY coatings, respectively. The direction of shearing stresses along the slopes is reversed during heat up cycle as compared to the cool down shearing direction thereby leading to an alternating shear stress.

SUMMARY

A steady-state heat transfer analysis of coated GRCop-84 revealed that both coatings provide adequate protection of the substrate. The NiAl coating's high thermal conductivity provided protection almost independent of the coating thickness. The temperature of the substrate hot wall temperature with a NiAl coating decreased by only 15 °C for a coating thickness ranging from 25.4 to 228.6 μm. The through thickness temperature difference is also small relative to the difference for the NiCrAlY top coat. In contrast, the NiCrAlY coating provides a better heat shield to the GRCop-84 substrate due to its low thermal conductivity, but at the expense of a high temperature difference in the coating reaching almost 578 °C at a coating thickness of 228.6 μm.

The residual stresses developed during cool down from plasma spraying showed that the Y-direction stresses are compressive for both coatings, while the stresses in the copper bond coat and the GRCop-84 are tensile. The stress magnitude for the NiAl coating is almost a factor of 2 smaller than the stresses for the NiCrAlY top coat. The presence of interfacial asperity introduces a X-direction stress along the peak and valley of the asperities as well as a shear stress along the slopes of the asperities. The stress perturbation is limited to a small region of less than 25 μm for a 101.6 μm coating.

The through thickness thermal stresses developed after exposure to a simulated rocket liner gas temperature are tensile in the NiAl top coat. The stress distribution for the NiCrAlY coatings is more complex due to the large thermal gradient developed from the low conductivity of the coating. The stress gradient in the NiCrAlY coating changes dramatically after heat up, and plastic yield occurs in the outer region of the NiCrAlY coating. Again, the presence of rough interfaces perturbs the Y-stress distribution as well as introducing X-direction stress along the peaks and valleys and shear stresses along the slopes.

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