CHAPTER 9

RESIDUAL STRESS ANALYSIS

9.1 INTRODUCTION

The residual stresses in plasma sprayed coatings play a major role in the durability of the coating (Kuroda and Clyne 1991). Residual stresses are of two types: Macro & Micro (Kandil et al 2001). Macro residual stresses exist in the part over a range larger than the grain size. These originate from non-uniform heating and cooling operations, mismatch of coefficient of thermal expansion between the top coat, the bond coat and the substrate, temperature gradients during deposition and densification, creep and oxidation of the bond coat during high temperature exposure (Nair et al 2004). Chemical reactions, precipitation or phase transformations also produce macro residual stresses. Meanwhile, crystallographically anisotropic thermal or elastic properties or mixtures of grains of different phases produce micro residual stresses. Their effective zone extends to a few grains. Gill and Clyne (1990) have divided the macro residual stresses in plasma sprayed coatings which result from the deposition process into quenching stress and thermal stress. For a material with a large coefficient of thermal expansion mismatch with the substrate (e.g., mullite and aluminum) the effect of the quenching stress is negligible, while for a material with a coefficient of thermal expansion close to that of the substrate (e.g., forsterite) the relatively small quenching stress can be the difference between a tensile and/or compressive stress. This chapter attempts to study the macro stresses arising in coatings.
Kokini et al (1996) modeled the thermal stress distribution in zirconia and mullite coatings under transient heating conditions. Their results showed that the temperature gradient which would develop under service conditions would generate a higher compressive stress at the surface of a duplex YPSZ coating than in a mullite coating under the same conditions. The compressive stress was expected to be relaxed through diffusive processes at the elevated service temperatures, leading to the development of tensile stresses in the coating after cooling back to room temperature. This tensile stress would then contribute to coating failure. Kokini’s calculations assumed a stress-free coating at room temperature before the system was exposed to the elevated temperature service conditions.

In the following sections the nature of these two types of stresses are explained to establish the connection between thermal spray process parameters, materials properties, and residual stress in thermal sprayed coatings. Finally, the residual stresses in the interface of the substrate and the bond coat and in the interface of the bond coat and the top coat are simulated using FEA software and the results discussed.

9.1.1 Quenching Stress

When a liquid droplet hits the substrate, it cools from the temperature of the molten droplet in-flight to the substrate temperature within a few microseconds (Heimann 1996). The shrinkage associated with cooling the newly formed splat from the melting (solidification) temperature to the substrate temperature is constrained by the attachment of the newly solidified splat to the substrate, resulting in the formation of a tensile stress within individual splats known as the quenching stress (Kuroda and Clyne 1991,Gill and Clyne 1990). The quenching stress is responsible for cracks in the individual particles (splats) perpendicular to the splat boundaries (Heimann 1996). The maximum quenching stress is:
\[ \sigma_q = E_c \times \alpha_c \left( T_{mc} - T_s \right) \tag{9.1} \]

where, \( \sigma_q \) = quenching stress

\( E_c \) = modulus of elasticity of the coating material

\( \alpha_c \) = coefficient of thermal expansion of the coating material

\( T_{mc} \) = melting point of the coating material

\( T_s \) = Substrate initial temperature

For a ceramic material like alumina, this value exceeds 1 GPa, although experimental studies show a value of a few tens of MPa’s (Kuroda and Clyne 1991). There are two main reasons for this huge difference: one is that stress build up would not start while the particle temperature is close to the melting point due to rapid stress relaxation by diffusive processes. Hence a temperature called the creep temperature is employed to calculate the cooling range instead of the melting point. This temperature is the lowest temperature at which the creep rate is significant in the material. For mullite this temperature is about 1000°C (Kokini et al 1996). Secondly, plastic deformation may occur in metallic materials and micro cracking in ceramics at sufficiently high stresses.

### 9.1.2 Thermal Stresses

Macroscopic stresses which occur between the coating and the substrate are of interest since these affect the adhesion of the coating (Heimann 1996) and their role in determining coating durability. The stresses referred to here as thermal stresses are generated when a system at a uniform initial temperature cools to a uniform final temperature (Gill and Clyne 1990). These stresses are due to a mismatch in the coefficient of thermal expansion between the coating and the substrate. Thermal stresses between two adjacent
layers can be approximated by the following equation given by Levine et al (Houck 1988).

\[
\sigma_c = \frac{E_c (\alpha_s - \alpha_c) \Delta T}{(1 - \nu_c)}
\]  

(9.2)

where, \( \alpha \) = linear coefficient of thermal expansion

\( \nu_c \) = Poisson ratio

\( E_c \) = modulus of elasticity and \( \Delta T \): Temperature gradient

Notation c refers to the deposit and s refers to the substrate.

9.1.3 Total Residual Stress

Kuroda and Clyne (1991) developed a model for the total residual stress in a thermal sprayed coating including both the quenching stress and the thermal stress arising from cooling the system to room temperature from the deposition temperature.

The following assumptions have been made in this model:

1. The coating thickness (\( h_c \)) is negligible compared to thickness of the substrate (\( h_s \)).

2. The substrate temperature is constant at \( T_s \) during spraying.

3. The sprayed deposit is quenched to \( T_s \) instantly.

4. The temperature of the substrate-deposit system remains uniform as it cools down to the ambient temperature \( T_0 \).
5. The interfacial bonding between the deposit and the substrate is good, and the material behaves elastically in the cooling period.

If the coefficient of thermal expansion of the substrate is higher than that of the coating, the thermal stress contribution in the coating would be compressive and the thermal stress for a coating having a higher coefficient of thermal expansion than the substrate would be tensile. If both materials have the same coefficient of thermal expansion (CTE), there would be no thermal stress contribution, and the residual stress would be equal to the quenching stress (Kuroda and Clyne 1991).

When \( \alpha_c < \alpha_s \), there is a temperature at which the residual stress changes from tension to compression; this temperature is called the transition temperature \( T_s^* \) (Kuroda and Clyne 1991). For preheating temperatures higher than \( T_s^* \), the residual stress is compressive. The model is shown below

\[
\sigma_r(T_0) = \left( \frac{\sigma q(T_s)}{E_d(T_s)} + (\alpha_d - \alpha_s)(T_s - T_o) \right) E_d(T_o) \tag{9.3}
\]

Where, \( \sigma_r \) = the final residual stress

\( \sigma q \) = the average of the lateral stress buildup in the splats

\( E_d(T) \) = Young's modulus of the coating at temperature \( T \)

\( \alpha_d \) = Thermal expansion coefficient of deposit

\( \alpha_s \) = Thermal expansion coefficient of substrate

\( T_s \) = Substrate temperature

\( T_o \) = Ambient temperature
9.1.4 Stress Relaxation

Stress relaxation (creep) behavior of ceramics can be described by the following empirical expression (Kokini et al 1996):

\[ \varepsilon_c = A \times \sigma^n \times e^{-\Delta H/RT} \]  

(9.3)

where, \( \varepsilon_c \) = strain rate, \( \sigma^n \) = Von Mises equivalent stress, \( \Delta H \) = activation energy, and \( A, n \) = constants. R is the gas constant and T is the temperature to which the material is heated.

When heating 500µm thick coatings of zirconia or mullite under identical heat fluxes, the surface temperature of the zirconia coating would be higher than that of the mullite coating because of the higher heat capacity and thermal diffusivity of mullite (Samadi and Coyle 2006). This results in a higher thermal gradient in the zirconia coating and as a result, a higher compressive surface stress is expected. In the steady state mode, because of the lower creep strain rate (1.32x10\(^{-20}\) s\(^{-1}\) for mullite vs. 3.25x10\(^{-7}\) s\(^{-1}\) for YSZ at 800°C and \( \sigma \) =100 MPa (Kokini et al 1996) there is no significant change in compressive stress for the mullite. However, the zirconia coating undergoes significant stress relaxation. Even if the surface temperature of mullite is high, no harm will occur.

Kokini et al (1996) showed that using low CTE materials, such as mullite, significantly reduces stress relaxation, resulting in a reduction in cracking. The stress relaxation behavior is related to stress-enhanced diffusive phenomena. The relative boundary sliding of plasma-sprayed splats and grains, and the stress redistributions around the splats and micro cracks are important mechanisms for ceramic coating shrinkage and stress relaxation. As a result of stress relaxation, the compressive stresses decrease during high temperature exposure.
Then upon cooling, tensile stresses develop as the coating tries to shrink. This tension causes the surface to crack and can lead to the initiation and propagation of interfacial cracks between the top coat and the substrate (or bond coat). The surface crack length increases with temperature and the normalized crack length increases with coating thickness decrease. Choules et al. (2001) investigated the effect of coating thickness on the thermal fracture behavior of ceramic coatings under high heat flux loading at constant surface temperature. This study showed that increasing the thickness of thermal barrier coatings decreases the number of surface cracks and increases the interface crack length up to a point and then the interface crack length decreased, which makes thick thermal barrier coatings more resistant to interface crack propagation.

9.1.5 Residual Stress Determination- X-ray Diffraction

There are a wide variety of methods for determining residual stress in coatings. Each measurement technique has its own advantages and disadvantages. One method, the X-ray diffraction method is explained below.

X-Ray diffraction stress measurement is based on the elastic deformations within a polycrystalline material. The deformations cause changes in the spacing of the lattice planes from their stress free value to a new value that corresponds to the magnitude of the applied stress. This new spacing will be the same in any similarly oriented planes with respect to the applied stress, and the crystal lattice therefore effectively acts as a very small strain gauge. The measurement itself is relatively straightforward and the equipment readily available. During a measurement the specimen is irradiated with high energy X-rays that penetrate the surface, the crystal planes diffract some of these X-rays according to Bragg’s law, and a detector, which moves around the specimen to detect the angular positions where diffracted X-rays are located, records the intensity of these rays at that angular position. Several
experimental methods can be used to evaluate the stresses within a material using this diffractometer technique, including the two exposure method, parallel beam method, \( \sin^2 \psi \) method, side inclination method and a variant of the two-exposure method whereby the inclined measurement is made at \( \psi = 60^\circ \) rather than at \( 45^\circ \). The most popular method is probably the \( \sin^2 \psi \) method. This has the advantage that inclined measurements are made at a number of angles \( \psi \) rather than at only one.

9.2 STUDY OF RESIDUAL STRESSES

The thermal properties of the duplex coating are good, and the durability of the coating is confirmed in the thermal shock tests and in the endurance test in an IC engine test rig and on road. The residual thermal stress build up during service is to be ascertained, which would give an understanding of the coating performance. This aspect has been attempted in this chapter. A numerical method was used to approximately calculate the residual stresses arising due to the service condition, as in an IC engine.

9.2.1 Numerical Modeling of the Thermal Stresses in Mullite Coatings under Service Conditions

9.2.1.1 Introduction

Experimental determination of residual stresses is very difficult and resorted to as a validation tool. Initially, numerical modeling and simulation is a good technique that can be adopted to calculate the residual stresses under service conditions. In this chapter, a numerical model has been developed and the stresses have been calculated under service conditions.
9.2.1.2 Model description

The model was divided into two physics: heat transfer and structural mechanics. The heat transfer part was solved first using the experimental parameters. The resulting temperature distributions were then used in the structural mechanics part to calculate the local stresses and strains.

To simulate the temperature and stress distributions to be expected under a thermal gradient reflective of service conditions in a duplex coating used in an IC engine, a cylindrical substrate was employed, with dimension of diameter 40 mm x thickness 6 mm.

The duplex coating, consisting of a bond coat of NiCr (150 µm) and a top coat of mullite layer (150 µm) on a thick (6 mm) substrate was modeled. Figure 9.4 shows the model of the duplex coating. Calculations were performed to determine the internal stresses arising in service. The results were compared with boron carbide coating on cast aluminum A 356.O. The reason for selecting boron carbide is that little work has been done on boron carbide coated cast aluminum for engine application and also the ceramic has excellent structural and thermal properties. A commercial finite element modeling software package (Ansys 11) was used for the study. The software package easily incorporated 2-D heat transfer calculations and a plane–stress assumption for stress and strain calculations.
9.2.1.3 Coupled thermal/structural analysis

Coupled field analysis is “a sequentially coupled physics analysis wherein the combination of analysis from different engineering disciplines interacts to solve a global engineering problem”. When the input of one physics analysis depends on the results from another analysis, the analysis is coupled.

Hence, in this study, in the preprocessing stage, thermal and structural environments are constructed separately to determine the coupled physics solution. The geometry is kept constant for the entire study and a single set of nodes will exist for the entire model. The geometry is created in the thermal environment, the thermal effects are applied. Later the structural effects are applied in the second structural environment. The element used for the two environments may be same or different, and if different a combination of elements should be used as per the standards established in the software. In this study the element used is solid brick with 8 nodes.
SOLID45 is used for the 3-D modeling of solid structures. The element is defined by eight nodes having three degrees of freedom at each node: translations in the nodal x, y, and z directions. The element has plasticity, creep, swelling, stress stiffening, large deflection, and large strain capabilities. In the second phase, the two environments are combined. The loads and constraints are applied in each case. In the post processing phase, the results, namely the deformation and the stress plots are viewed.

9.2.1.4 Material properties

Literature values were used for all material properties of the duplex coating (Juliana Anggono 2005). The material property values used in the modeling are given in chapter 3, Table 3.3.

9.2.1.5 Heat transfer boundary conditions

To generate a hot-face temperature resembling the engine situation using known guidelines (Kokini et al 1996), a thermal flux of 350 kw/m² is applied to the top surface of the coating while the back surface of the substrate is maintained at 400 K. The heat flux is assumed to produce an ambient temperature of 600°C as shown in the figure 9.5.

Figure 9.2 Ambient temperature acting on the coated model
The temperature on the top of the piston due to convection will be around 250°C (Parvathi 2003). A ΔT of 50° C is assumed in service in the coating system and the temperature of the base will be 200° C, due to which the thermal stresses will build up. Heat transfer between the solid material and the ambient atmosphere occurs by convection:

\[ Q = h \times a \times (T_1 - T_2) \]  

(9.5)

where, \( Q \) is the heat flux in kW/m²,
\( h \) is the convective heat transfer coefficient in kW/m² °C,
\( a \) is the area of cross section exposed to the heat in m²,
\( T_1 \) is the ambient temperature, taken as 600°C for this study,
\( T_2 \) is the surface temperature of the coated surface, taken as 250°C in this study.

Heat transfer within the coating system occurs by conduction

\[ Q = k \times a \times (T_1 - T_2) \]  

(9.6)

where, \( Q \) is the heat transfer in kW /m²,
\( k \) is the heat transfer coefficient in kW/m² °C,
\( a \) is the area of cross section in m²,
\( T_1 \) is the coating surface temperature, taken as 250°C for this study,
\( T_2 \) is the substrate temperature, taken as 200°C in this study.

9.2.1.6 Mechanical boundary conditions

Material response was assumed to be perfectly elastic with no plastic deformation. The temperatures were assumed to be below creep temperatures and all mechanical parameters are a function of temperature. To
simulate the stresses under a thermal gradient reflective of service conditions, the model was fixed at the circumference as the case in an IC engine piston, and allowed to expand in the Y-direction only as shown in Figure 9.6.

![Figure 9.3 Mechanical boundary condition](image)

9.2.1.7 Meshing

A Lagrange-Quadratic mesh was chosen as the mesh method. This means that a quadratic polynomial is used to interpolate in each element and that the function, but not its normal derivative, will be continuous from one element to the next (Lagrange). This is the default mode for solving solid mechanics problems with the finite element method. The geometry of the model and the meshing is shown in Figure 9.7.
Figure 9.4  Geometry and meshing of the model

9.2.1.8  Results and discussion

The temperature gradients, the deformations and the residual stresses developed in the coating in service are shown in the Figures 9.8 to 9.11 below.
Figure 9.5  Plot of mullite coating without bond coat (100 microns thick) Top– temperature plot, Bottom – deformation plot
Figure 9.6  Plot of mullite coating with bond coat (200 microns thick)
Top – temperature plot   Bottom – deformation plot
Figure 9.7 Plot of Boron carbide coating without bond coat (100 microns thick) Top – temperature plot, bottom – deformation plot
Figure 9.8  Plot of boron carbide coating with bond coat (200 microns thick) Top – temperature plot, bottom – deformation plot
The results of the numerical simulation studies are shown in the table 9.2. Four types of coating systems have been studied. As zirconia has been studied by many researchers, boron carbide, a ceramic with excellent mechanical and thermal properties has been studied.

Table 9.1 Numerical simulation results of the residual stresses

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Description</th>
<th>Deformation in ‘m’</th>
<th>Residual stress in MPa (min)</th>
<th>Residual stress in GPa (max)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Mullite coating on cast Al 356.0 without bond Coat (single layer coating)</td>
<td>0.488 x 10^{-4}</td>
<td>127</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>Mullite coating on cast Al 356.0 with bond Coat (duplex coating)</td>
<td>0.512 x 10^{-4}</td>
<td>70.9</td>
<td>5.8</td>
</tr>
<tr>
<td>3</td>
<td>Boron Carbide coating on cast Al 356.0 without bond Coat ( single layer coating)</td>
<td>0.537 x 10^{-4}</td>
<td>65.7</td>
<td>8.3</td>
</tr>
<tr>
<td>4</td>
<td>Boron Carbide coating on cast Al 356.0 with bond Coat ( duplex coating)</td>
<td>0.536 x 10^{-4}</td>
<td>52.1</td>
<td>5.4</td>
</tr>
</tbody>
</table>

1. Clearly the results show that both deformation and residual stresses are both low in the case of duplex coated specimens of both mullite and boron carbide, when compared to the single layer coatings. Also, the stresses and deformations are lower in the case of mullite and smaller regions are affected, when compared to those of boron carbide coating.

2. The plots reveal that the stresses are more in the single layer coatings due to the mismatch in the elastic modulus and the thermal expansion coefficients of the coating and the base materials.
3. The resulting stress values are high. The deformations are very less in all the cases with an average of 0.5 x 10^{-4}m.

4. The residual stress is compressive in nature, since \( \sigma_c < \sigma_s \).

5. The results showed that the temperature gradient which develops under service conditions, would generate a higher compressive stress at the surface of the single layer coatings than in the duplex coating, under similar conditions. Kokini et al (1996) modeled the stress distribution in zirconia and mullite coatings under transient heating conditions. The temperature gradient produced a higher compressive stress in zirconia coatings. The compressive stresses are expected to be relaxed through diffusive processes at the elevated service temperatures, leading to the development of tensile stresses in the coating after cooling to room temperature, which will contribute to coating failure. But this does not happen in mullite coatings due to higher creep resistance.

6. Even if the mullite top layer in the duplex coating is exposed to a higher surface temperature the material has good resistance to creep deformation and hence less prone to surface cracks.

9.2.2 Results and Discussion

Shown in Figure 9.3 are micrographs of the coating showing, voids, discontinuities, coating cavities and pores which might have arisen due to the residual stresses. The numerical simulation revealed that residual stresses may arise during service, due to the mismatch in the thermal and mechanical properties of the coating and the substrate. Since the numerical solution is an approximate method, the actual residual stress buildup should be ascertained
by experimentation for validating the simulated results. This has been done by endurance test of the IC engine coated with mullite. The results were good showing no apparent failure. This may due to the good creep resistance and crack growth resistance of the mullite coating and also due to the crystalline microstructure of the coating with less amorphous content.

1. Large Pores
2. Coating cavities
3. Coating discontinuities
4. Voids in coating

Figure 9.9 Microstructure of the coating showing defects

9.3 CONCLUSIONS

Macro residual stresses comprising of quenching stresses and thermal stresses were studied in this chapter. Since the thermal stresses are more significant, an attempt was made to study the thermal stresses arising in service. When the residual stress exceeds the adhesion strength of the coating on the substrate, the coating delaminates. In this study the mullite duplex
coating has mean adhesion strength of 20 MPa and clearly less than the residual stress buildup during service as per the simulation study and hence unsafe. But the creep resistance of mullite is very high and the material will not permit stress relaxation and initiation and propagation of cracks. Also, the endurance test on road has shown good results of the duplex coating. Since the simulation is an approximation, and also since the analytical models does not consider the creep behavior of the coating material, the results of the endurance test can be taken as proof of the life of the coating. Another solution to this problem is to adopt a functionally graded coating with improved adhesion strength and reduced thermal residual stresses.