EVALUATION OF THE RESIDUAL STRESSES IN ADVANCED COMPOSITE CERAMIC COATINGS USING X-RAY DIFFRACTION AND FINITE ELEMENT TECHNIQUES

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Abstract: *The aim of this work is to evaluate the residual stresses in advanced composite ceramic coatings (60wt% Al_2O_3 – 40wt% SiO_2) was produced by thermal spraying coating (flame spraying) on the mild steel substrate (AISI 1050) steel. The bond coat used in this work was AlNi alloy between metallic substrate and advanced composite ceramic coatings which was implemented by flame spraying technique. The thickness of bond coating was (150μm) and for composite ceramic coating was (450 μm). the residual stresses evaluated by X-Ray diffraction technique were compressive residual stresses (-62.6099), while by finite element method were compressive residual stresses (-68.491). The percentage of agreement between the residual stresses evaluated by X-Ray diffraction technique and finite element technique was (91.509%).*

KEYWOEDS: ADVANCED CMPOSITE CERAMIC COATINGS, X-RAY DIFFRACTION TECHNIQUE, FINITE ELEMENT METHOD

1. Introduction

Increased use of thermal spray coatings, especially for high-temperature environmental resistance, requires confidence in coating durability, i.e., resistance to cracking, debonding, and spallation, both during application and in service. Residual stresses are known to play an important role in coating durability; for example, tensile residual stresses typically increase the susceptibility to cracking and debonding. Many studies have been devoted to the measurement of residual stresses in coatings [1-4]. Residual stresses develop during cooling of a thermal spray coating due to the mismatch of thermal expansion coefficients of the coating and substrate. Depending on the relative magnitudes of the thermal expansion coefficients of the coating and substrate [5-7] residual stress can be either tensile or compressive Parameters that strongly affect the magnitude of residual stresses are coating and substrate temperature during spray deposition and properties of the coating such as thickness, roughness and porosity. Experiments have shown that residual stresses increase with coating thickness and deposition temperature [8]. Thermal barrier coatings (TBC_s) are the best way to protect components of gas turbine engines and the demand for such coatings is becoming more important as higher temperature engines are being developed [9-14]. Generally, the residual stresses of thermally sprayed coatings are induced by different mechanisms and sources [15-17]. In a thermal spray process with a high flame temperature, such like flame spray, plasma spray, or arc spray, fully and partially molten particles striking onto the surface of the substrate, are flattened, solidified, and cooled down in a very short period of time (few microseconds). After their solidification and adhesion onto the surface of the substrate, the contraction of the splats can be hindered by substrate material or the underlying solidified coating material, which results in tensile stresses which are called intrinsic, deposition, or quenching stress. Due to an extremely high temperature difference, a high theoretical residual stress in the order of up to 1 GPa can be induced. However, due to the many relaxation mechanisms, such as the sliding of the splats, micro cracks, plastic deformations, and material creep, the experimentally measured values are much lower (<100 MPa) [18]. X-ray diffraction was used as a complementary technique; it can determine stress only in a thin surface layer,

whereas the penetrating power of neutrons enables through-thickness stress profiling without any material removal [19].

This work aims to evaluation of the residual stresses in advanced composite ceramic coating (60%wt Al_2O_3 - 40%wt SiO_2) using X-ray diffraction technique (XRD) and the residual stresses calculated by finite element method (FEM).

2. Materials and method

2.1 Materials and parameters of the spraying processes

The coatings were applied by thermal spraying method (flame spraying) in air on the plain-carbon steel (AISI 1050), cylindrical substrate that’s dimensions were 15 mm in diameter and 10 mm in height. The flame spraying system is designed and implemented in the welding laboratory of Mechanical Engineering Department, College of Engineering, University of Diyala, Iraq using spray gun the heat flame is produced by the burning of oxygen and acetylene, where the molten powder is carried out in the gas mixture and is attached to the surface to be coated by the high temperature of the torch which can raise to 3000 Cº. It is required to control the pressure of the gases to obtain the flame equal to the speed of the powder rush. The oxygen pressure should be adjusted according to the spray gun used no more than 4 bar and the acetylene pressure not more than 0.7 bar before spraying process. Two coating layers were used in this work are the bond coat from (AlNi) alloy to reduce mismatch of thermal expansion coefficient between substrate and composite ceramic coating as a top coating layer. The conditions of deposition process are listed in Table1.

***Table 1** Operating parameters during coating deposition process*

Operating Parameters	Values
Oxygen pressure	4 bar
Acetylene pressure	0.7 bar
Distance	20 cm
Powder feed rate	7 cm^3/min
Particle size	Mish (100-300)
Temperature substrate	(300 - 450) C°

2.2 Residual stress analysis

2.2.1. X-Ray stress evaluation

XRD-based residual stress measurements were made using standard dspacing vs. sin2ψ techniques using Shimadzu X-Ray Diffractometer type XRD-6000 and CrKα radiation. The $\sin^2\psi$ method [20, 21] was used to determine the residual stresses in this work, the change of a lattice plane distance (d spacing) of a phase, i.e., the peak shift of the corresponding reflection, was measured for tilt ψ-angles between 0° and 45°. To calculate the residual stresses the linear regression of the plot (d spacing) versus $\sin^2\psi$ and the X-ray elastic constants. The coating and substrate physical properties (elastic modulus, Poisson's ratio, and coefficient of thermal expansion), thickness of the top coating, bond coat and substrate are shown in the table 2. The deposition temperature used in the present work during coating process for the topcoat and bond coat was 850C°.

***Table 2** The physical properties of substrate, bond coat and topcoat [22-25]*

Physical properties	Substrate	Bond coating	Top coating
Yong's modulus (Gpa)	200	105	64.167
Poisson's ratio	0.33	0.315	0.206
Thickness	10 (mm)	150µm	400µm
Thermalexpansion coefficientα, µƐK^{-}	12.6	11.9	7.6

From Shimadzu X-Ray Diffractometer XRD-6000 chart, will be getting on the following values are shown in the table 3.

***Table 3** Shows the relationship between 2Ɵ & ψ to the topcoat ($60\%Al_2O_3+40\% SiO_2$)*

2Ɵ	*ψ*
156.966	*0*
156.825	*15*
157.007	*30*
157.483	*45*

By Brag Law (nλ = 2d sinθ) may be calculated (d), where n=1, λ= 2.28970 A° and Ɵ (0, 15, 30, 45) degree. From the figure1 may be calculated the linear slop of the plot $d_{spacing}$ versus $\sin^2\psi$.

The stress can then be obtained from the following equation:

Ϭ= (E/(1+v)) *1/do (∂d/ (∂ 〖sin〗 ^2 d)) (1)

From figure1 the slop ∂d/ (∂ 〖sin〗 ^2 d)) =-0.00239,
$d_\circ$ =2.02712 A°
from Eq. (1), the value of the Residual stresses is:
Ϭ = - 62.6099 Mpa

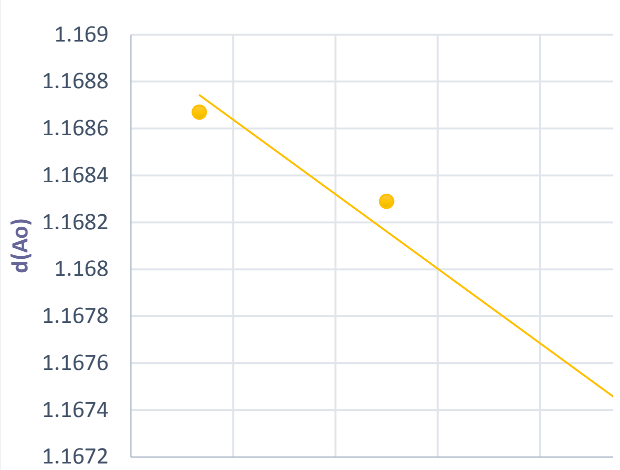

***Fig. 1** Relationship between ($\sin^2\psi$) and $d_{spacing}$ (Å).*

2.2.2. Finite element model

To evaluate the residual stress distribution within coating(s) after flame thermal spray, a finite element model was developed using ANSYS 15. The physical specimen tested experimentally is a cylindrical shape plain-carbon steel substrate of 10 mm in diameter and 15 mm in height, with layers of coatings deposited on the substrate surface. Finite element model of the simulation is considered as two-dimensional simulation. The element type 182 was selected for the analyses. Figure 2 shows atypical model used in the analysis. The thermal load applied as the decrease in temperature from the initial temperature at coating 850 C° to room temperature of 25 C°, where the specimen was assumed to be stress free. Table 2 summarizes the types thickness of coatings with their material properties considered in the present work. The specimen was modelled to have a 150 µm AlNi layer as a bond coat with a total thickness of coating system 650 µm. The substrate/bond coat and bond coat/top coat interfaces were assumed to be flat, neglecting the effect of grit blasting prior to deposition process. Perfect bonding between layers of sprayed materials is assumed. Homogeneous material properties are assumed.

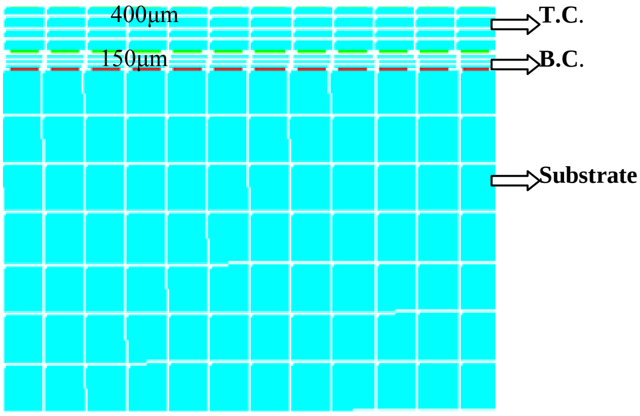

***Fig. 2** The geometry of the model*

3. Results and discussion

3.1. Residual stress measurement—XRD results

It can be referred from from Eq. (1) that in topcoat (60%wt Al_2O_3-40%wt SiO_2) was subjected to compressive residual stresses (-62.6099 Mpa). This residual stresses were evaluated in the surface layer of coating adherent to the substrate. Thickness of topcoat layer conforming to the X-ray penetration was observed 450 µm. The study was carried out at several sites of each coating and the residual stresses were always determined along two perpendicular directions corresponding to azimuth angles of 0º and 120º. The results showed for each sample characteristics of a plane-equiaxial and compressive stress state, with constant values at sites far from the borders or irregularities. The results presented in the remainder of the study confirm this feature.

The level of the residual stresses in the topcoat surface was related to characteristics of composite ceramic coating (60%wt Al2O3-40%wt SiO2) deposited by flame spraying technique. The parameters considered were the substrate material (AISI 1050), the substrate thickness (10 mm), and a bond coat of NiAl (150µm). As can be observed, the level of the residual stresses remains constant for all the samples inside the error bars. This behavior can be related to the stress relief by extensive micro-cracking during spraying. The coating flaws, porosities and microcracks have an important effect on the stress release and only quenching stresses remain in the finished deposit [18].

3.2. Residual stress measurement—FEM results

Figures 3, 4 show the results of FE simulation of residual stresses on the topcoat surface can be seen. The figures show the residual stresses in plane plastic strain within the composite ceramic coating (60%wt Al_2O_3 - 40%wt SiO_2) layer and the steel substrate. In this case, the maximum plastic strain is induced into the coating (60%wt Al_2O_3 - 40%wt SiO_2) layer. However, the bond coat is significantly affected as well, while only a minor influence on the steel substrate can be found.

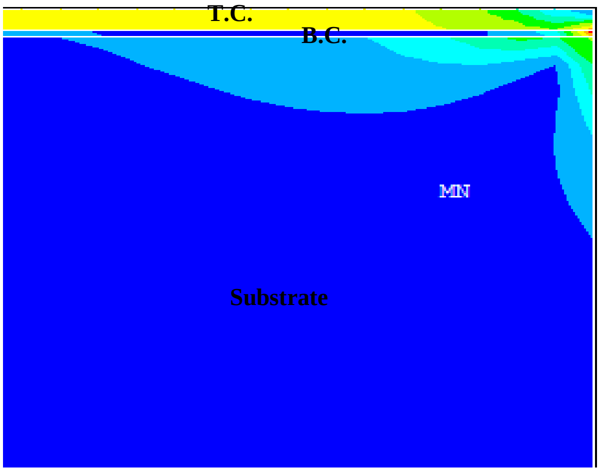

Fig. 3 *Effect distribution of residual stresses in layers*

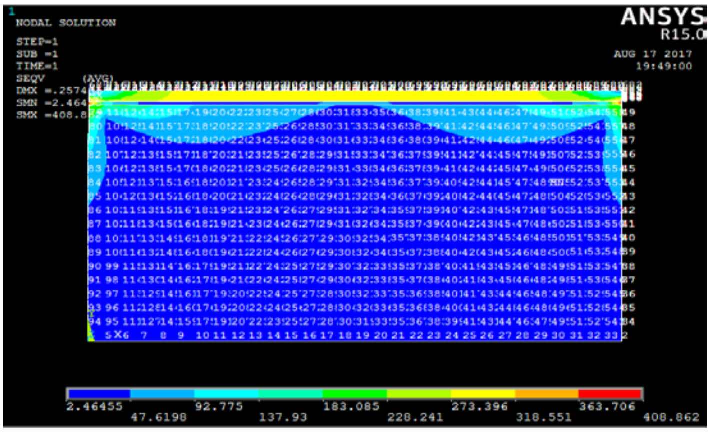

Fig. 3 *Shows analysis of FEM and distribution of nods*

It can be seen from above results that in top coat layer (60% wt Al_2O_3 - 40%wt SiO_2) topcoat was subjected to compressive residual stresses (-62.6099 Mpa). These results were in a reasonable agreement in sign with the stresses given by FEM (-68.491 Mpa) although the calculated stresses tend to be slightly higher than the measured values. As well, the stresses in axial direction calculated by FEM were much higher than the measured values. This could be attributed to the effect of interface roughness of specimen. It should be noted that for the reason of simplicity, FEM performed in this study assumed flat interfaces between dissimilar coating layers materials. On the contrary, it has been shown that surface roughness generates higher out-of-plane stress (axial direction) [25]. Thus, it is reasonable to obtain a higher axial stress from the X-ray measurement.

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