

**EFFECT OF THERMAL SPRAY COATING PROCESS
PARAMETERS ON THE DEVELOPMENT OF RESIDUAL
STRESSES IN CERAMIC COATINGS**

BY

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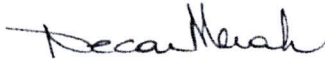
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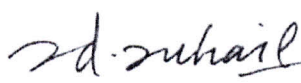
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Dedicated to my family

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ABSTRACT

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In this work, a 3D stochastic model coupled with a finite element (FE) code is used to investigate the development of residual stresses in thermal spray coatings. The residual stresses of a thermally sprayed yttria-stabilized zirconia (YSZ) coating applied on stainless steel substrates are used for this work. The formation of the coating layers was simulated with a 3D stochastic model, SIMCOAT. Four YSZ coating models were developed. The first three models were built with a similar average thickness, but different layers (one-, two-, and three-layer coatings) were obtained by changing three process parameters: the material feed rate, the gun velocity, and the total number of passes. Two 2D slices of each 3D model were taken and converted into FE models using an in-house Python code. An FE simulation was then used to study the combined effect of these process parameters on the development of residual stresses. The variation of in-plane stresses through the thickness for each model was obtained, and a comparison between the developed stresses was conducted. The results show that each coating layer is subjected to compressive stress at its top surface and tensile stress at its bottom surface during the deposition. The deposition stress profiles show that reducing the number of coating layers is better in terms of reducing the fluctuations in expansion/contraction rates. After the deposition, the permanent stress is compressive in ceramic coatings (YSZ) due to its low thermal expansion coefficient and tensile in the stainless steel substrate. The profiles of the final residual stress reveal that the

thermal mismatch stress is the dominant source and constitutes the major part. This model allows the prediction of the interaction between the sources of residual stress which cannot be predicted experimentally. The fourth stochastic model was converted into a 3D FE model, then the residual stress profiles parallel and perpendicular to the gun movement were predicted. The stress profiles obtained in the 3D analysis are following the same pattern as in the 2D analysis indicating the validity of plane stress assumption. The results were compared with actual residual stress readings measured by the hole drilling method. The developed methodology was effective for understanding the effect of the coating process parameters on the development of residual stresses and can be used to optimize the coating process parameters to obtain the desired residual stresses.

ملخص الرسالة

الاسم الكامل: علي عبد الباقي جاد المولى

عنوان الرسالة: تأثير معاملات عملية الطلاء بالرش الحراري على تطور الاجهادات المتبقية في الطلاءات الخزفية

التخصص: هندسة ميكانيكية

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في هذا العمل ، يتم استخدام نموذج عشوائي ثلاثي الأبعاد مقروناً بنموذج العناصر المتناهية (FE) لدراسة تطور الإجهادات المتبقية في طلاءات الرش الحرارية. تم اختيار الإجهادات المتبقية في طلاء زركونيا الإيتريا المستقرة (YSZ) والمثبت حرارياً على ركائز الفولاذ المقاوم للصدأ لهذا العمل. تمت تشكيل طبقات الطلاء باستخدام (سمكوت) وهو برنامج مطور لنمذجة الطلاء الحراري. تم إنشاء أربعة نماذج طلاء من الزركونيا. تم بناء النماذج الثلاثة الأولى بمتوسط سماكة متشابهة تقريباً ، ولكنها تختلف في أعداد طبقات الطلاء (نموذج ذي طبقة واحدة وذي طبقتين وذي ثلاث طبقات) ، تم الحصول عليها عن طريق تغيير ثلاث معاملات لعملية الرش: معدل تغذية المواد وسرعة الرشاش والعدد الكلي للأنشواط. تم أخذ شريحتين ثنائيي الأبعاد لكل نموذج وتحويلها إلى نماذج FE باستخدام رمز تم إنشاؤه بواسطة Python. ثم تم استخدام نموذج العناصر المتناهية FE لدراسة التأثير المشترك لمعاملات هذه العملية على تطور الإجهادات المتبقية. تم الحصول على تغير الإجهادات عبر سمك كل نموذج ، وتم إجراء مقارنة بين هذه الإجهادات. أظهرت النتائج أن كل طبقة طلاء تتعرض لإجهاد انضغاطي على سطحها العلوي وإجهاد شد على سطحها السفلي أثناء الترسيب. أظهرت منحنيات الإجهاد الترسيبي - الإجهاد الناشئ أثناء الرش - أن تقليل عدد طبقات الطلاء أفضل من حيث تقليل التقلبات في معدلات التمدد / الانكماش. بعد الترسيب ، يكون الإجهاد انضغاطياً في الطلاء الخزفي (YSZ) بسبب معامل التمدد الحراري المنخفض لمادة الطلاء ، بينما تعرضت ألواح الفولاذ لإجهاد شد. تكشف منحنيات الإجهاد المتبقي النهائي أن الإجهاد الناشئ نتيجة عدم التوافق في الخصائص الحرارية هو المصدر المهيمن ويشكل الجزء الرئيسي. يسمح هذا النموذج بالتنبؤ بالتفاعل بين مصادر الإجهاد المتبقي التي لا يمكن التنبؤ بها معملياً. تم تحويل نموذج الطلاء العشوائي الرابع إلى نموذج العناصر المتناهية ثلاثي الأبعاد FE ، ثم تم نمذجة الإجهادات المتبقية المتوازية والمتعامدة مع حركة الرشاش. تتبع منحنيات الإجهاد التي تم الحصول عليها في التحليل ثلاثي الأبعاد نفس النمط كما في التحليل ثنائي الأبعاد الذي يشير إلى صحة افتراض الإجهاد المستوي. قورنت النتائج مع قراءات الإجهاد المتبقية الفعلية المقاسة بطريقة حفر الثقب. كانت المنهجية التي تم تطويرها فعالة لفهم تأثير معاملات عملية الطلاء على تطور الإجهادات المتبقية ويمكن استخدامها لتحسين معاملات عملية الطلاء للحصول على الإجهادات المتبقية المطلوبة.

CHAPTER 1

INTRODUCTION

1.1 Background

Thermal barrier coatings (TBCs) were invented in the 1960s to lower the temperature of hot components [1-2]. In the mid-1970s, the first successful testing of TBCs was carried out in the area of turbine engines [3]. In the 1980s, they were used on the vane of aircraft gas turbine engines to increase the operating temperature [3-4]. Since that time, they have been widely used in the field of aircraft engines, gas turbine blades, and diesel engines [5–9]. TBCs are expected to have low thermal conductivity. The main aim of applying TBCs is to provide thermal insulation to hot sections that operate under high temperatures [10–14]. They can achieve a temperature drop (100-200 °C) at the substrate surface [2, 7, 12, 15, 16]. The inlet temperatures of the turbine can be increased 100 -300 °C resulting in increasing the efficiency [7, 12, 17]. In the past 50 years, nickel-based superalloy materials obtained an increase in engine operational temperature about 100 °C [4]. In current days, an inlet temperature of more than 1500-1600 °C is achieved in some turbines and is expected to reach 1760 °C. It was found that the use of TBCs has resulted in an increase in the engine thrust up to 5% and efficiency up to 1% [12]. The protection from severe operational conditions prolongs the life of the hot components, thus improving the reliability of engines [18]. In addition, TBCs can protect the underlying materials from oxidation, corrosion, and cyclic thermal stresses, which involve fatigue and creep phenomena [19–23]. The demand for raising the efficiency of engines and improve their performance is increasing in the context of higher

operating temperature, longer service life components, and lower emissions. The efforts made in improving the performance of engines resulted in rapid development in TBC technology.

The conventional TBC systems (Figure. 1) consist of three layers:

1. An outer insulating ceramic topcoat (TC) to provide thermal insulation to the underlying substrate. Materials used as a TC should exhibit the following properties: (1) Low thermal conductivity. (2) High melting point, so that it can resist high operational temperatures without melting. (3) No phase transformation below operating temperature because phase transformation involves volume change and cracks inside the coating, thus failure of the coating [4, 24, 25]. Yttria stabilized Zirconia (6-8 wt% YSZ) is one of the most widely used materials as a TC. It possesses excellent thermal shock resistance, a relatively high coefficient of thermal expansion (CTE), and low thermal conductivity [1, 24, 26, 27]. The selection of YSZ as a TBC material is mainly based on the reality that the zirconia is a refractory oxide. The identification of yttria is that it is a stabilizer, especially under thermal cycling conditions. YSZ has temperature-independent low thermal conductivity, because of high point defect concentration present due to substituting of Zr^{4+} ions by Y^{3+} ions in the fluorite structure, creating small spaces between point defects [28].
2. Metallic bond coat (BC) to protect the substrate from oxidation and improve the adhesion of the TC. A BC material should meet the following requirements: (1) Resistance to interdiffusion with the substrate. (2) High creep strength. MCrAlY is the typical material used as a BC [24, 29–31].
3. Thermally grown oxides (TGO) that develops at the interface between the TC and the BC due to oxidation of the BC at high temperature during the operational service [24].

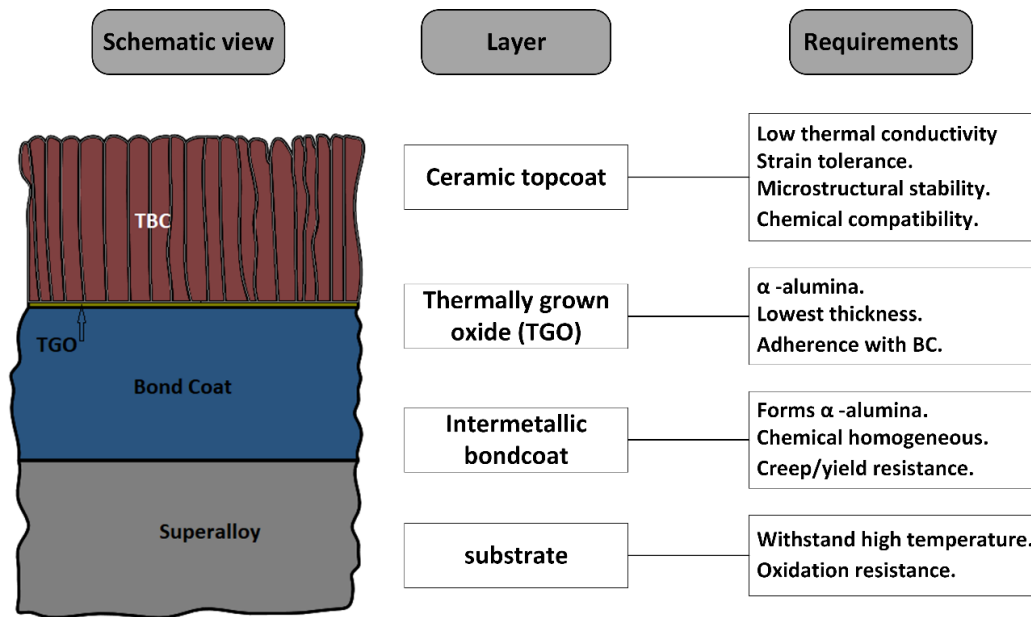


Figure 1 The major elements of a thermal barrier coating system and their requirements

1.2 Applications

TBCs have been extensively used in the aerospace industry. There is an increased demand for aero-engines and turbines, which resulted in an increased demand for more reliable components. TBCs are applied to the hot sections of the turbines such as vane bases, combustor liner (cans), splash plate, fuel injector and transition ring to increase the thermal efficiency and prolong the hot components life. In diesel engines, TBCs are applied to components exposed to high-temperature fatigue such as piston crowns to extend their life. In high-performance engines, TBCs are used on cylinder heads, piston crowns, valve, and exhaust ports. TBCs also have been used on brake pads to provide insulation from hydraulics thus improving brake fade characteristics [32, 33].

1.3 Objectives

Ceramic coatings are widely used in many engineering applications, especially applications related to components operating at elevated temperatures. One of the main issues relates to ceramic coatings is the development of residual stresses due to quenching and the thermal mismatch between the deposited coating layers and the substrate. The present study aims to:

- Generate various 2D FE models with different process parameters, and to compare the development of residual stresses among them.
- Develop a 3D FE model with real surface topographies in order to predict residual stress profiles parallel and perpendicular to gun movement.

1.4 Motivation for research

One of the technological challenges that face TBCs produced by thermal spray coating is the development of the residual stresses through the thickness of the coatings. The residual stresses influence the quality and the lifetime of the coatings, through affecting many factors controlling the performance of the TBCs like adhesion strength, wear performance, bond-coat oxidation, and microcrack formation. Therefore, understanding the behavior of the residual stresses is important and attracted much of the researchers' attention [34–37] The evolution of the residual stresses in thermal spray coatings is a complex phenomenon that induced as a result of nonuniform heating and cooling during manufacturing and processing. They are strongly influenced by coating process parameters and material types. Therefore the coating process parameters should be carefully controlled to maintain a good coating quality. TBCs usually are deposited in several number of layers, the stress developed in each layer is affected by the deposition of the subsequent layers. The rate of contraction of each layer is different from the others due to the difference in the time of deposition and thus temperatures. The interaction between the coating layers and the effect of

the number of layers on the development of the residual stress is not well investigated in the literature, Various analytical and computational models have been developed to simulate the residual stresses development through the coating thickness. Most analytical models are very limited and are based on many assumptions that are not always valid. In computational models, there are two directions of modelling residual stresses, the first direction is modeling the residual stress at the micro level. In this case the principles of the fluid dynamics are used to model the deposition of few particles. They cannot be applied to the whole coating particles due to the computational cost. the second direction is the macro-modeling approach which is assuming that the coating layer is continuous and homogeneous. Some of the researchers adopting this approach assumed that the coating layers interfaces are wave-shaped and others used flat interfaces. In general, there is a lack of studies investigating how the number of passes affect the residual stress development. This study investigates the effect of the progressive (layer-by-layer) deposition on the residual stress development over the time and the interaction between the sources of the residual stresses (Quenching and thermal mismatch stresses).

1.5 Methodology

In this study, four stochastically generated FE models are presented to simulate the residual stresses induced during the spraying of YSZ on stainless steel. The first three models were developed by varying three process parameters (gun speed, feed rate, and number of passes) while keeping the same average total thicknesses: one-layer, two-layer, and three-layer coatings of YSZ applied on stainless steel. To visualize the simulation of coating structure, SIMCOAT was linked with TECPLOT which provides the data of the 3D simulation of the coating structure in terms of several planes, each plane divided into small cells. The coordinates and porosity values of each cell were stored in a data spreadsheet. Then the data of two 2D slices of each model were taken

and converted into a 2D FE model using an in-house Python code. The developed FE models represent a 2D geometry of the coatings with accurate details of the surface roughness and a clear distinction of the interfaces between the coating layers and can be imported into any commercial FE code. The coating process is then simulated by depositing the layers progressively (layer-by-layer deposition) and solving the conduction/convection heat transfer that takes place during the coating process. The residual stress distribution is then compared between the three cases to understand the mechanism of residual stress development between the coating layers. In the fourth model, the roughness of each layer was extracted from TECPLOT as a cloud of points and plotted into SOLIDWORKS using a visual basic script. Solid 3D components (the first layer, the second layer, the substrate) were imported into ABAQUS as a 3D FE model. Then the residual stresses parallel and perpendicular to the gun movement were simulated.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction and historical overview of thermal spray

Thermal spraying is a technology that is employed to generate a stream of coating particles and deposit them on a substrate. Thermal spray techniques aim at improving the performance of components and increasing their life. Thermal spraying was invented for the first time by Max Ulrich Schoop (1870-1956) at the beginning of the 20th century [33]. He discovered that when a metal, in the form of powder, is heated and converted to molten particles, can form a coating upon collision of molten particles onto a surface. At the beginning, only low-melting metals, such as tin and lead, were used. Some years later, a thermal spray device was developed that can spray metal wires. In this device, a flame generated by combustion of fuel with Oxygen was used in melting metal wires, then the melted metal is atomized and accelerated towards a substrate by a compressed gas. This method is named flame spray. Later the device was modified to accept powdered materials. Based on the principle of the flame spray high-velocity oxygen fuel technique (HVOF) was introduced at the beginning of the 1980s. To protect the components subjected to corrosive environments, a new spraying technique based on using the electric energy was introduced by Schoop [33] to accept new types of metals as coating materials. That technique was electric arc, which can accept spraying metals with high melting points such as steel, stainless steel, and zinc. The electric arc is the basis of the second family of spraying techniques. The third family of spraying techniques is known as cold spraying and is based on using gas-dynamic techniques, in

which the powdered metals are accelerated to speeds of 300 to 1200 m/s using nitrogen or helium as the process gas [33].

2.2 Thermal spray techniques

Different processes are employed to produce ceramic coatings in industrial applications such as thermal spraying, physical vapor deposition, chemical vapor deposition, etc. Thermal spray coating process is used to apply nonmetallic or metallic coatings. These coating processes are divided into three categories: plasma spray, electric arc spray, and flame spray, with a number of techniques falling under each other as shown in Figure 2. A brief description of some thermal spray processes is given below.

2.2.1 Flame spray

Flame spray was the first thermal spray technique developed. The hot flame is generated from the combustion of fuel gas in oxygen. The fuel can be oxyacetylene mixtures of hydrogen, and propane to obtain combustion about 3000 °C. Mostly oxyacetylene mixtures are used and they work at atmospheric pressure. The coating can be in the form of powders, wires, or cords. The particle velocity is less than 100 m/s. The feedstock material is melted by the flame then propelled by the flame and air jet towards the workpiece [32, 33, 38, 39].

2.2.2 Detonation gun

This technique was originally developed in 1955 by Union Carbide. The feedstock powder is introduced into a long tube (450-1350 mm) closed at one end. Combusting gases, acetylene or hydrogen with oxygen, are injected inside the tube. The mixture is ignited by a spark resulting in a high-pressure wave (2 MPa) propelling the particles, which are heated by the combustion gases.

The particle velocity is between 800-1200 m/s. This method produces dense and well-bonded coatings [33, 38, 39].

2.2.3 High-velocity oxygen fuel (HVOF)

HVOF is similar to the detonation-gun technique. In both techniques, fuel gases are combusted in a pressurized chamber. The difference is that the combustion here is continuous while in the previous technique is cyclic. Gases are introduced inside the combustion chamber under 0.3-0.4 MPa pressure. Then the exhaust gas passes through a small-diameter tube resulting in supersonic flame velocities. The feedstock material is injected inside the barrel axially or horizontally by a carrier gas resulting in a high speed of particles [33].

2.2.4 Plasma spray

This process has been considered as an effective and economical technique for producing ceramic coatings. In this process, an ionized gas is used to melt and propel the feedstock material. An inert gas, typically argon or argon-hydrogen mixture, passing through an electric field is heated to very high temperatures (6000-10000 K). Then, the gas is ionized by the electric arc to produce plasma, which can be defined as electrically charged particles. The feedstock material injected in the high-temperature plasma will immediately melt, then the molten droplets are accelerated toward a prepared substrate surface [2].

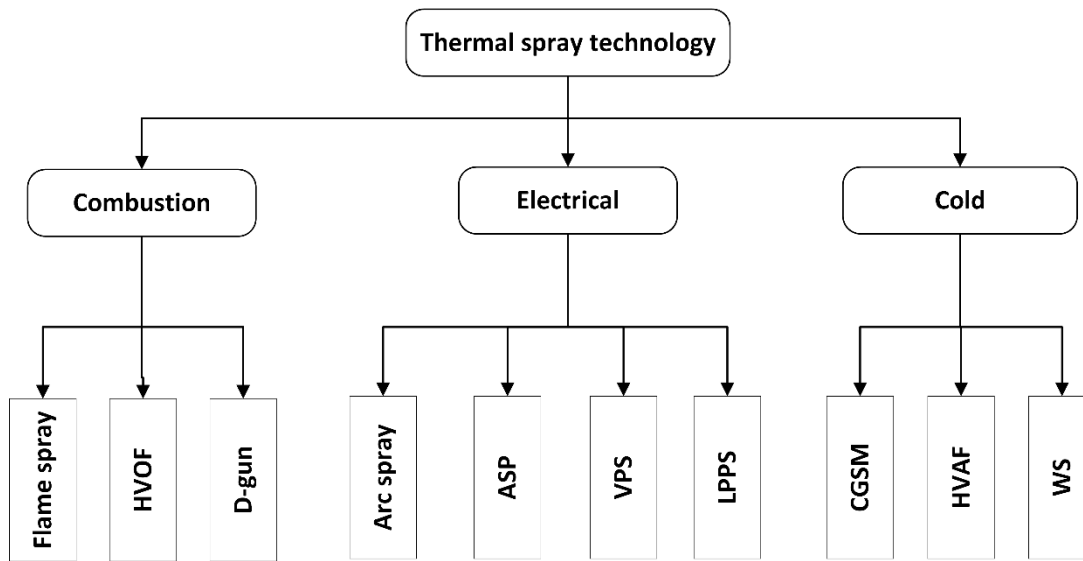


Figure 2 Family tree of thermal spray technology

2.3 Microstructure of coatings produced by thermal spraying

All thermal spray methods use a heat source to heat the coating material to a very high temperature until melting or semi melting occurs, then the molten particles are accelerated toward a prepared substrate surface [32]. Upon landing on the substrate surface, the particles strike the surface, flatten, rapidly solidify [2], and then mechanically and chemically bond to each other as the coating thickness accumulates [40–42]. The rapid cooling of the flattened particles (splats) results in a huge contraction of the splats, which in turn leads to structural defects and inter-splat cracks [43–45].

The structure of the coating produced by the thermal spraying process is greatly different from the structure of the bulk materials. The microstructure of the coating consists of a large number of layers called lamellae (layered structure). The lamellae are composed of a few layers of splats, where the structure inside the grain is columnar. Besides the lamellae structure, the coating

includes a large number of voids and pores, which have different shapes and sizes and are randomly distributed. The pores develop when the spaces between the contracted splats are not filled by the subsequent splats. This is believed to be the main source of pores. Vertical microcracks and horizontal delamination are also present. The vertical micro cracks arise from the weak adhesion or bad contact between splats or between lamellae. It can be said that the incomplete filling of interstices, the imperfect contact between splats and unmolten particles and cracks formed by solidification, relaxation of the quenching stresses, and thermal stresses contribute to the formation of the porous, defective coating microstructure [2, 40, 46]. Because of such structure, the thermo-mechanical properties of the coating differ from those of the corresponding bulk material [2]. Figure 3 shows a schematic view of typical thermal spray coatings.

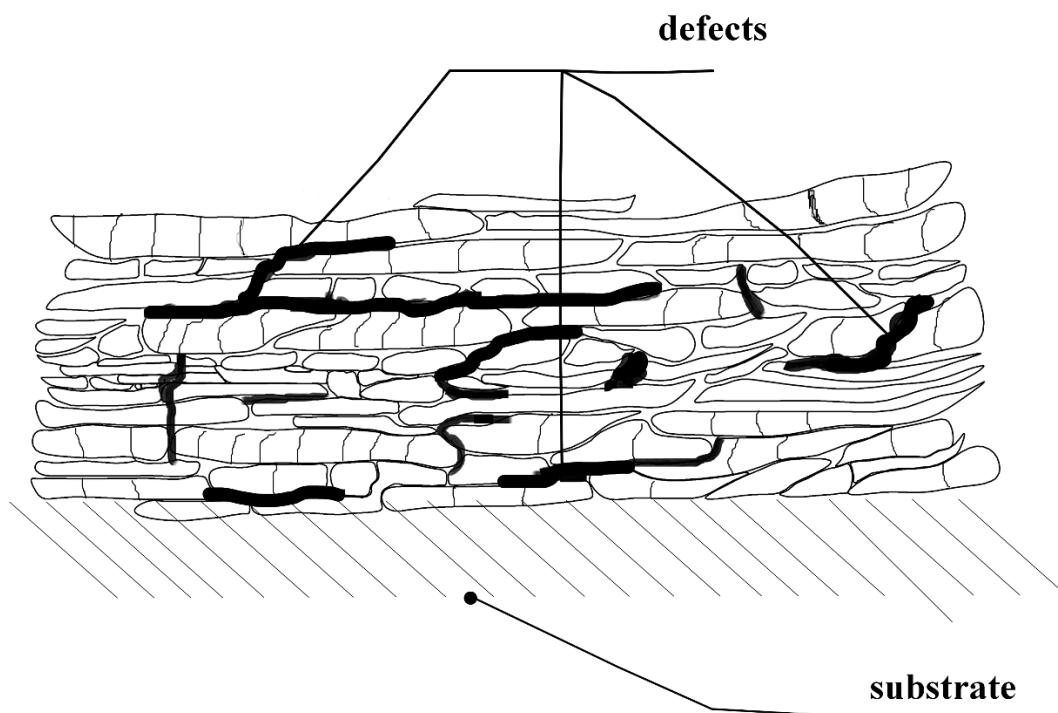


Figure 3 The microstructure of thermal spray coatings.

2.4 Simulation of thermal spray coatings

Physical properties of thermal spray coatings, such as microstructure, adhesion to the substrate, porosity, and surface roughness were found to be sensitive to a large number of process parameters such as gun speed, droplet size, temperature, solidification rate, and substrate material. To obtain uniform properties for thermally sprayed coatings, and to maintain good coating quality, coating process variables should be carefully controlled. Conducting experiments to study the effect of these parameters on the structure of the coating is expensive and time-consuming since new materials are required, and a large number of experiments should be run [47, 48].

The computational models have been built based on studying and analyzing the fluid dynamics and heat transfer associated with the impingement and solidification of the molten particles. Zhao et al. [49, 50] investigated the dynamics and heat transfer of the droplet when it strikes the substrate surface until it is spreading and flattening, forming a splat. They assumed that the droplet deformation is completed before the starting of solidification. Poulikakos et al. [51] divided the process of spray deposition into four regions. In The first region, the coating material is heated to a very large temperature until melting occurs with good fluidity. The second region is called the atomization region in which the liquid stream is disintegrated and converted into a spray. The third region is called the spray region in which further disintegration occurs and the spray transports into droplets. The last region is called impact or deposition region in which the droplets strike the surface of the substrate and solidify on it. The fluid dynamics and heat transfer occur in all four regions. In the spray region, convective cooling takes place, which might lead to partial solidification of the droplets prior to impact. Megaridis et al. published a numerical study on this region assuming laminar and axisymmetric flow conditions. Mostaghimi and Ghafouri-Azar [52] introduced a complete numerical model, which simulates three processes: spray droplets such as

velocity, temperature, droplet size and impact point, splat formation, and final coating structure covering the porosity and coating roughness. Flattening or deformation behavior and solidification rates are determined by the characteristics of spray particle (temperature, velocity). The shape of splats formed after droplet impact was assumed as a cylindrical disc, its diameter was computed from an analytical model based on Monte Carlo technique. The measurements of diameter, velocity, and temperature of particles performed by DPV2000 monitoring system have shown that the properties of these particles can be represented by a normal probability distribution. Computer models have been developed to optimize the process variables and predict the coating features due to difficulties in experimental optimization methods.

2.5 Residual stresses in TSCs

The major problem in thermally sprayed ceramic coatings on metallic substrates is the development of residual stresses due to the dynamics of the coating particles involved in the spraying process, and the difference in mechanical and thermo-physical properties between the coating and substrate materials [53]. Residual stresses occur during and after the coating deposition process. Residual stresses represent one of the technological challenges that face TBC industries. These stresses are inevitable results of the manufacturing and fabrication process and cannot be avoided [54]. It is important to understand the behavior of the residual stresses because they influence the thermal and mechanical properties of the coating, such as adhesion strength, thermal shock resistance, and coating service life [55]. The relationship between the residual stresses and coating longevity has been investigated in the literature; for example, McGrann et al. [56] studied the influence of the residual stresses on the fatigue life of thermally sprayed coatings and found a direct relation between the residual stresses and fatigue life. Araujo et al. [57] revealed that residual stresses play an effective role in coating adhesion. The failure of TBCs after exposure to several

thermal cycles can be attributed to the residual stresses developed during the coating process, the oxidation of the bond coat, the thermal mismatch between coating and substrate materials, sintering, and creep [58, 59].

2.6 Sources of residual stresses

2.6.1 Quenching stresses

These stresses occur due to the rapid solidification of splats upon their landing on the substrate surface or the previously deposited coating layers. The shrinkage (occurring within 10-100 μm) of the solidified splats is restricted by their adhesion to the underlying layer, thus tensile stress is induced inside the current deposited layer [54]. This process is called quenching or primary cooling. Figure 4 shows a schematic view of the development of this type of stress. The quenching stresses is a unique and important source of residual stresses. They have a significant effect on the structure of the coating. The value of quenching stress is a function of the properties of particles striking the substrate surface and the substrate temperature. It becomes independent of the substrate material when the coating accumulates and reaches a thickness of more than 10 microns [60, 61].

2.6.2 Thermal mismatch stresses

Thermal mismatch stresses occur after the deposition is complete and the coating has cooled to room temperature. These stresses are induced by the difference in thermal expansion coefficients between the deposited layer and substrate material. The residual stresses can be either compressive or tensile, depending on the materials and the number of coating layers [2]. It has a macro-level effect because the deposited splats can be considered as a continuous solid [55]. It has a larger influence and constitutes the major part of the final residual stresses. The residual stresses due to

thermal mismatch after deposition in a common coating system, ceramic/bond coat/substrate, are compressive in the ceramic TC because of its low coefficient of thermal expansion [2].

2.6.3 Peening stresses

Peening stresses occur due to the impact of the molten particles on the underlying coating layers. It was found in coating layers deposited by HVOF, D-gun, and cold spraying and not effective in plasma spray [62]. It is usually compressive due to the reaction forces induced by high-velocity impacts [39]. Kuroda et al. [63] studied the peening effect of the HVOF sprayed particles. They found that the intensity of the peening action and the resultant compressive stress induced by HVOF sprayed particles increase with the kinetic energy of the sprayed particles. Their results have shown that the residual stresses at the coating surface are low and often in tension, while the stresses inside the coatings are in a high level of compression. The absence of peening action at the last deposited splats leads to a low value of stress at the surface. Peening stress reduces the influence of the tensile quenching stress and transfer it to compressive stress within and beneath the deposited layer. Peening stress has a significant effect on the resultant residual stress, particularly in metallic coatings deposited by the high-velocity thermal spray process. Figure 5 schematically summarizes the development of peening stresses.

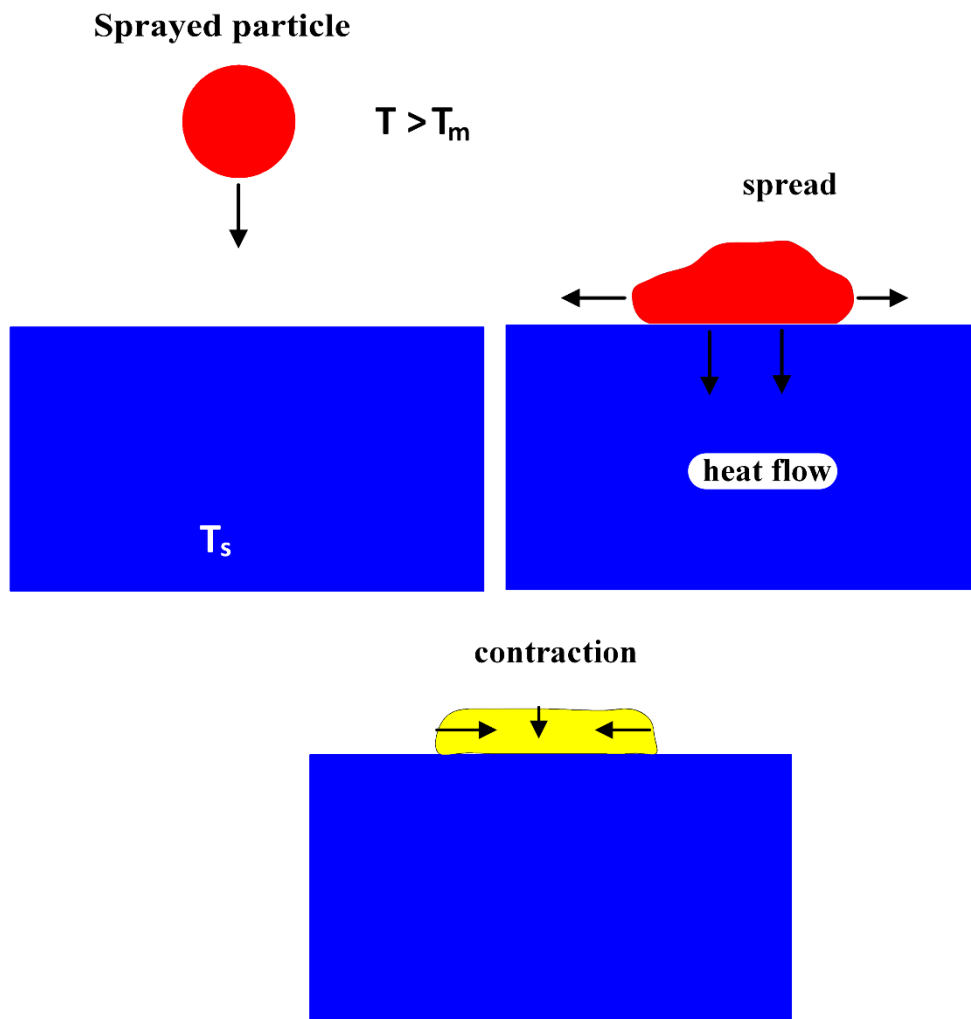


Figure 4 Quenching stress developed during splat solidification

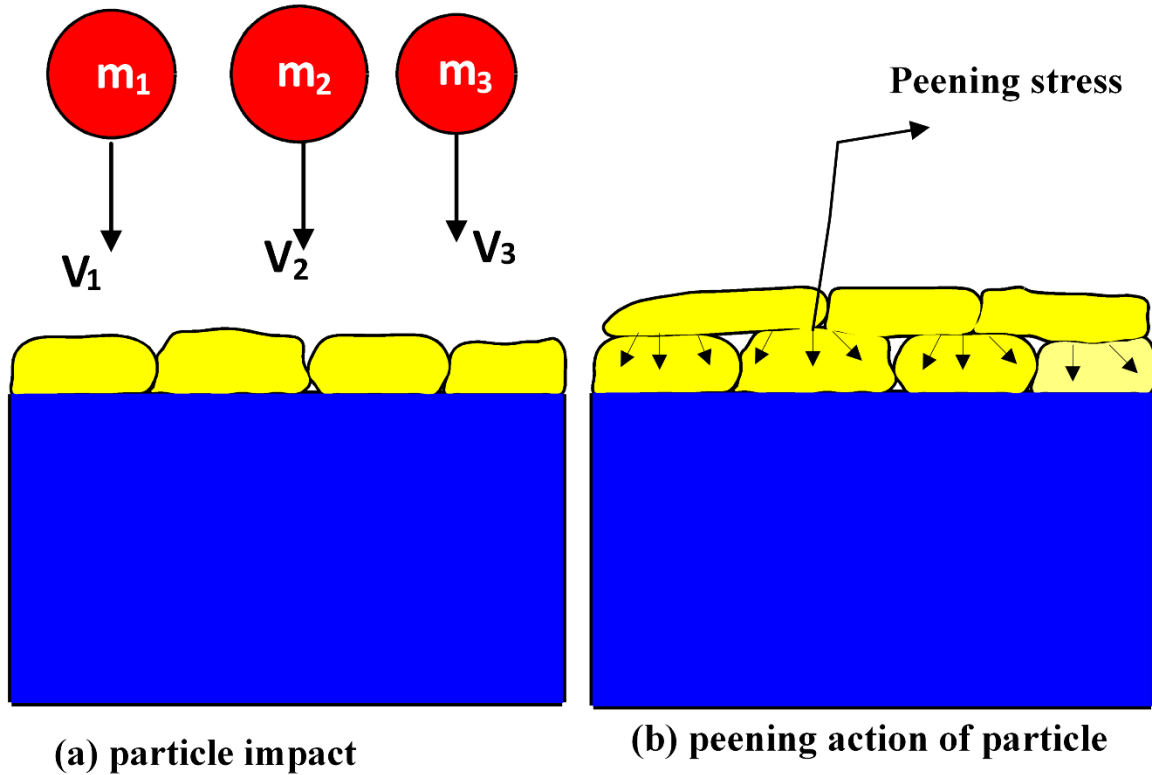


Figure 5 Development of peening stresses

2.7 Measurements of residual stresses

Various experimental techniques have been developed to determine the residual stresses. They have been classified into destructive and non-destructive methods. Destructive techniques involve material removal to evaluate internal stresses. One of the most widely used destructive techniques is hole drilling which involves drilling a small hole onto the coated material and monitoring stress relaxation by strain gauges mounted around the hole. The incremental hole-drilling method can be employed to measure the residual stress profile through the coating thickness. It involves drilling the hole in a series of small steps and measuring stress relaxation at each step [64]. It is applicable to all types of materials and is based on assumptions that the analyzed material is isotropic, elastic, and machinable [65]. However, it has some difficulties in mounting the strain gages. It is not

possible to access the whole hole regions with the strain gages. This limitation has been solved by combining optical approaches with hole drilling to measure stress relief [66]. The curvature method is another technique that is frequently used to estimate the residual stresses induced by coating processes. The deposition of a layer results in curving the substrate. Measurement of the resulting curvature caused by the addition of the coating layers can be employed in estimating the induced stresses [67]. Another destructive method is the sectioning technique, which relies on cutting and removing small slots from the specimen. The specimen will deform due to unbalanced internal stresses and strain gauges are used to measure the stress relief. This method has been widely used to evaluate residual stresses in structural carbon steel, aluminum, and stainless steel [65].

The non-destructive methods measure stresses without damaging the component or specimen. They usually measure some factor that is related to stress. They include X-ray diffraction, neutron diffraction, and the ultrasonic method. They have been used increasingly in parts subjected to fatigue damage. In many structural parts, such as bridges and aircraft, periodic inspection of internal stresses is required to avoid major damage or failure [65]. In components that are subjected to several kinds of loads, after long term service, internal stresses might concentrate in small regions, and values of stresses may become greater than the design value, which may lead to structural failure. The destructive techniques are not suitable for in-service components since they involve material removal. The non-destructive techniques are found to be reliable and effective in measuring the internal stresses and provide useful information about the performance of the in-service components [68].

2.8 Modelling of residual stresses

The issue with the mentioned experimental techniques is that they do not predict a detailed stress profile along the thickness of the coating. They only give the average value of the residual stresses. Additionally, many are difficult to apply for thin coatings. Various analytical and computational models have been suggested to simulate the variation of residual stresses through the coating thickness [69]. Tsui and Clyne [70] developed an analytical model to predict the residual stress distribution based on the concept of misfit strain. The model combined the stresses due to splat quenching and thermal contraction between coating and substrate during cooling. To obtain an accurate stress distribution, the coating deposition is considered as a progressive process (layer-by-layer deposition). It allows examining the effect of varying the number of coating layers on the residual stress distribution. A comparison between the block deposition (considering the deposition as a single layer) and the progressive deposition has been conducted and the results have shown a significant difference in the quenching stress level and the gradient between the two cases. This has been explained as that, in progressive deposition, the tensile quenching stress at the top of each layer is progressively reduced by the deposition of the subsequent layer. The residual stress distribution can be obtained directly by the material properties, the intrinsic stress, and the specimen dimensions. Zhang et al. [71] proposed an analytical model to predict residual stresses in elastic multilayer coating systems based on force and moment balances. The total strains of the coating and substrate are obtained from combining the stress strain and the bending strain, the quenching stress was neglected. The analytical model developed by Hsueh et al. [72] was based on the same concept as the Zhang model. They introduced a closed-form solution taking into account different elastic moduli for each coating layer. Most analytical models have been

developed based on the theory of elasticity, with several assumptions considered to derive the solution.

Recently, computational models have become more common. One commonly used numerical method for predicting residual stresses is the finite element (FE) method [54]. Some researchers simulate the residual stress evolution during the coating buildup at the micro-level [73–76]. They use the concept of fluid dynamics and heat transfer to simulate the deposition of a few particles. Such computational models focus on the droplet itself and analyze its thermal and mechanical behavior during the deposition. These computational models are limited to several droplets and are not practical to apply them for the whole coating process due to a large number of deposited droplets and the computational cost associated. Others simulate the residual stresses developed during deposition as well as the residual stresses due to the thermal loading cycle during service assuming that the TC is continuous and homogeneous, with a wave-shaped or flat interface [77–81].

The birth-kill finite element method has been used to consider both deposition and postdeposition stresses. The birth-kill technique is commonly applied to simulate the layer-by-layer growth of the deposition stresses (quenching). Killing (or deactivating) an element is obtained by reducing the values of material properties such as conductivity or stiffness to almost zero. This is done by multiplying these properties by a reduction factor mostly taken as 1×10^{-6} . In birth (reactivation), the element is multiplied by a reduction factor equaling unity [54].

CHAPTER 3

THE STOCHASTIC GEOMETRICAL MODEL

3.1 Introduction to SIMCOAT

The thermal spray process (Figure 6) can be simulated by SIMCOAT, a software that simulates the formation of thermal spray coatings as a function of process parameters. It predicts the thickness, roughness, and pores of the coating. The software uses a 3D stochastic model based on Monte Carlo technique. Figure 6 shows a stochastic view of the thermal spray process. The coating material is introduced to the thermal spray system in the form of fine particles (powder), where they are heated above the melting point, changed into small droplets, then accelerated at high speed towards a prepared substrate surface. When the molten particles impact on the surface being coated, they flatten, solidify, and bond to each other forming a thin layer. Inspection of this thin layer has shown that it is built up of thin lamellae, with large number of cracks and voids. The model spreads the molten particles on the surface being coated by generating random values of their properties (process variables). The model assumes that these properties follow a random distribution with user-defined means and standard deviations. The shape of splats formed after droplet impact is assumed as a cylindrical disc, with its diameter being computed from an analytical model.

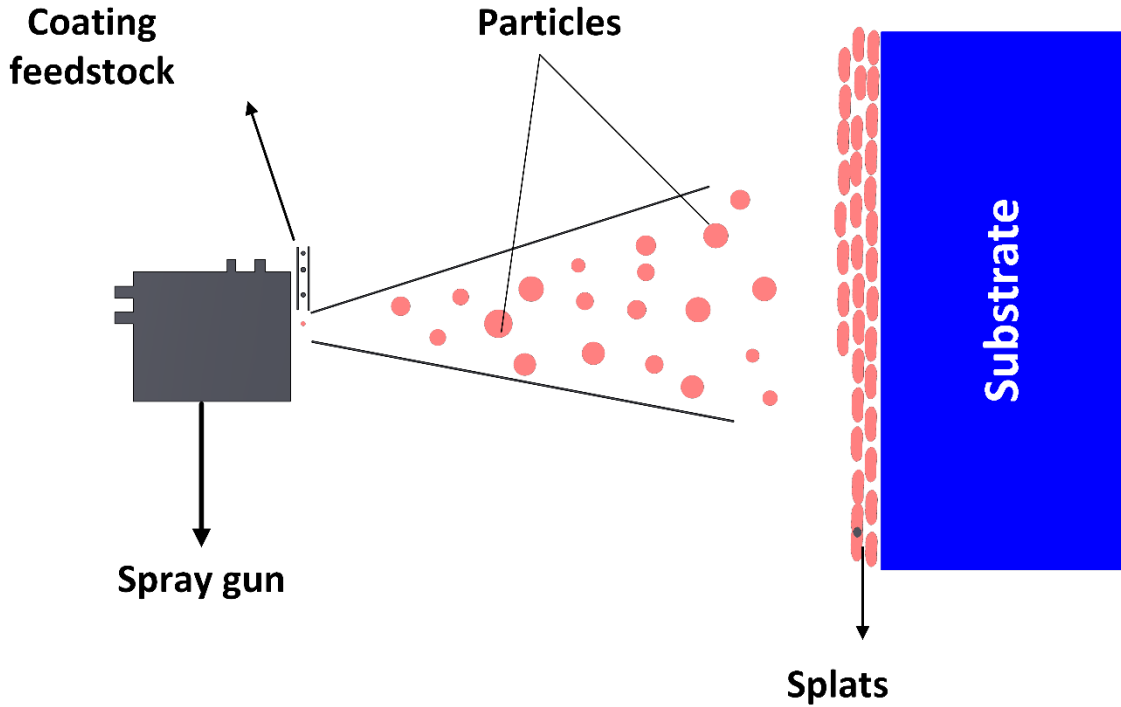


Figure 6 Schematic diagram of the thermal spray process

3.2 Numerical model

It has been reported that the properties of the thermal spray coatings are strongly dependent on coating process parameters. In this model, it was assumed that the values of particle temperature (T), speed (V), diameter (D), splat peripheral detachment, and impact point coordinates have random distributions. It was found from measurements that the values of the velocity and the temperature of the particle can be represented by a normal probability distribution termed by (μ, σ^2) with probability density function given by [47, 82]:

$$g(x) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(\ln x - \mu)^2\right) \dots\dots\dots(1)$$

Where g is a distributed variable, μ is the mean of the population and σ is the standard deviation of the population [82].

The particles landing positions were defined by using a spherical coordinate system as following:

$$x_c = Z \tan(\omega) \cos(\theta) \dots\dots\dots(2)$$

$$y_c = Z \tan(\omega) \sin(\theta) \dots\dots\dots(3)$$

where

Z: the distance between the gun and substrate.

ω : disperse angle.

θ : azimuthal angle.

3.3 Splat shape

This model assumes that the spherical droplet flattens upon impacting the solid surface and forms a cylindrical disc. Since the velocity, temperature, and the size of each droplet are given, it is possible to analytically predict the final shape of the splat. Pasandideh-Fard et al. [83] studied the dynamics of the droplet impact on a solid surface. They used energy conservation equations before and after impact to develop an expression for the maximum spread factor

$$\xi_{max} = \frac{D_{max}}{D_0} = \sqrt{\frac{We+12}{\frac{We}{\sqrt{Re}} + We\sqrt{3St/(4Pe)}}} \dots\dots\dots(4)$$

where We is the Weber number

$$(We = \rho V_0^2 D_0 / \sigma) \dots\dots\dots(5)$$

ξ_{max} is the maximum spread factor, D_{max} is the maximum splat diameter, D_0 is the droplet diameter before impact, Re is the Reynolds number, and St is the Stefan number.

The interaction between splats was determined by the distance between the droplet impact point and the center point of the closest previously deposited splat (L):

$$L = \text{Min}(l_n) \dots \dots \dots (6)$$

where l_n is the distance between the droplet impact point and the center of all previously deposited splats and is determined as follows:

$$l_n = (x_{c,n} - x_{c,q})i + (y_{c,n} - y_{c,q})j \dots \dots \dots (7)$$

where $x_{c,n}$, $y_{c,n}$ are the coordinates of the impact droplet.

Four possible scenarios (Figure. 7) have been developed to obtain the droplet overlaps based on experimental work and results of droplet impact simulations. The following rules were employed to select the splat shapes:

$$\left\{ \begin{array}{l} 0 \leq l < \frac{7D_m}{8} \dots \dots \dots \text{splat No. 1} \\ \frac{7D_m}{8} \leq l < D_m \dots \dots \dots \text{splat No. 2} \\ D_m < l \leq \frac{9D_m}{8} \dots \dots \dots \text{splat No. 3} \dots \dots \dots (8) \\ \frac{9D_m}{8} < l \leq \frac{D_n + D_m}{2} \dots \dots \dots \text{splat No. 4} \\ l > \frac{D_n + D_m}{2} \dots \dots \dots \text{no overlap} \end{array} \right.$$

where D_m is the diameter of the closest previously deposited splat, and D_n is the diameter of the current splat. In the case of no overlap, the splat will be disc-shaped and its diameter is obtained

from equation (4). In the case of splats interaction (noncircular splats), the shape is obtained using equation (8) [77].

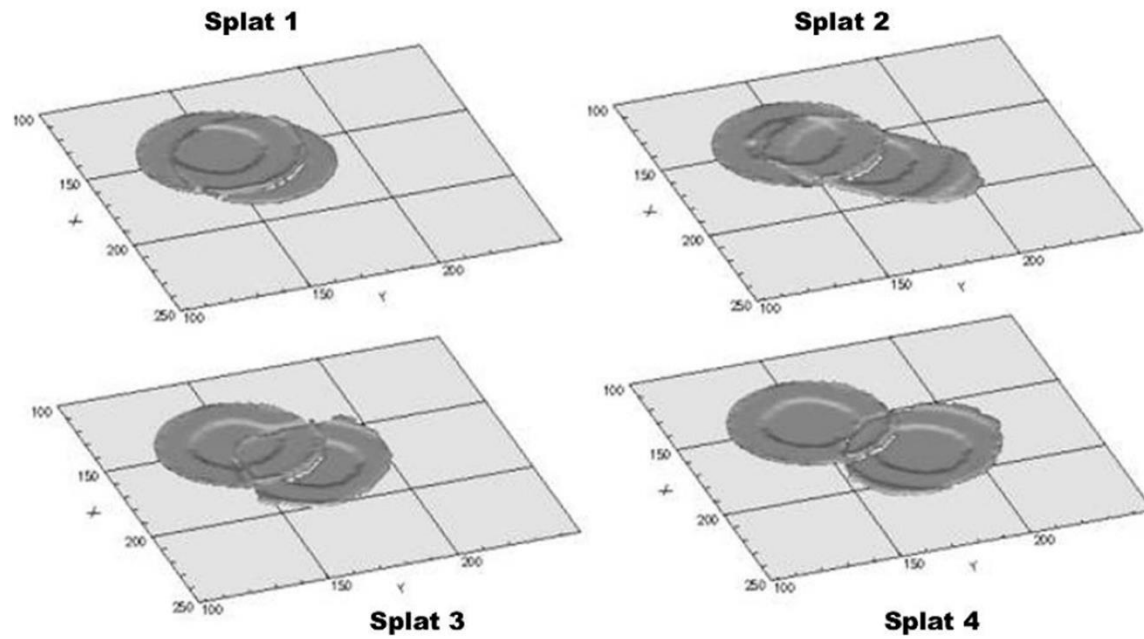


Figure 7 The four possible scenarios of droplets overlap [47].

3.4 Formation of pores

Several sources of coating porosity have been specified, they include curling up at the periphery of splats due to thermal stresses, the presence of satellite droplets around the splat, the existence of unmolten particles, and pores due to incomplete filling of interstices.

Ghafouri et al. [47] assumed in the old version of the stochastic model that the development of porosity is completely caused by curling up of splats. Xue et al. [84] reported that in ceramic coatings, the presence of micro-cracks release the thermal stresses and reduce the effect of splats curling up. They reported that the main and most important source of porosity in ceramic coatings is the incomplete filling of interstices. This is because the surface tension prevents the molten droplets from penetrating the previous coating layer and filling small gaps between splats as illustrated in Figure. 8. The current SIMCOAT version automatically considers the incomplete filling of interstices as the main source of the coating porosity. SIMCOAT also provides additional options of pores curling up model, unmolten particle model, and satellite droplet model. In this work, those additional options were not considered since a ceramic coating is considered and a preheated substrate (700°C). according to Hamideh et al. [85], the effect of satellite droplets can be neglected when the substrate temperature is high.

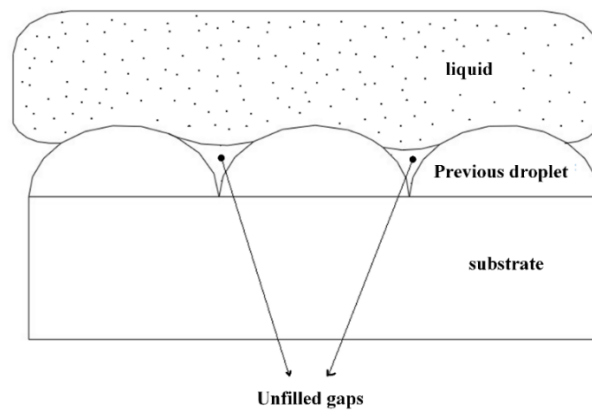


Figure 8 Contact between the molten droplet and rough surface: unfilled voids due to surface tension

3.5 Coating build-up

The coating is formed as the splats accumulate on each other, with small gaps between them leading to porosity. SIMCOAT defines the computational domain using three-dimensional cartesian grid. The domain (Figure. 9) is divided into small equal cells to track the position and shape of the coating surface. The volume fraction, which is the fraction of the cell occupied by the coating material, is used to define the coating structure [82].

$$f_{i,j,k} = \frac{1}{\Delta x_i \Delta y_j \Delta z_k} \int_{\Delta x_i} \int_{\Delta y_j} \int_{\Delta z_k} f_s dx dy dz \dots \dots \dots (9)$$

where $f_{i,j,k} = 1$ when the cell is filled completely with the material, $f_{i,j,k} = 0$ when the cell is completely empty or the whole volume of the cell is a pore, and $0 < f_{i,j,k} < 1$ when the cell is partially filled.

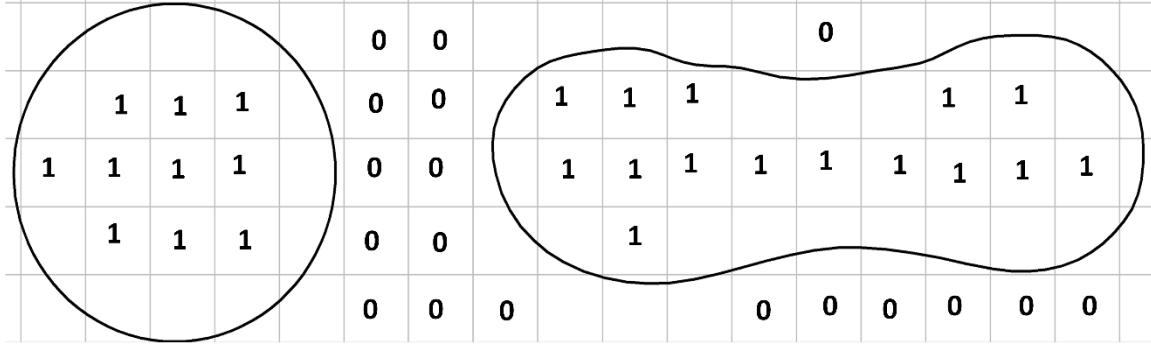


Figure 9 Discretization of splats in the computational domain

3.6 SIMCOAT input data

SIMCOAT uses the coating process parameters as input data to simulate the coating structure.

Figures 10-13 show the input data required by SIMCOAT. The input data includes [85]:

- The substrate properties: the length and width of the substrate, and the maximum number of grids in the three directions.
- The inflight conditions of the particles and their transportation properties: the mean values of particle diameter, temperature, velocity, and dispersion angle, and the standard deviation of each value.
- The conditions of the spray gun: the initial position, standoff distance, and step size.
- The properties of the coating material

Computational Domain

Help ?

1. Specify the length of the calculation domain in each direction [m]:

X- direction (Length)

Y-direction (width)

2. Specify the number of grids on the substrate in the X, Y, and Z (coating), directions:

IMAX:

JMAX:

KMAX:

Cancel < Back Next >

Figure 10 Computational domain input data

Stochastic Data

Help ?

1. Give the droplets' velocity, m/s:		3. Give the droplet's temperature, C:	
1.1 Mean velocity	219.00	3.1 Mean temperature	2606.00
1.2 Standard deviation	55.00	3.2 Standard deviation	225.00

2. Give the droplets' size, microns:		4. Give the spray dispersion angle, degree:	
2.1. Mean diameter	50.000	4.1 Mean angle	0.00
2.2 Standard deviation	10	4.2 Standard deviation	20.00

5. Give a random seed number: 500

Cancel < Back Next >

Figure 11 Stochastic data

Spray Gun

Help ?

1. Material loading rate, kg/s: 0.40000E- 1.1 What is the deposition efficiency, %? 70

2. Is the gun moving? ☒ Yes ☐ No

If the gun is stationary, what is the total time for the coating process, s? 0.10000

3. If the gun is moving, does it have a constant speed?

☒ Yes ☐ No

Note that if the speed of the gun is not constant, it is assumed that the gun moves in a sinusoidal pattern. Give the gun velocity in the Y direction, m/s: 0.00000

3.1 Gun velocity in the X direction, m/s: 0.63500

3.2 Gun step size in the Y direction, m: 0.00560

4. Total number of passes: 5

5. Spray gun distance from the substrate, m: 0.10000

6. Initial gun position, m:

- In the X direction: -0.01000

- In the Y direction: 0.00000

Cancel < Back Next >

Figure 12 Spray gun input data

Coating Properties

Help ?

1. Substrate temperature, C

2. Please specify the droplet material:

Alumina
Molybdenum
Nickel

File Name

If you use another droplet material rather than those listed above, you must create a "property" file as described in the Manual, before starting the code.

Cancel < Back Next >

Figure 13 Coating properties input data

3.7 The first three models of Ytria-Stabilized Zirconia (YSZ)

In this study, SIMCOAT has been used to simulate the coating deposition process and the final coating structure. Three coating models were generated. The following three process parameters were varied: the material feed rate, the gun speed, and the total number of passes, while the other parameters were maintained constant. The substrate size was 1 by 1 mm, and the coating material was selected to be Ytria stabilized Zirconia (YSZ). The computational domain was divided into 1000 cells in the X direction, and the code automatically specifies the number of cells in the Y

direction (1000 cells in this case) from the already assigned substrate dimensions and No. of cells in the X direction.

Table 1 lists the statistical information used in the three models. The particle's diameter, velocity, and temperature are the most important parameters that influence the coating microstructure. The main temperature of the particle was selected to be above the melting point of YSZ, which indicates higher deposition efficiency [85]. The spray dispersion angle can be specified from the diameter covered by the gun and the distance between the substrate and the gun. It was assumed that it has a normal distribution with a mean that lies along the axis of the spray gun. Its standard deviation was chosen to be 2.5 degrees, and a number of models were run in order to select the relevant dispersion angle standard deviation. It was observed that when using a value smaller than 2.5 degrees, concentration of the particles in certain regions of the substrate took place, resulting in a rough coating system. When using larger values, the particles scatter out of the substrate, since a relatively small computational domain (1x1 mm) was used. The selected value was chosen to give good distributions of the particles. Hamideh et al. [85] reported that the standard deviation of the dispersion angle is normally less than 10 degrees. Table 2 lists the spray gun positions; SIMCOAT assumes that the gun is moving in the X direction (velocities will be reported in the following sections) to complete one pass, then it steps 0.5 mm in the Y direction to start the next pass. After covering the whole substrate, the gun will move back half of the step size along the Y direction and starts moving in X direction to build a new layer [82]. In the passes following the first pass, the gun will return to use the original step size until covering the new layer. The initial gun position was chosen half of the step size (-0.25 mm) in order to overlap passes, to serve good particles distributions, and to avoid the formation of peaks. Since the initial gun position is out of the substrate, and the step size is half of the substrate width, three passes are

needed to cover the whole substrate and create the bottom layer. each following layer is created in two passes since the initial gun position corresponds to the edge of the substrate.

Table 1 Coating process parameters for the three models

Particles' information	Mean/value	Standard deviation
Droplets' size (diameter in micron)	50	2
Droplets' temperature (Celsius)	2550	5
Droplets' velocity (m/s)	219	5
Dispersion angle (degree)	0	2.5
Spray gun distance from substrate, mm	80	-
Initial gun position in X direction, mm	-0.25	-
Initial gun position in Y direction, m	0	-
Step size in y direction, mm	0.5	-

3.7.1 Single-layer model

Table 2 lists the material feed rate, the total number of passes, and gun velocity assigned to this model. The combination of these parameters was selected to produce a coating thickness of approximately 200 microns. According to the gun step size, its initial position, and substrate dimensions, three passes were needed to cover the substrate and create one layer. It was assumed that the gun is moving in the X direction at a constant speed. Figure 14 (a) shows a 3D plot of the deposition, where the legend illustrates the coating thickness. The results of the run are reported in Table 3.

3.7.2 Two-layer model

In this model, two parameters were changed while obtaining an approximate thickness of 200 microns. The material loading rate was decreased while the total number of passes was increased. According to the step size and the initial gun position, five passes are needed in order to create two layers. The gun velocity was left constant at 0.25 m/s. The parameters are listed in Table 2. Table

3 shows the results of the simulation. Figure 14(b) shows an isometric view of the two-layer YSZ coating over the substrate.

3.7.3 Three-layer model

Since the number of layers is increasing, the spray gun has to increase and/or reduce the material feed rate in order produce thinner layers. Both were changed in this case to increase the total number of passes. The parameters are listed in Table 2. The final coating structure is shown in Figure 14 (c). The percentage of pores, the average thickness, and roughness are listed in Table 3.

Table 2 Variation between process parameters for the three models

Parameter	Model		
	Single layer	Two layers	Three layers
Gun velocity in X Dir., m/s	0.24	0.25	0.3
Total NO. of passes	3	5	7
Material loading rate, Kg/s	0.0009(54 gr/min)	0.0006(36 gr/min)	0.00055(33 gr/min)

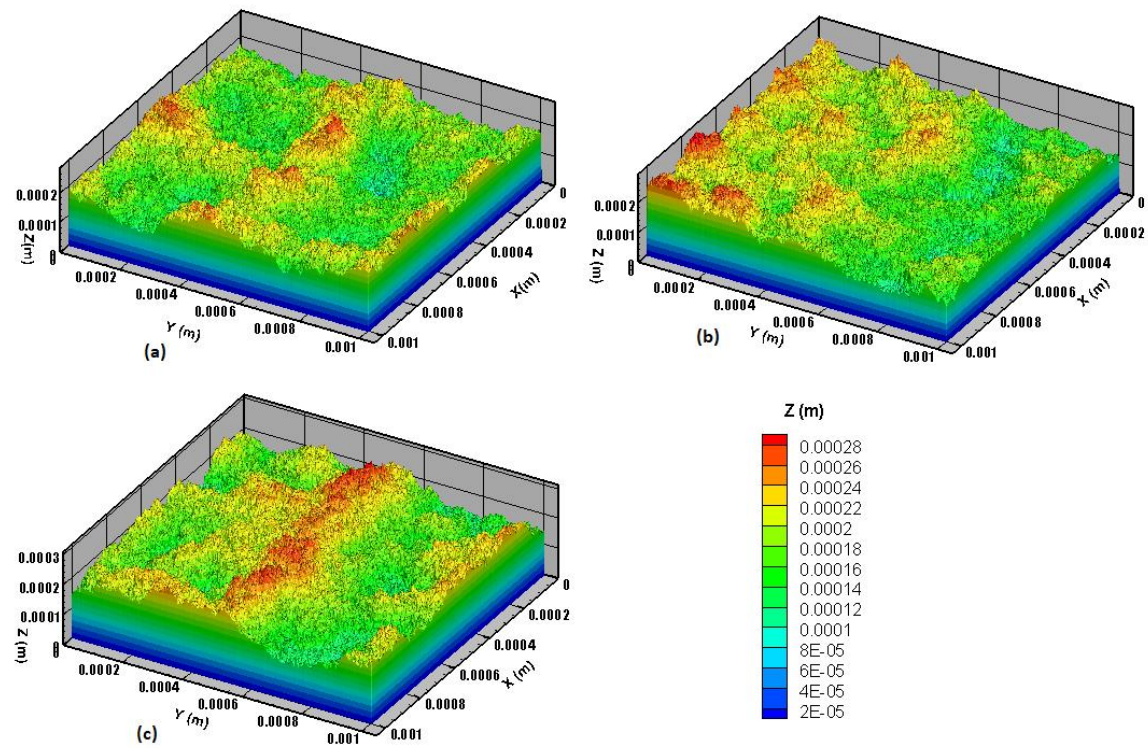


Figure 14 An isometric view of YSZ coating. (a) single-layer (b) two-layers (c) three-layers models.

Table 3 Coating simulation results for the first three models

Parameter	single-layer model		Double-layers model		three-layers-model	
	X Direction	Y Direction	X Direction	Y Direction	X Direction	Y Direction
Porosity, %	1.01	1.076	1.0391	1.21629	0.9779	0.934
Thickness, μm	171	200	171	191	188	247
Roughness, μm	28	13	25	17	29	12

3.8 The fourth model of Yttria-Stabilized Zirconia (YSZ)

In this model SIMCOAT4.5 has been used to simulate the spraying of YSZ particles on stainless steel, figure 15 shows an isometric view of this model. The substrate size is 1 by 1 mm. the statistical information (mean and standard deviation) about the initial particle's conditions (temperature, velocity, and diameter) has been directly assigned to the software as shown in table 4. It should be noted that the software can accept the particle's information from the DPV2000 measurements. The computational domain was discrete into 1000 by 1000 cells in the X and Y directions to obtain a high resolution of the coating structure. SIMCOAT provides two options of the spray gun movement: constant speed and sinusoidal gun movement over the substrate. The former option was selected in which the gun is moving in x-direction along the substrate surface and the gun velocity in the Y direction is zero. When the gun moves from one edge ($X=0$) to the corresponding edge ($X=L$) of the surface being coated, it completes one pass after that it will step along the Y direction as much as one step size and move back along the X direction to make another pass. The gun will continue moving back and forth over the substrate until it is completely covered. In order to obtain a smooth coating surface, the gun must provide a good distribution of the particles. The location of the landing for each droplet is obtained from the dispersion angle and the standoff distance (distance between the gun and substrate). The dispersion angle was assumed to have a mean equals zero degree which lies on the gun axis. the particle distribution is strongly dependent on the standard deviation of the dispersion angle which was selected as 2.5 degrees, as mentioned above this value gives good distributions of the particles. The simulation results for this model are listed in table 5.

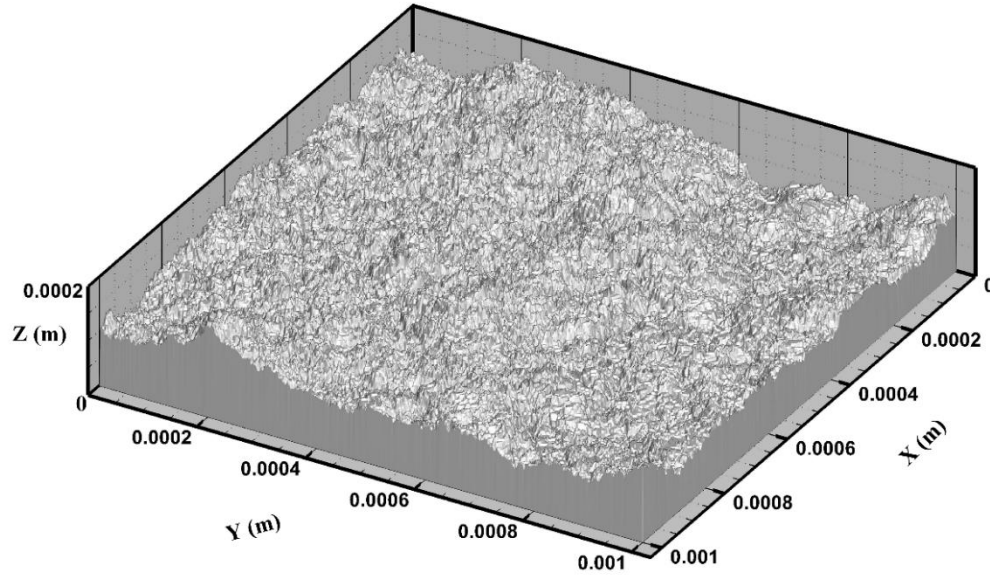


Figure 15 Isometric view of YSZ coating for the fourth model

Table 4 Process parameters for the fourth model

Particles' information	Mean/value	Standard deviation
Droplets' size (diameter in micron)	50	2
Droplets' temperature (Celsius)	2550	5
Droplets' velocity (m/s)	219	5
Dispersion angle (degree)	0	2.5
Initial gun position in X direction, mm	-0.25	-
Initial gun position in Y direction, m	0	-
Step size in y direction, mm	0.5	-
Total No. of passes	5	-
Gun velocity in X Dir., m/s	0.4	-
Material loading rate, Kg/s	0.0006	-

Table 5 Coating simulation results for the fourth model

Parameter	Result	
	X Direction	Y Direction
Porosity, %	1.35	1.64
Thickness, μm	107	124
Roughness, μm	23	15

CHAPTER 4

2D RESIDUAL STRESS DEVELOPMENT MODELS

4.1 FE model

To simulate the thermal stresses developed by the thermal spraying process, the simulated coating geometry must be converted into an FE model. An in-house code was built to extract the coating roughness and convert it into text format, then a python code was written to convert the text file into a 2D CAD geometry that can be imported into any commercial FE software. SIMCOAT was linked with TECPLOT [86] to provide data visualization (Figure 14). TECPLOT provides the data of the 3D simulation of the coating structure in terms of several planes, each plane divided into small cells. The coordinates and porosity values of each cell were stored in a data spreadsheet. Each model includes 100 planes (indexed from 1 to 100) parallel to the XZ plane. Two slices (planes) were selected, indexed as 5 and 30 of each model parallel to the X-axis. Only the roughness values were extracted, while geometrical porosity was neglected by assuming that the coating surface was completely solid. Adding pores would be of importance to studies investigating crack propagation, which could be an extension of this work. As for predicting the deposition residual stresses between the coating layers, it is reasonable to assume that the effect of geometrical pores can be neglected. However, it is important to note that the material properties are those of the material with the pores presented within them. 2D FE models are considered because they represent the worst case in terms of strength. The average thickness was calculated for each model (listed in Table 4), and all models had very close thickness values. The substrate

thickness was set to 0.5 mm. Plane 30 of the one-, two-, and three-layer models is shown in Figure 16. ABAQUS [87] was used as the FE solution tool to conduct the stress analysis. In the one-layer model, the coating is adhered to the substrate with tie constraints at the interface. In the two- and three-layer models, tie constraints are applied between the substrate and the bottom layer and between subsequent layers.

Periodic boundary conditions are applied at the edges (figure 17). Material properties of stainless steel and YSZ, assigned to the substrate and coating, respectively, are listed in Table 5. To consider stress relaxation due to plastic deformation, plastic properties were defined for both coating and substrate. The initial temperatures for the substrate and the coating were set to 700 and 2550 °C, respectively. Coupled temperature–displacement transient analysis with multiple time steps was conducted. During spraying, heat transfers from the molten particles by two mechanisms. The first is conduction to the substrate, or the previously deposited layer, due to the higher initial temperature of the molten-sprayed particles. During solidification, the latent heat associated with the phase change from liquid to solid is released and conducted to the underlying layers and substrate. The second mechanism is the heat loss at the bottom surface of the substrate and the top surface of the coating due to natural convection cooling. In the two-layers and three-layers models, the layer-by-layer buildup was assumed. Model change interaction was applied to deactivate and reactivate elements to simulate the deposition of the two and three coating layers using the birth-kill FE technique. In the two-layer model, the top layer was deactivated (killed) in the first step and reactivated in the second step. At the third time step, natural convection was applied to cool the assembly to room temperature. In the three-layer model, the middle and top layers were activated in the second and third steps, respectively. In the fourth time step, the coated substrate was cooled. To conduct the analysis, the models were discretized into small elements, as

shown in Figure 16, with a more refined mesh at the rough surfaces to capture the geometrical details of the roughness. The number of elements and type of elements for each model are listed in Table 4. Plane stress analysis was conducted for each case.

Table 6 Average thickness & number of elements of the selected slices

Model	Plane	Average thickness micron	Thickness STD, micron	Total No. of Elements	Type of Elements	
					CPS4RT	CPS3T
single-layer model	plane 5	190	19	11343	10839	504
	plane 30	188	22	11050	10516	534
two-layers model	plane 5	219	22	9527	9302	225
	plane 30	220	23	9955	9713	242
three-layers model	plane 5	189	25	9283	9029	254
	plane 30	189	21	8945	8606	339

Table 7 Material properties of YSZ & stainless steel [88][89]

Property	YSZ	301 Stainless Steel
Density, (Kg/m ³)	5890 @ liquid & solid state	7900
Latent heat, (J/Kg)	7.07E+05	-
Specific heat, (J/Kg K)	713 @ liquid state 580 @ solid state	477
Thermal conductivity, (W/m K)	2.32 @ liquid state 2.0 @ solid state 9.68E-6 @ 20 °C.	14.1 16.6E-6 @ 100°C.
Coefficient of thermal expansion, (1/°C).	10.34E-6 @ 1000°C. 11E-6 @ 2527°C.	17.6E-6 @ 300°C. 18.6E-6 @ 500°C. 19.5E-6 @ 700°C.
Elastic modulus E (GPa)/ Poisson ratio	63.4/0.21 @ 20°C. 28.33/0.21 @ 2000°C. 26.67/0.21 @ 2522°C. 3E-3/0.4 @ 2532°C. 3E-3/0.4 @ 3000°C.	200/0.3 @ 700°C. 0.2/0.4@1400°C.
Melting point,(°C).	2527°C.	
Heat transfer coefficient of air (W/m ² K)	20	20
Yield strength (MPa)	30 (tensile) 300 (compressive)	Johnson-Cook parameters: A=310, B=1000, C=0.07, n=0.65, m=1

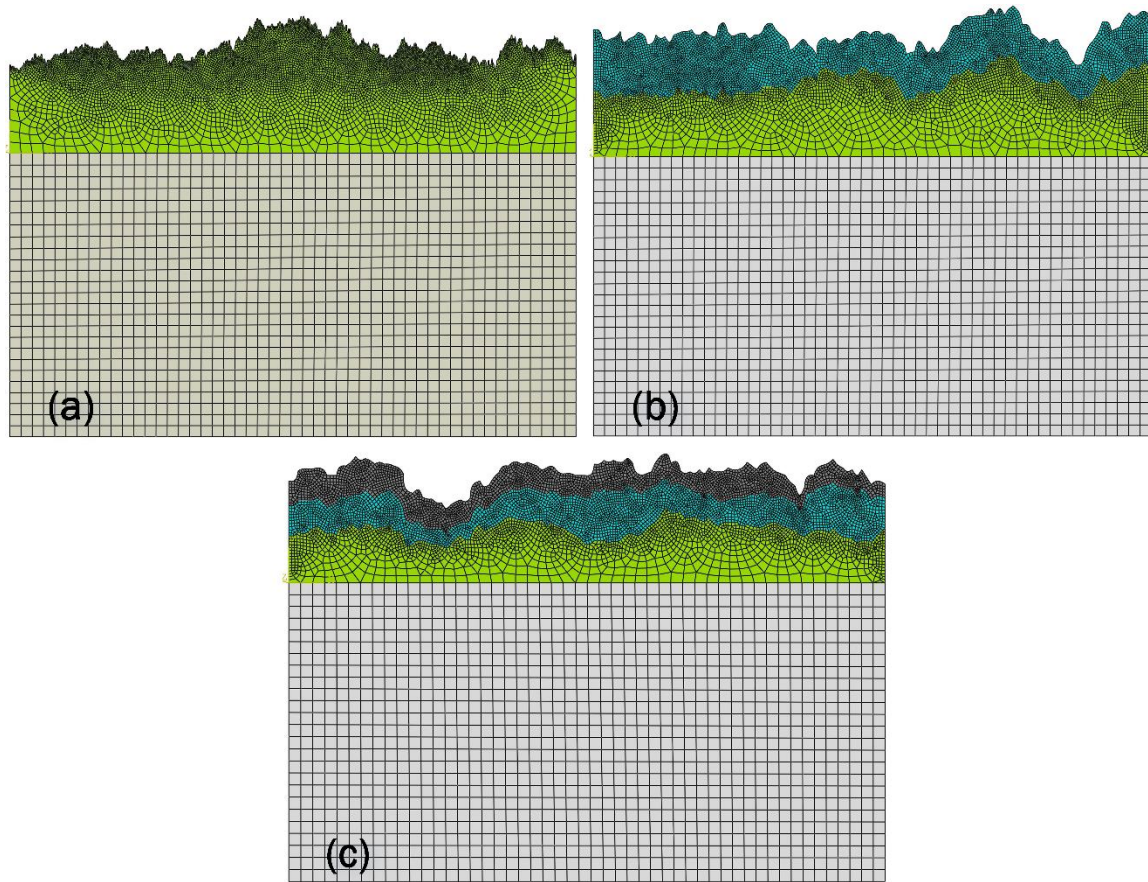


Figure 16 Meshing of slices No. 30 (a) single-layer model (b) two-layer model (c) three-layer model.

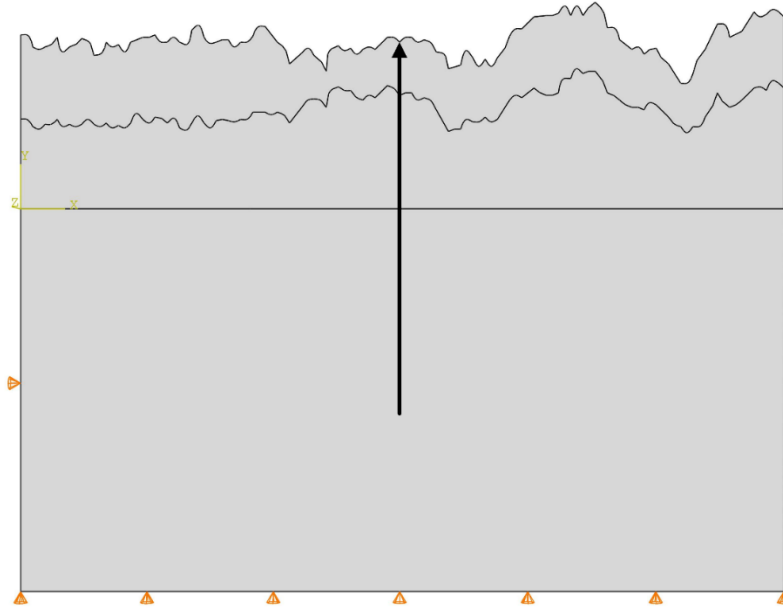


Figure 17 Applied boundary conditions and path created for residual stress variation along thickness.

4.2 Results and discussion

The thermal stresses developed due to the thermal mismatch between the substrate and coating materials, during and after deposition, for one-, two-, and three-layer models are investigated in the longitudinal direction. For each case, a path starting from 0.3 mm substrate depth up to the top surface of the coating was created. It was located exactly in the middle of the substrate length to exclude the effect of the free boundaries (Figure 17). Figures 18, 19, and 20 show the stress distribution contours for the three models before and after cooling, while Figures 21, 22, and 23 show the residual stresses before and after cooling for the middle path shown in Figure 16.

Figure 18(a) shows the quenching stress distribution, while Figure 18(b) shows the residual stresses due to the thermal mismatch at the end of the cooling step of the one-layer model. These stresses are graphically shown in Figure 21. The stresses developed in YSZ coating because of quenching are tensile with a maximum value around 108 MPa, while those generated in the coating

because of thermal mismatch are mostly compressive with a maximum of 135 MPa. In the thermal stress profile, the stress is also higher at the coating–substrate interface and decreases close to zero at the free surface. It has been reported that the maximum stress is always at the interface [64, 90] and that the residual stresses developed inside the coating particles upon its deposition and rapid solidification are always tensile. Adhesion to the substrate or previously deposited splats restricts particle contraction and induces tensile stresses [2]. The low magnitude of the quenching stress is attributed to the plastic material properties, which are considered to have a stress relaxation effect due to interfacial sliding and microcracking associated with the ceramic coating [2, 61].

The residual stresses developed in the two-layer model during the deposition and cooling are shown in Figures 19 and 22. The stresses developed after the deposition of the bottom and the top layers are shown in part (a). As with the one-layer model, the deposition of the bottom layer induces tensile stresses. However, the stress values show a significant increase in quenching stresses. Stokes and Looney [91] analytically studied the dependence of the quenching stress on the deposited thickness and found that increasing the deposited coating layer's thickness reduces tensile quenching stresses. This effect can be clearly observed by comparing Figure 19 (a) and 19 (b). Moving to the deposition of the top layer, there is a clear significant change in the deposit stress profile. The stress at the upper part of the bottom layer has changed from tensile to compressive, while the compressive stresses in the substrate decreased to zero. This can be explained in that continuing the deposition of material on the top of the previously deposited layer will develop compressive stress under the current deposited one. The contraction of the new particles is impeded by the old underlying solidified splats. The stress-free state produced in the substrate can be attributed to the balance between the tensile and compressive stresses that occurred within the coating layers. Figures 20 and 23 show the stress contours and profile for the

three-layer model. Similarly, the stresses are higher at the interface between the substrate and coating, where spallation usually occurs. The maximum stresses developed at the interface are 350 and - 134 MPa on the substrate and coating sides, respectively. The residual stress change in the coating/substrate may result in cohesion loss and consequently reduce the coating longevity.

Figure 20 (a), (b), and (c) shows the distribution of stresses developed during the deposit of three YSZ layers on the stainless steel substrate. In this case, the gun is moving fast, thus producing thin layers. The increase in quenching stresses within the coating layers confirm what was written previously about the stresses' dependence on coating thickness; the quenching stresses are highest (around 130 MPa) on the coating side. Usually, microcracking associated with ceramic materials is believed to reduce the quenching stresses to lower values compared with metals [61]. The resultant residual stresses in the three-layer model are shown in Figure 20 (d).

There is no difference in the final residual stresses developed in the three coating models. This can be explained because the mismatch of the thermal expansion coefficients of the different materials is the dominant source of the residual stresses here. In most regions on the coating side, the final stresses are around -135 MPa. Thermal mismatch stresses are compressive in ceramic coatings because they possess a low thermal expansion coefficient compared with the underlying substrate. Although the final residual stresses are almost the same in the three coating models, they have different maximum stress locations that would affect the crack initiation and propagation, and hence, the microstructural details due to their different process parameters. The results show that depositing a certain coating thickness using different sets of process parameters leads to different quenching stress distributions. The same study was conducted for the second slice (slice No. 5); the combined results for each slice are shown in Figure 24 (a) and (b).

The results show no major difference between the curves in each figure, which indicates an independence of the results in terms of the plane selection and that the 2D slice selection provides general results for the whole coating. Abubaker et al. [88] experimentally studied the internal stress induced in YSZ coating applied to stainless steel. They used the incremental hole-drilling method to determine the residual stresses. Their coating sample was deposited in six passes with a final coating thickness of 150 microns. Stresses acting in YSZ coating are plotted in Figure 24. Stress profiles obtained in our work are in close agreement with those measured experimentally. It is important to note the difference in process parameters and hence the differences in values. However, the change between the tensile and compressive states and the behavior of the residual stresses was the same.

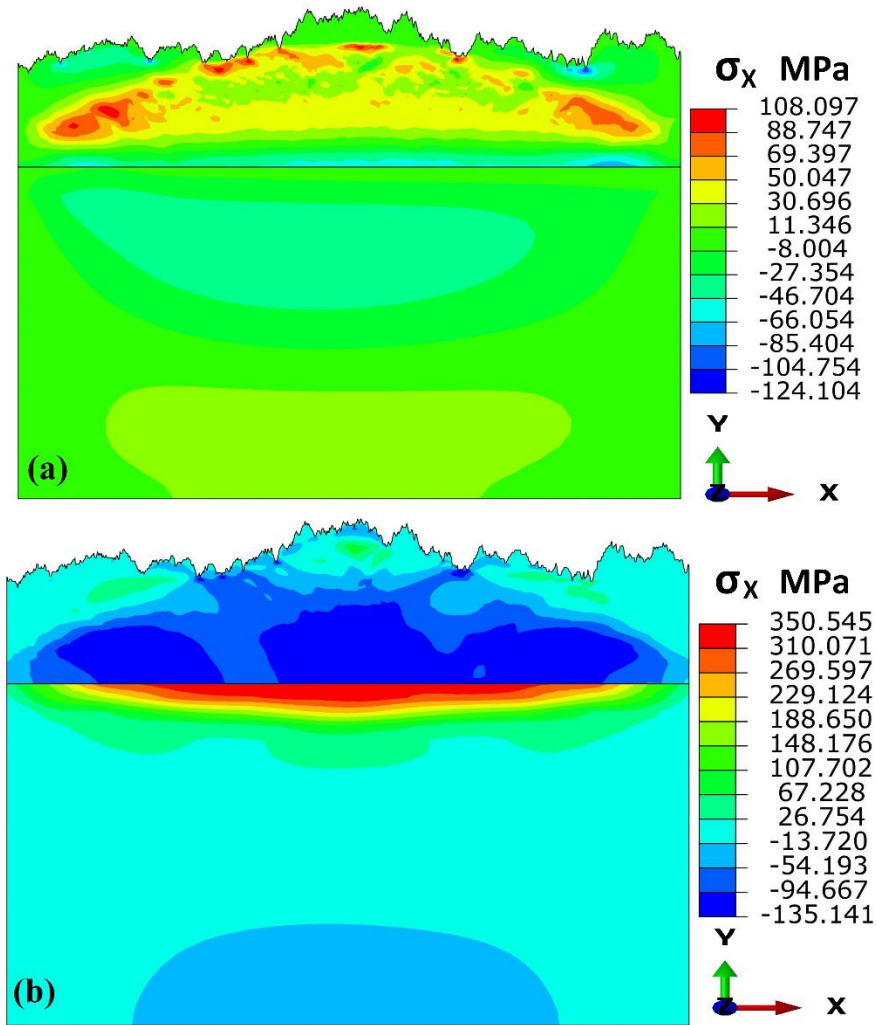


Figure 18 Residual stresses in the one-layer model: (a) quenching and (b) final thermal stresses

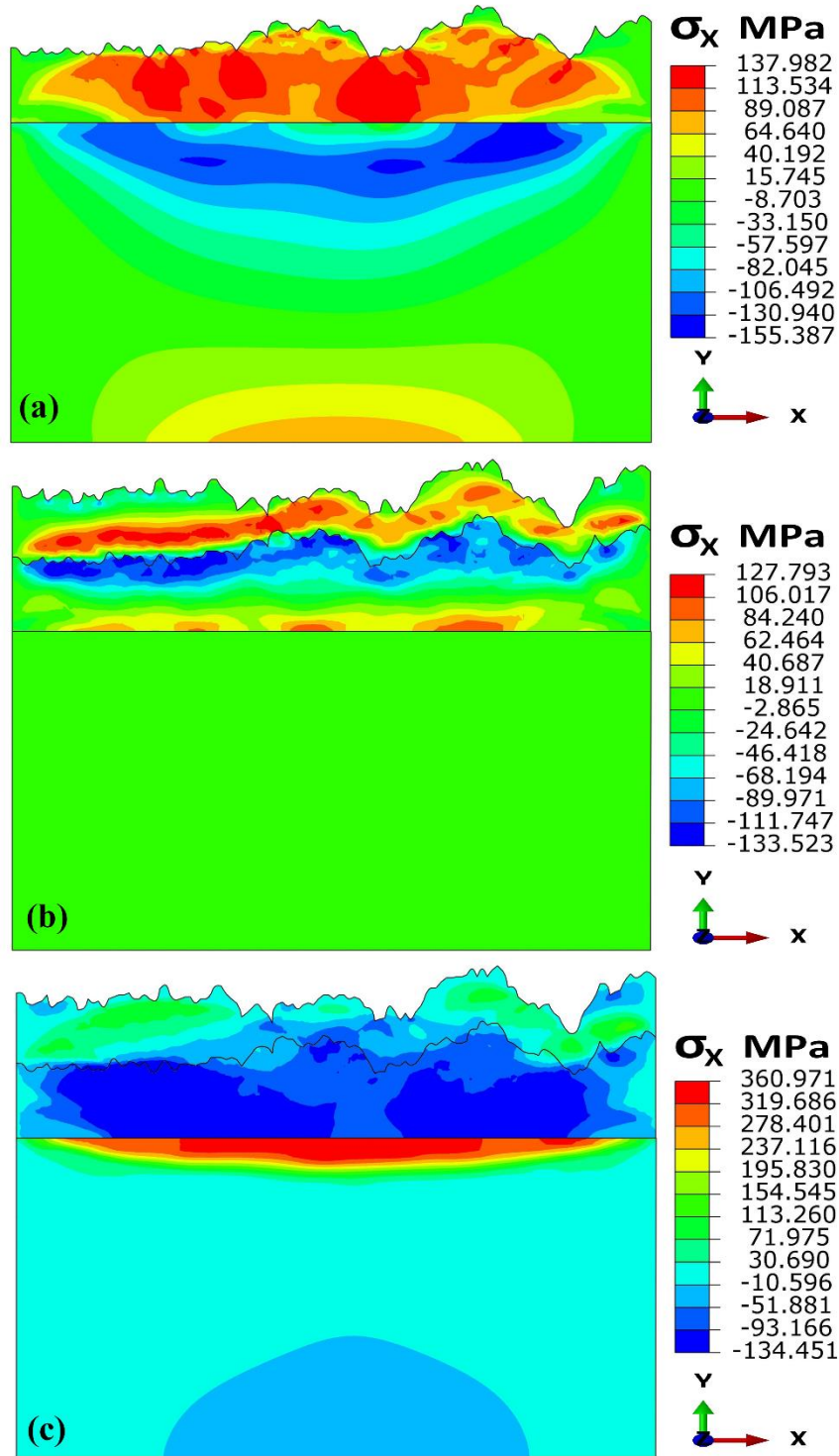


Figure 19 Residual stresses in the two-layer model: (a) quenching of the bottom layer, (b) quenching of the top layer, and (c) final thermal stresses

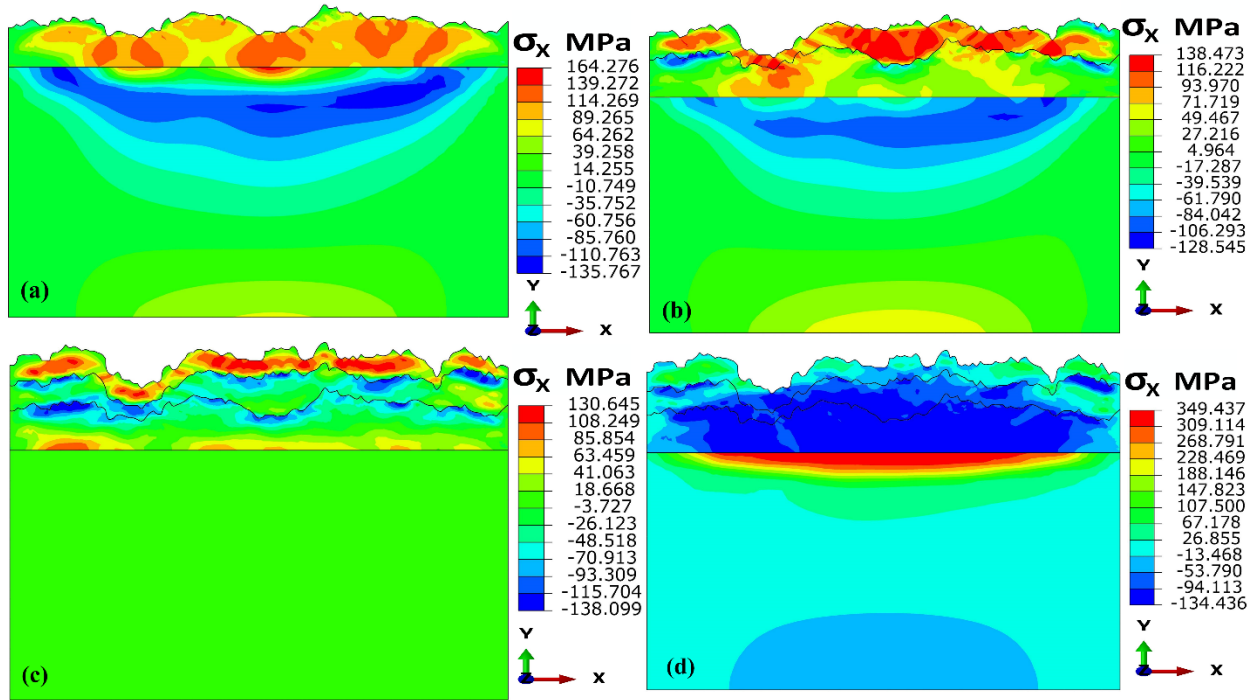


Figure 20 Residual stresses in the three-layer model: (a) quenching of the bottom layer, (b) quenching of the top layer, and (c) final thermal stresses

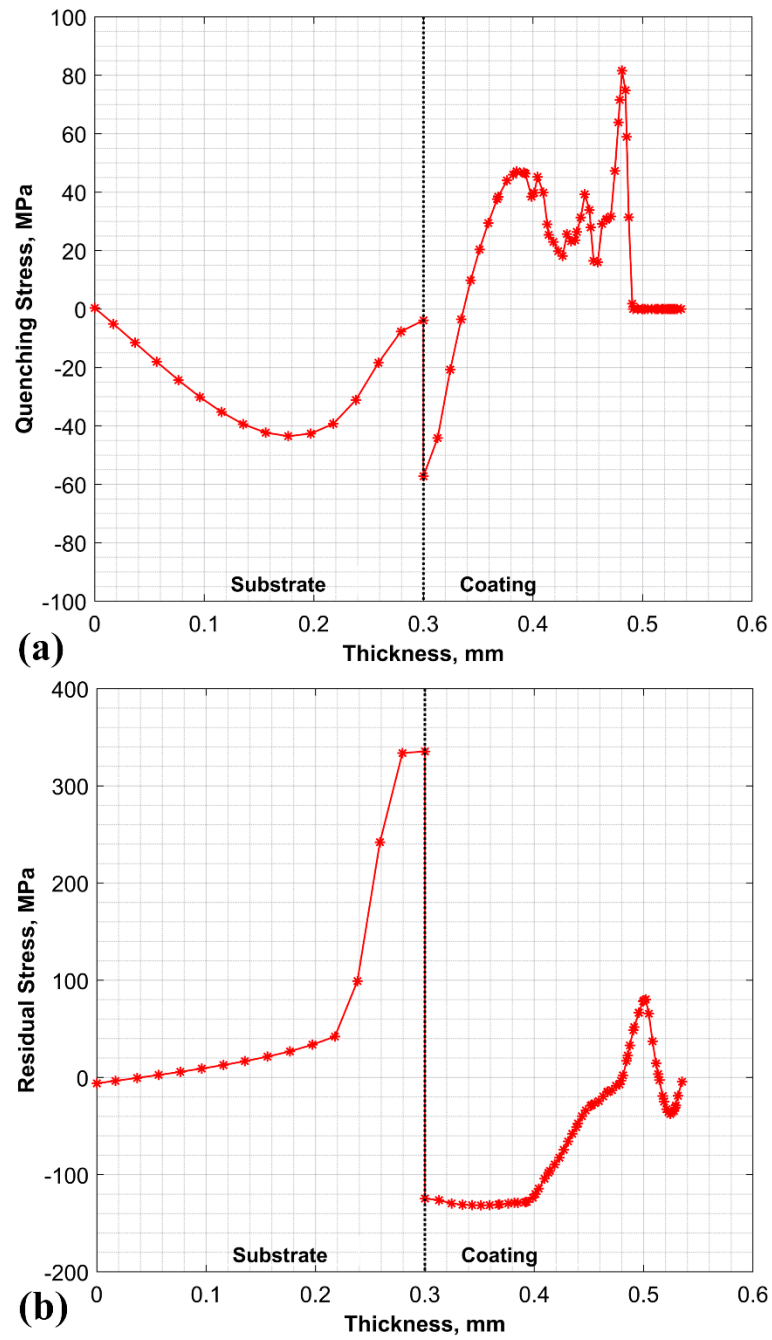


Figure 21 Residual stresses in the one-layer model: (a) quenching and (b) final residual stresses

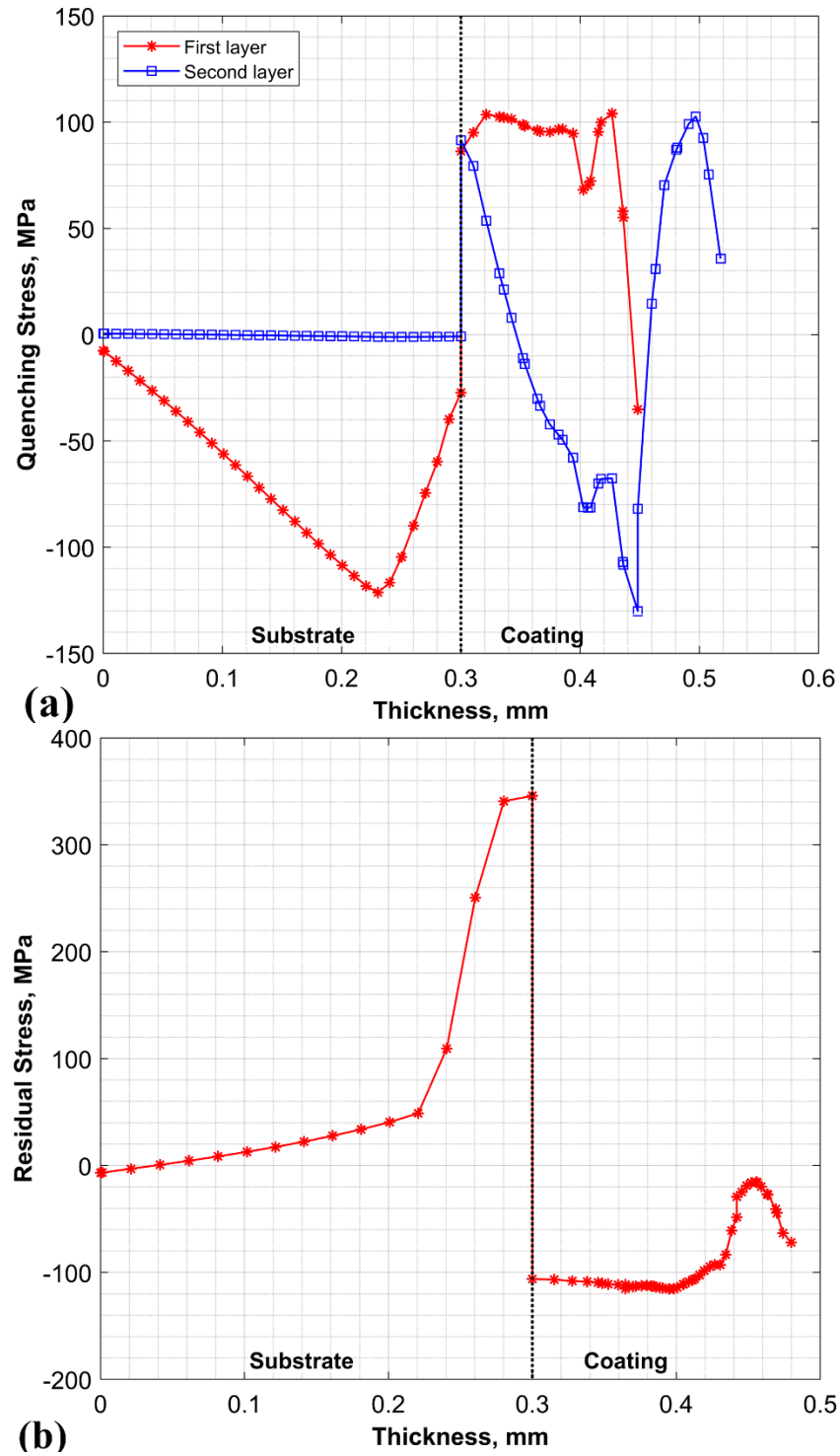


Figure 22 Residual stresses in the two-layer model: (a) quenching and (b) final residual stresses

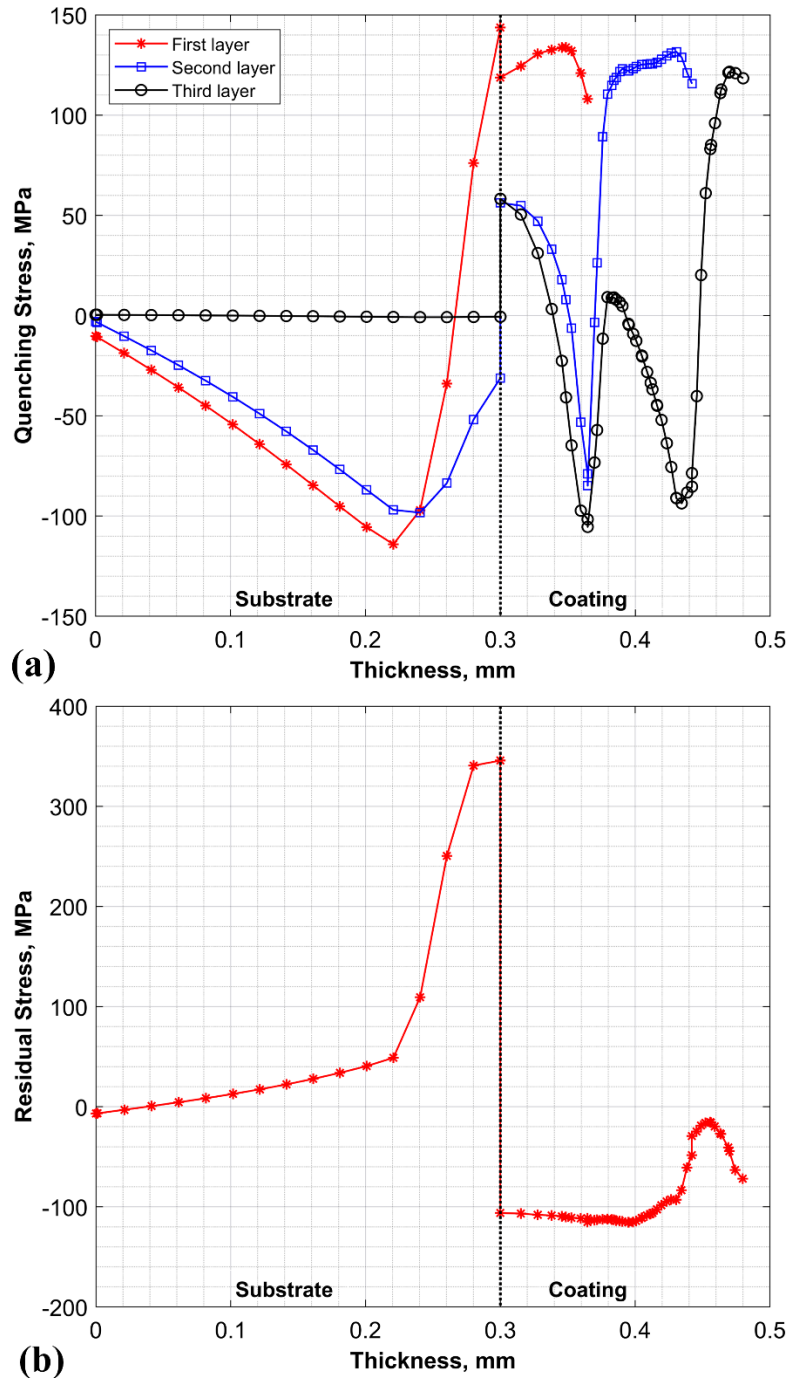


Figure 23 Residual stresses in the three-layer model: (a) quenching and (b) final residual stresses

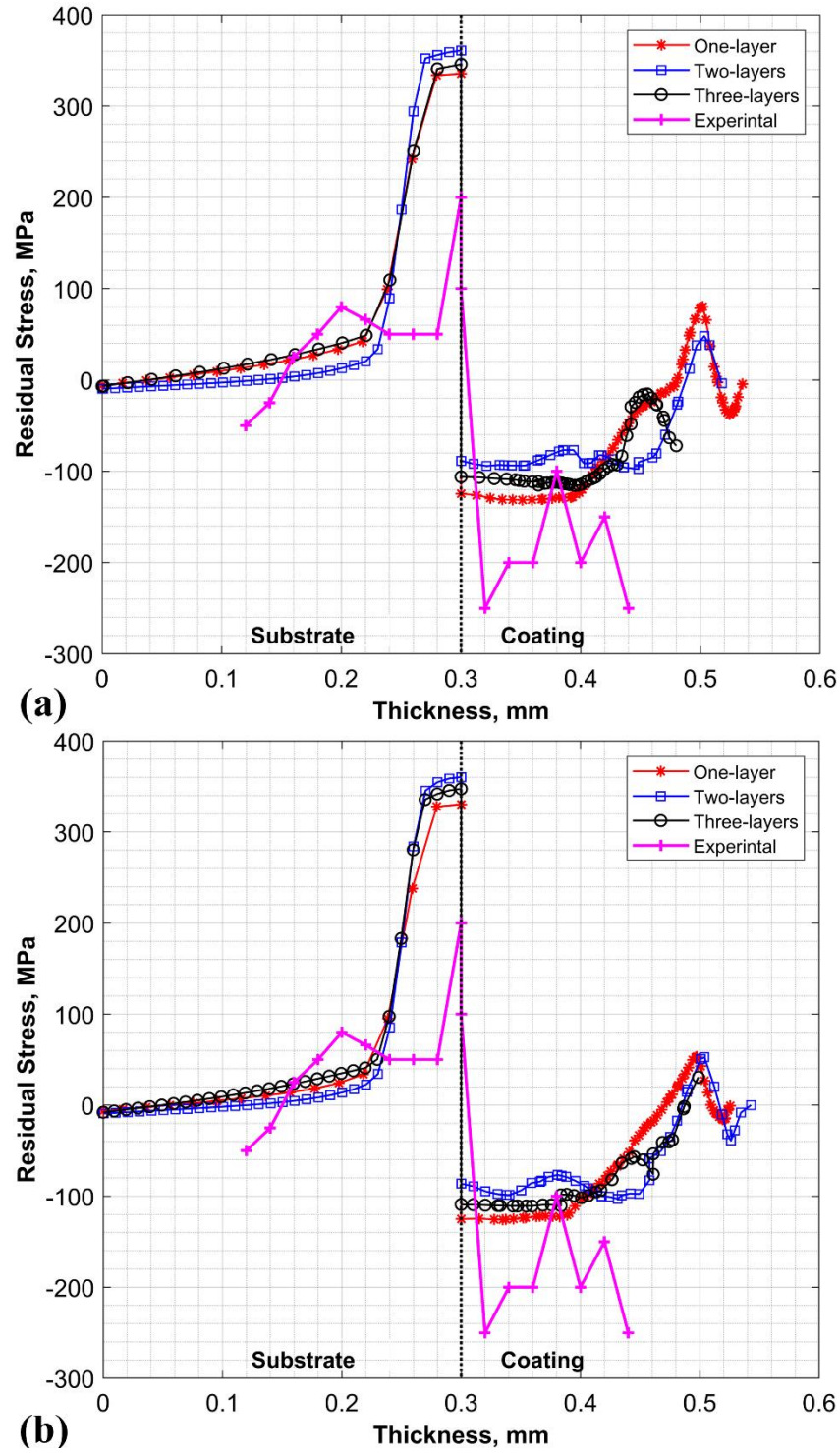


Figure 24 Thermal residual stresses in the one-layer, two-layer, and three-layer models and experimental values for (a) slice 30 and (b) slice 5

CHAPTER 5

3D RESIDUAL STRESS DEVELOPMENT MODEL

5.1 3D FE model:

To evaluate the residual stress distribution within the YSZ coating layer after thermal spraying on a stainless steel substrate, a 3D FE model was developed using commercially available software ABAQUS. The data of the geometry used in this analysis were extracted from the fourth coating model. As mentioned in chapter 3, the dimensions of the coated surface are 1x1 mm, however only a small section with dimensions 0.25x0.06 mm, as shown in Figure 25(a), was selected due to very high computational time needed for the full model. The roughness of each layer was extracted from TECPLOT [86] as a cloud of points and plotted using a visual basic script as a set of closed lines at different planes. 61 planes, 1 micron apart, were plotted and then filled in SOLIDWORKS [92] assuming linear interpolation. Solid 3D components (the first layer, the second layer, the substrate) with STEP extension were imported into ABAQUS as three separate parts. The effect of porosity was neglected. The total coating thickness is around 100 microns. Tie constraints between the coating and substrate and between coating layers were applied, and perfect contact between the three parts was assumed. The model-change technique was applied to simulate the progressive growth of the coating (layer-by-layer deposition). Two time steps were created to simulate the deactivation/activation of the elements. In the first time step, the second layer is in the deactivation state using the kill-birth method. In the second time step, the second layer is activated again to simulate its deposition. In the last time step (third step) the whole model is

cooled down to room temperature assuming natural heat transfer convection. The coupled temperature-displacement analysis was applied to simulate the thermo-mechanical behavior of the thermal spray coating. The material properties have been assigned as in the 2D analysis. As mentioned before, the material properties of both the coating and the substrate are temperature-dependent. A 3D FE mesh was generated using a tetrahedral element of type C3D4T as shown in Figure 25(b). The number of elements for each layer is summarized in Table 6. the mesh was refined at the coating interfaces and surface because of the small roughness features involved. Before deposition, a pre-heating of substrate material is usually carried out to minimize the deposition stresses and to improve the adhesion strength, thus in this analysis, the substrate is assumed to be preheated to 700°C

Table 8 Type and No. of element 3D model

layer	No. of Elements	Type of Elements
First	151579	C3D4T
Second	338078	
substrate	23075	

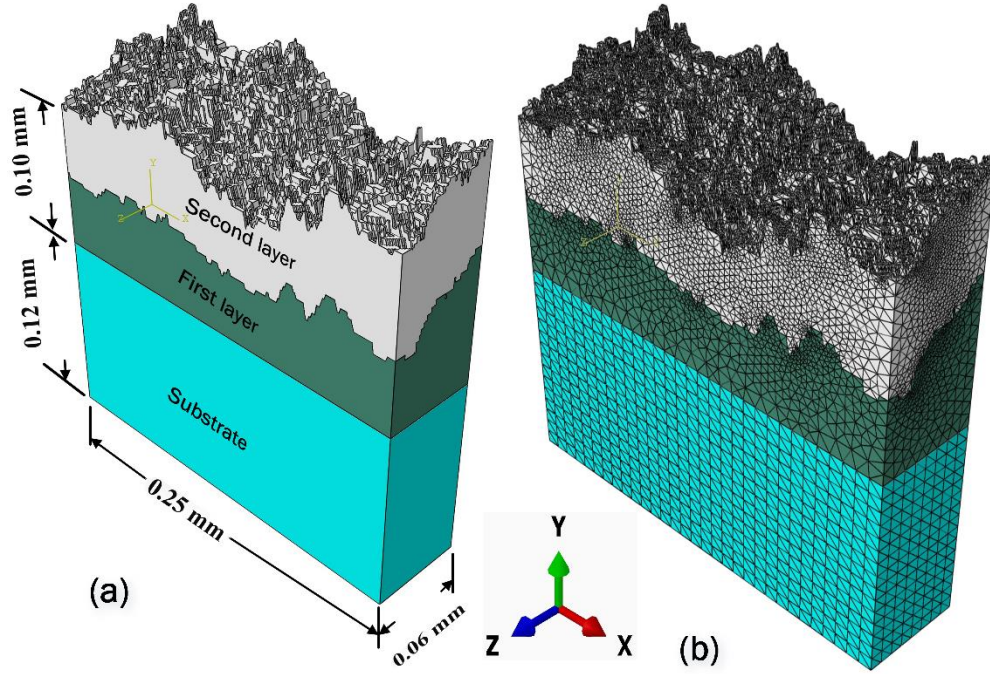


Figure 25 The 3D model: (a) dimensions (b) mesh

5.2 Results and discussions:

The thermal stresses developed at deposition and post-deposition for the two-layers 3D model are investigated in both X and Z directions. Starting with the longitudinal direction, three paths starting at substrate depth of 0.05 mm and going through the coating thickness up to the coating top surface were defined at the middle plane parallel to XY ($Z=0.03$ mm) as shown in Figure 26. These three paths were selected to track the thermal stress variation along the thickness of the coating. Numerical data for the thermal stress profiles along the aforementioned paths were extracted at the time of the second layer deposition as well as after cooling down the whole coating system to room temperature. Figure 27(a) shows the residual stresses after the deposition of the second layer. It can be seen that the three defined paths are following the same pattern, indicating no significant stress variation in the X direction. Starting with the first layer, tensile stresses are

induced in most regions and have a maximum value of around 80 MPa. It was widely reported that the rapid solidification of splats upon their landing on the substrate surface, or the previously deposited coating layers, develops tensile stresses. The shrinkage of the solidified coating layer is restricted by their adhesion to the underlying layer, thus a tensile stress is induced inside the current deposited layer. However, the top section of this layer developed compressive stress with a maximum value of 130 MPa near the interface. This is due to the deposition of the second layer. The contraction of the second layer during its solidification develops compressive stresses below the coating layers interface. Figure 27(b) shows the deposition stress distribution in the transverse direction (Z-direction) at the end of the second layer deposition. It is obvious that it has the same behavior as the longitudinal stress except for the low value of the compressive stresses at the coating layers interface. This is attributed to the short width compared with the length of the coating layers as the simulation was carried out assuming continuous coating layer. The deposition stress profiles discussed above were extracted from the stress contours shown in figure 29. Figures 28 (a) & (b) show the stress distribution in the longitudinal and transverse directions respectively at the end of the cooling cycle. It is clear from Figure 28 (a) & (b) that the substrate residual stresses are almost zero far away from the coating, and highly tensile closer to the interface. On the other hand, the residual stresses are highly compressive in the coating near the interface and become tensile in the second layer then decline to zero near the free surface. Thermal mismatch stresses are compressive in ceramic coatings because they possess a low thermal expansion coefficient compared with the underlying substrate.

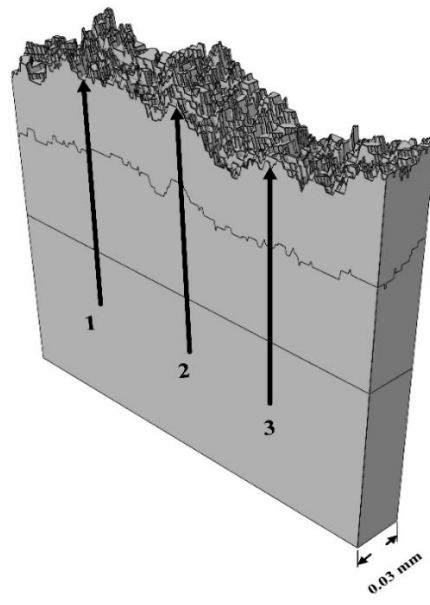


Figure 26 The three paths fixed at the middle of XY planes

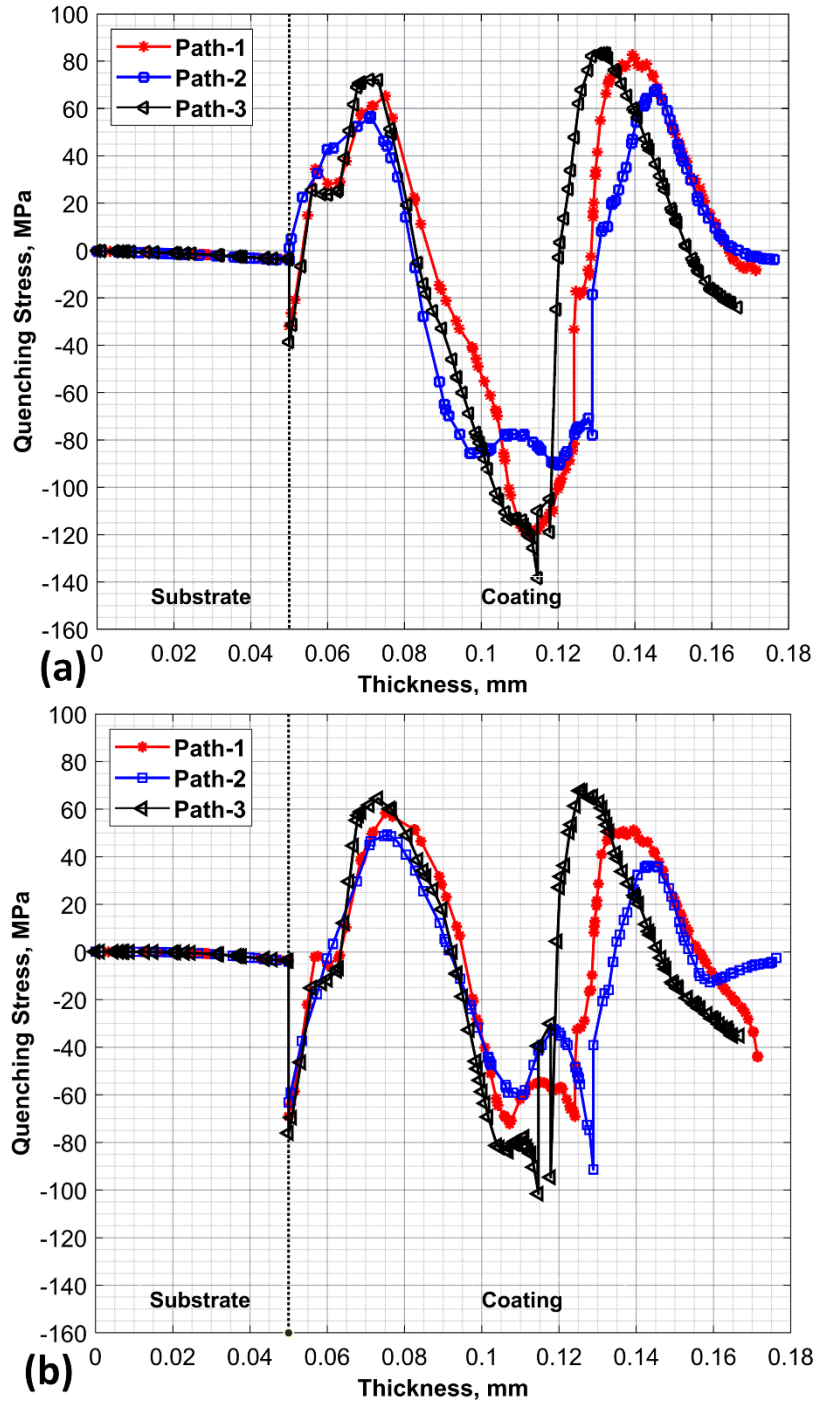


Figure 27 The stress profiles after the deposition of the second layer along the three paths (a) σ_x (b) σ_z

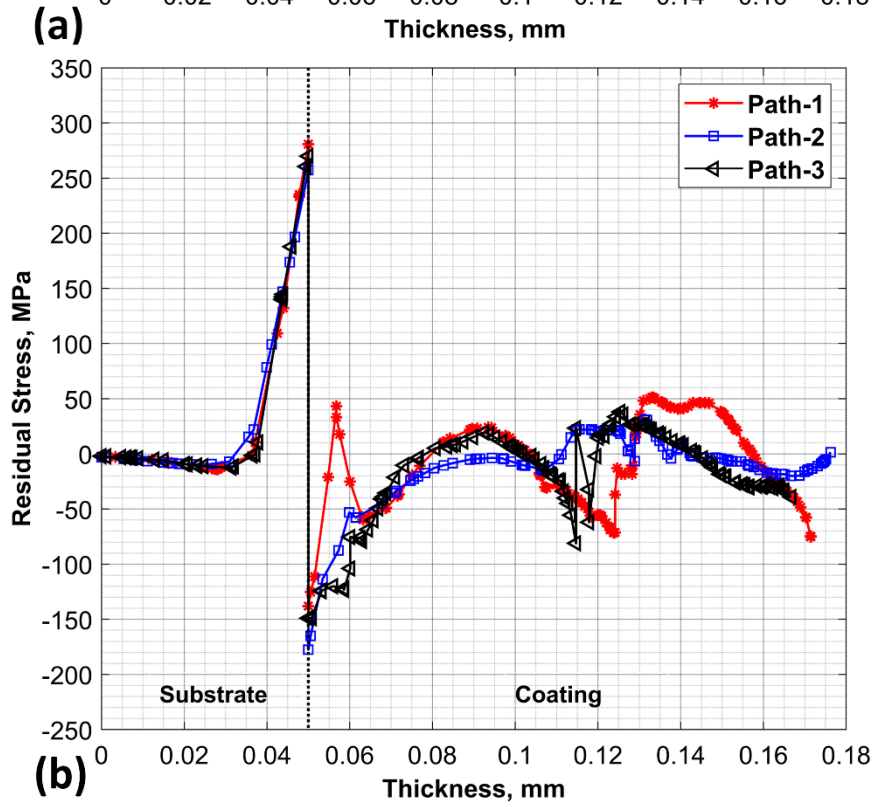
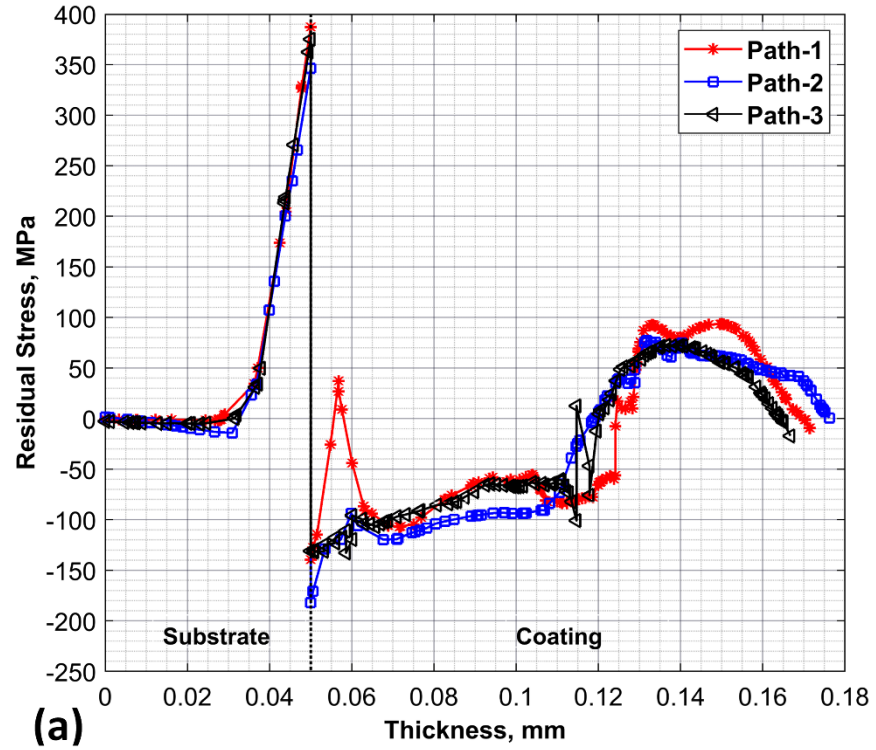


Figure 28 The post-deposition stress profiles along the three paths (a) σ_x (b) σ_z

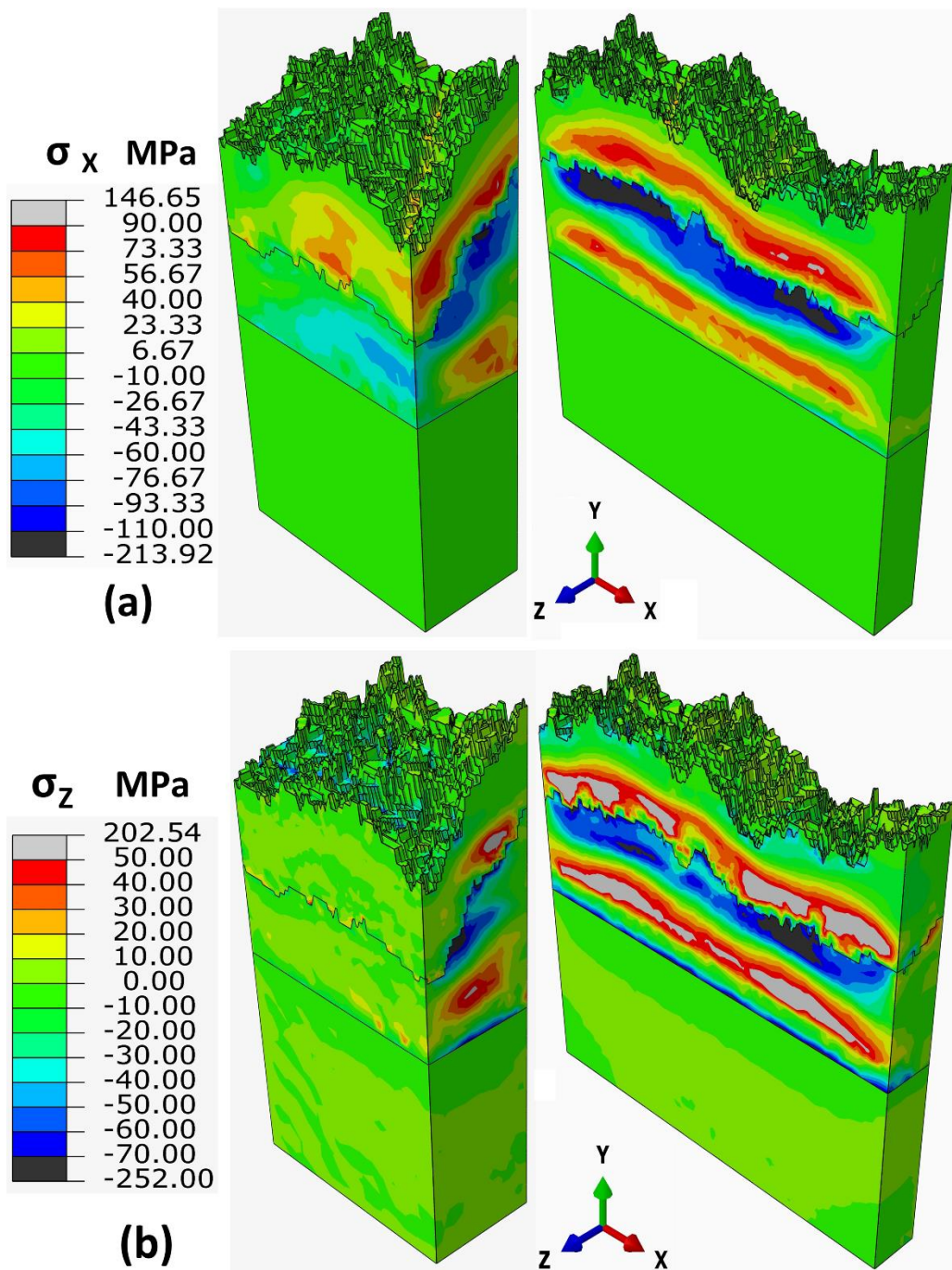


Figure 29 The quenching stress contours after the second layer deposition (a) σ_x (b) σ_z

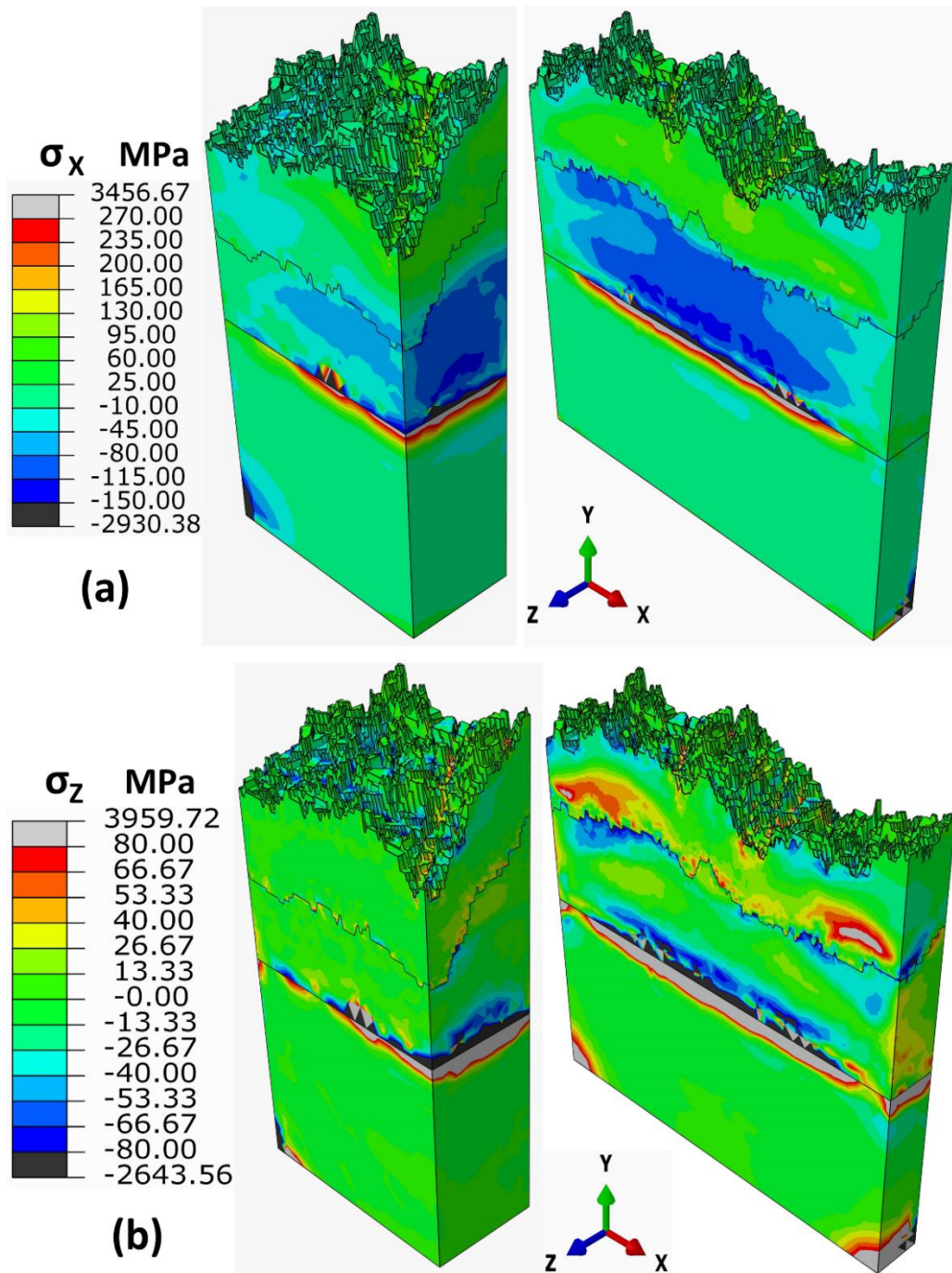


Figure 30 The post-deposition stress contours (a) σ_x (b) σ_z

CHAPTER 6

CONCLUSION

6.1 Conclusion

This work presented a detailed computational model to investigate the combined influence of the coating process parameters on the residual stresses development for thermal spray coatings. The model adopted a macro-model approach, that treats the bulk of sprayed layers as a continuous solid instead of modeling the deposition of single consecutive particles. The residual stresses predicted using the model were obtained for the quenching stage and the thermal mismatch during the cooling stage. The results showed that in progressive (layer-by-layer) deposition, the tensile quenching stress at the top of each layer is progressively changed to be compressive by the deposition of the subsequent layer. Although the quenching stress has no significant effect in constituting the final residual stress profile. It will qualitatively affect the microstructure of the coating and would also affect the crack initiation and propagation. The three models are showing the difference between the progressive deposition (multi-layer deposition) and block deposition (single-layer deposition). The proposed model is an effective method for bridging the gap between the stochastic modeling of thermal spray coatings and finite-element modeling of thermal stresses, crack propagation, fatigue etc. it enables utilizing of coating microstructures formed stochastically for creating a detailed FE geometry that can be imported to any commercial FE software to model the coating deposition process or the thermal loads associated with the operation processes.

6.2 Future work

The methodology presented in this work allows for the use of a stochastic model that is based on experimental data as well as a 3D droplet model to generate detailed coating geometry based on chosen thermal spray coating process parameters. The work presented here does not account for porosity. The coating was assumed as a solid continuous layer. In future porosity can be added to prepare a 3D porous FE model and it can be employed to study the development of the cyclic thermal stresses and fatigue life prediction for different coating systems. The process parameters were examined in terms of the number of layers produced to achieve the same average coating thickness, but a separate study can also be performed on the individual process parameters.

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