



Diploma Thesis

ANALYTICAL TREATMENT OF RESIDUAL STRESSES IN MUTLILAYER COATINGS

carried out for the purpose of obtaining the degree of Master of Science (MSc or Dipl.-Ing), submitted at TU Wien, Faculty of Mechanical and Industrial Engineering, by

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Affidavit

I declare in lieu of oath, that I wrote this thesis and performed the associated research myself, using only literature cited in this volume. If text passages from sources are used literally, they are marked as such.

I confirm that this work is original and has not been submitted elsewhere for any examination, nor it is currently under consideration for a thesis elsewhere.

Vienna, June, 2017

Signature

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Abstract

Multilayer thin films have been widely used as optical coatings, semiconductor devices and resistant coatings. They are used to control the mechanical, optical, thermal and electrical properties of a system. Residual stresses in coatings arising due to the manufacturing process in many cases are undesirable because they may lead to through-film cracking or interfacial delamination. It is therefore of great benefit to be able to calculate the residual stress level after the manufacturing process.

The aim of this thesis is to develop an efficient analytical approach to determining residual stress distributions in multilayer systems. The model should be able to simulate systems comprising several hundred layers where each layer possesses a thickness of a few nanometers.

To achieve such multilayer systems the layers are deposited onto a substrate by physical vapor deposition. After the manufacturing process residual stresses in the coating as well as in the substrate can be observed. There are two primary causes of residual stresses in a multilayer system. Stresses which are generated from the film growth process and stresses due to a thermal mismatch of the coefficient of thermal expansion when the system is cooled down from manufacturing temperature to room temperature. The analytical approach is based on Euler - Bernoulli beam theory. With a force and moment balance the stress distribution in the multilayer system can be obtained.

The presented approach provides a tool of high efficiency compared to Finite Element models. Not only for predicting the residual stress state in the actual system but also for parametric studies to find a optimum layer structure.

Kurzfassung

Multilayer - Beschichtungen finden Verwendung als Beschichtungen in vielen Bereichen beispielsweise in elektronischen Geräten, optischen Beschichtungen und Halbleiterbauelementen. Sie verbessern die mechanischen, optischen, thermischen und elektronischen Eigenschaften des beschichteten Materials. Die bei der Herstellung entstehenden Eigenspannungen sind teilweise unerwünscht da sie einen erheblichen Einfluss auf die Leistungsfähigkeit der beschichteten Komponenten haben. Die entstehenden Eigenspannungen können zum Versagen des Mehrlagensystems durch Rissbildung, Delamination oder Abplatzen führen. Deshalb ist es von besonderem Interesse, den Eigenspannungszustand nach dem Herstellungsprozess bestimmen zu können.

Ziel dieser Arbeit ist die Erstellung eines analytischen Modells zur Berechnung von Eigenspannungen in mehrlagigen Beschichtungen mit einigen hunderten Lagen, wobei die einzelnen Schichtdicken im Nanometerbereich sind.

Die Beschichtung wird mittel physikalischer Dampfphasenabscheidung auf ein Substratmaterial aufgebracht. Die Eigenspannungen entstehen einerseits durch den Schichtwachstumsprozess und andererseits entstehen thermische Spannungen durch die unterschiedlichen Wärmeausdehnungskoeffizienten beim Abkühlen von der Fertigungstemperatur auf Raumtempteratur. Das analytische Modell soll dazu dienen den Einfluss von verschiedenen Parametern, wie zum Beispiel Beschichtungs- und Substratmaterial, auf den Eigenspannungszustand in den Schichten und im Substrat zu berechnen. Der analytische Ansatz basiert auf der Euler-Bernoulli Balkentheorie. Mithilfe eines Kraft und Momenten Gleichgewichts werden die entstehenden Eigenspannungen berechnet.

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Chapter 1

Introduction

1.1 Definition of a multilayer system

Thin coatings or multilayer thin films, containing different materials are often used as protective coatings for certain technological applications. Multilayers consisting of two or more periodically alternating materials in the nanometer range, referred to as superlattice films, possess remarkably high hardness values compared to their single layer constituents. Within multilayer systems, different layer materials with variable layer thickness can be realized [9]. To achieve such multilayer systems the layers are deposited onto a substrate or onto previously deposited layers by the two main manufacturing techniques, physical (PVD) or chemical vapor deposition (CVD). During the manufacturing process residual stresses arise in deposited multilayer systems and can cause delamination or cracks. Hence they strongly influences the mechanical behaviour, the performance, and the lifetime of such multilayer systems. These stresses occur basically due to (i) intrinsic stresses, which are caused by the manufacturing process, (ii) thermal stresses, caused by different coefficients of thermal expansion (CTEs), when the multilayer is cooled down from its production temperature to room temperature and (iii) extrinsic stresses, introduced by the environment [8].

1.2 State of the Art

Thin films which have been deposited on a substrate are usually in a nonzero stress state. Initially, Stoney [19] studied a thin film deposited on a thick substrate in his seminal paper "The Tension of Metallic Films Deposited by Electrolysis". He derived a formula which illustrates the relationship between the curvature κ of the system and the stress in the thin film $\sigma^{(f)}$:

$$\sigma^{(f)} = \frac{E_{\rm s} h_{\rm s} \kappa}{6h_{\rm f} (1 - \nu_{\rm s})} \tag{1.1}$$

where the subscripts s und f denote the substrate and the film, respectively. The parameters E, h and ν stand for the Young's Modulus, the thickness and the Poisson's ratio. The Stoney formula has been widely used in comparisons with experimental work in which the film stress can be derived from curvature measurements [7]. The main assumptions of the formula are (i) film thickness $h_{\rm f}$ and substrate thickness $h_{\rm s}$ are small compared to the lateral dimensions of the sample; (ii) the thickness of the film is much smaller than the thickness of the substrate; (iii) the substrate material is taken to be isotropic, homogeneous, linearly elastic and the film material is isotropic [6].

Since that time major efforts have been devoted to analyzing thermal stresses in multilayer systems. Mostly the analysis is referred to classical beam bending theory. Strain continuity is required at the interfaces between the layers. Hsuch [11] developed an analytical approach for thermoelastic stress in multilayer systems where he decomposed the total strain into a uniform strain component and a bending strain component. Independent of the numbers of layers the following three unknowns are used: (i) the uniform strain component; (ii) the radius of curvature and (iii) the location of the bending axis. Zhang [25] developed a model for predicting thermoelastic stress in multilayer systems with only two variables. The reference strain at the interface between substrate and first layer and the curvature radius of the neutral axis of zero normal strain are taken as unknowns. Tsui and Clyne [22] developed an analytical approach to predicting residual stresses due to differential thermal contraction and intrinsic stresses. The analysis considers the influence of both the substrate and the coating and it is based on force and momentum balance. Therefore they added the multilayers layer wise to the substrate and after adding each layer the deposition stress was obtained. Subsequently the thermal stress can be superimposed on the calculated intrinsic stresses. A comparison with a numerical model for plasma sprayed systems demonstrate good correlation with the analytical model of Tsui and Clyne. Schoengrundner et al. [18] made use of the ion beam layer removal (ILR) method applied to a cantilever fixed on one side. The layers, which are deposited on the upper side of the substrate, are removed step by step. The deflection, which depends on the stress distribution, and the remaining film thickness are measured for each milling step with a scanning electron microscope (SEM). The deflection is used to determine the residual stresses according to an analytical approach using Euler-Bernoulli beam theory. Each previously removed layer is then added in a reverse analysis step. With a force and momentum balance the residual stress distribution of the system is obtained. Furthermore the analytical predictions and the results from the experiment are compared with a three-dimensional Finite Element model. The residual stress distribution is modified using a least square algorithm until the deflection of the FE-model reaches the value achieved in the experiment.

1.3 Aim of the present study

The aim of the present study is generating an analytical approach for predicting residual stress distributions in multilayer systems due to thermal stresses and intrinsic stresses generated by physical vapor deposition. The model is able to simulate systems with up to a few hundred layers, where each layer shows a thickness of a few nanometers. The analytical approach is based on classical beam theory. With a force and moment balance the stress distribution in a multilayer system can be obtained. Furthermore, the main part of the thesis is to comprise an efficient parameter study to predict the influence of various material properties and process parameters. The following parameters definitely or possibly affect the performance of multilayer systems: (i) material properties of the layers and the substrate; (ii) thickness of each deposited layer; (iii) number of deposited layers; (iv) cooling process.

The thesis is organized in the following way. The second chapter gives an overall introduction on thin films including deposition techniques, growth evolution of thin films, typically observed residual stresses in thin films, as well as methods for residual stress measurement. The third chapter covers the development of an analytical modelling approach for predicting the residual stress state of layered systems. This approach is compared with the analytical model developed by Hsueh [11]. The computational results and discussion are shown in the fourth chapter, where the concepts described up to that point are used. Finally the conclusions are summarized in the fifth chapter where ideas for further work in this field are also presented.

Chapter 2

Theoretical background

2.1 Thin film deposition technique

Physical vapor deposition (PVD) and chemical vapor deposition (CVD) are the most common methods for depositing thin films onto a substrate atom by atom. The most fundamental difference between these two techniques is the way the vapor necessary for the deposition process is supplied. Within the framework of this thesis only the PVD process is discussed further.

2.1.1 Physical vapor deposition

Physical vapor deposition is based on physical processes for transferring atoms from a solid or liquid material onto a substrate. To control the vapor composition the process is executed in a vacuum chamber. All PVD processes consist of three steps for the formation of thin films: (i) Transformation from condensed phase to the vapor phase; (ii) transferring of vapor from source material to the substrate; (iii) condensation, nucleation and growth of a thin film on the substrate.

Depending on the process of the phase transition from solid to vapor, the deposition techniques can be divided into four main categories: sputter deposition, arc vapor deposition, ion plating and arc vacuum deposition. Within this thesis only sputter deposition and arc vapor deposition (cathodic arc) are explained.

A schematic sketch of the basic sputter process is depicted in Figure 2.1. A sputtering system consists of an anode (substrate) and a cathode (target) which are located in a vacuum chamber. In the sputtering process atoms are removed from the surface of a target by momentum transfer from bombarding particles. These particles are usually gaseous ions, typically Ar, accelerated out of a plasma. The ions result from the collision of electrons with the gas in the chamber. An additional effect of the collision is the creation of free electrons. These electrons cause further collisions. The high potential difference between the cathode and the anode leads to an acceleration of the ions towards the target. The ions strike the target and atoms are ejected. The sputtered atoms are transferred to the substrate surface where they form a thin film by means of condensation [7].

Arc vapor deposition uses a high current, low voltage arc to vaporize the source material and deposit the vaporized material onto the substrate. Usually the substrate is biased to accelerate the ions towards its surface. The arc vapor deposition process is used to deposit decorative and hard coatings.[14]

Additionally, the substrate temperature influences the rate of film growth. A high substrate temperature enhances the growth of single crystal films on the substrate surface. A low substrate temperature generates a less coherent film growth and will possible result in amorphous film growth. [7]



Figure 2.1: Schematic showing the basic feature of a sputter deposition system [7]

2.2 Thin film growth

The growth of polycrystalline thin films, schematically depicted in Figure 2.2, is characterised by different processes of structural evolution: Nucleation, island growth, coalescence of islands, channel growth and thickness growth. The comprehensive description of these five stages can be based on the basic structure forming phenomena: nucleation, crystal growth and grain growth. These primary phenomena are summarized in the following.

In the nucleation phase the primary nucleation (condensation) starts the film growth on the substrate surface. The arriving vaporized particles migrate over the surface until they find an energetically optimal position. Condensation and film growth start over the entire substrate surface simultaneously, while secondary nucleation initiates



growth locally, in later stages of the film formation.

Figure 2.2: Schematic illustration of the fundamental growth process of the thin film microstructure [16]

The second phenomenon, crystal growth, describes the fundamental structure forming process which incorporates the adatoms into the condensed phase when further material is deposited. It takes place continuously during the whole process of film growth. Basically there are two cases of crystal growth of polycrystalline thin films: (i) discrete single crystals are dispersed on the substrate surface in the early stages of film growth directly after nucleation and (ii) the growth of crystals which are a part of a polycrystalline structure.

The third fundamental phenomenon of structure evolution, grain growth, is characterized by further growth of the crystals when two contacting single crystals experience a collision and coalesce to a single-crystal island of increased size. Crystals with lower energy per atom absorb the neighbouring crystals to minimize the overall interface and surface energy [1, 15, 16].

2.3 Origin of residual stress in thin films

Residual stress usually refers to an internal stress distribution present in a structure when all external boundaries of the structure are free of applied traction. The presence of residual stress implies that, if the system would be relieved of any constraints, it would change its dimensions and/or would deform. Film stresses are usually divided into two main groups, intrinsic and extrinsic stresses.

Intrinsic stress is generated due to the growth process, when a film is deposited on a substrate or an adjacent layer. The stress distribution due to growth stress strongly depends on the material properties of the constituents, on the substrate temperature during deposition, the growth flux and the growth chamber conditions.

Extrinsic stress arises from a variety of different physical effects. In this thesis only the thermal expansion mismatch between the constituents is considered and therefore explained. The mismatch of the coefficients of thermal expansion between individual phases results in differential thermal contraction and expansion stresses due to cooling or heating processes [7].

Both extrinsic and intrinsic stress contribute to the final residual stress state in thin films and they should not be thought of as acting alone [3]. Extrinsic stresses in terms of thermal residual stresses and intrinsic residual stresses are discussed in more detail in Sections 2.3.1 and 2.3.2, respectively.

2.3.1 Thermal residual stresses

Thermal residual stresses are generated when the mulitlayer system is subjected to a temperature change due to a mismatch between the coefficients of thermal expansion of the substrate and the coating. An elastic multilayer system is sketched in Figure 2.3a, where n layers of individual thickness t_i are bonded progressively to a substrate of thickness $t_{\rm s}$. The first layer is in direct contact with the substrate. The system is cooled from its production temperature to room temperature. The coefficients of thermal expansion (CTEs) for the substrate and the individual layers i are α_S and α_i , respectively. If the individual layers and the substrate are not connected to each other the system experiences an unconstrained differential shrinkage, see Figure 2.3b. Different thermal strains, $\alpha_S \Delta T$ and $\alpha_i \Delta T$, arise in the substrate and the individual layers. Due to the fact the individual constituents are connected with each other displacement compatibility at the interface is required. If $\alpha_S > \alpha_i$ a decrease in temperature causes the substrate to contract more strongly than the layers. Consequently uniform tensile/compressive stress are imposed on the individual layers and the substrate such that the strain in the multilayer system is constant, see Figure 2.3c. However the system is still not in mechanical equilibrium. If the structure can deform freely, bending of the system occurs due to the asymmetric stress in the system, depicted in Figure 2.3d [11].



Figure 2.3: Schematic showing bending of a multilayer system due to thermal stresses

Coefficients of thermal expansion

Thermal expansion is the tendency of a material to change its dimensions with a temperature change. It is characterized in terms of coefficients of thermal expansion (CTE), which state the relative amount by which a material expands or contracts. The linear CTE α_l and the volume CTE α_v at constant pressure P are defined as

$$\alpha_l = \frac{1}{l} \left(\frac{\delta l}{\delta T} \right)_P \qquad \alpha_v = \frac{1}{V} \left(\frac{\delta V}{\delta T} \right)_P \tag{2.1}$$

where V is defined as the volume and l defines the length of the gauge region. Due to the fact that the CTE is a function of the temperature, the range over which it is calculated must be defined. Both CTEs are intrinsic to a given material at a given temperature and independet of the amount of the material. The most common unit for CTE is K^{-1} [17].

2.3.2 Intrinsic residual stresses

Every growth step, explained in 2.2, is an essential step of unique film forming processes that causes growth stresses which can either be tensile or compressive. In this section the stress generation in polycrystalline films produced by vapor deposition is discussed. The development of the average film stress during the growth process is depicted in Figure 2.4, as proposed in [3]. First a compressive stress is generated in the initial island stage (stage I), then tensile stress is induced during island coalescence and grain growth (stage II). Finally compressive stress is imposed during deposition on continuous film thickening (stage III). In the following discussion the mechanisms which are responsible for this compressive-tensile-compressive evolution are described based on the findings in [3].



Figure 2.4: Schematic diagram of average film stress versus mean thickness of the film during the growth process [3]

Stage I: Compressive stress prior to island coalescence

A curvature change of a coating-substrate system can already be observed in the early stage of film growth. A compressive stress occurs in the film before the islands have coalesced into a continuous thin film. This can be explained by the islands being more dense (having a smaller lattice parameter) compared to a bulk crystal of the same material at the same temperature. When a growing island reaches a critical size it becomes rigidly attached to the substrate. By further growth the lattice parameter increases approaching the bulk density. However, the atoms of the islands which are closest to the substrate can no longer relax freely. They are constrained to the initial island size lattice parameter. Atoms further away from the surface of the substrate are less constrained. This surface stress induces an average compressive stress in the system. A schematic sketch of the islands before coalescence is shown in Figure 2.5.

Stage II: Tensile stress due to island contiguity

The second stage, as shown in Figure 2.5, describes the effect when two neighbouring growing islands touch and coalesce. Such a mechanism was proposed by Hoffmann [10], who argued that the stress is observed to become tensile when two neighbouring islands are closing the gap between them. By forming grain boundaries the surface energy is reduced. Since the islands need to close a gap, the strain energy needed must be less than the reduction of the surface energy. Due to the connection between the islands a continuous layer is formed and an average tensile stress is induced.

Stage III: Compressive stress during continued growth

After further growth to form a fully continuous film a compressive stress state starts to replace the tensile stress. Chason *et al* [4] suggested an explanation for the generation of compressive stress which takes the role of grain boundaries into account. The appearance of compressive stress indicates that there must be an excess number of atoms in the film. Due to a continuous deposition flux and the existence of grain boundaries a non-equilibrium is maintained at the growth surface. The energies of the arriving atoms may not be sufficient for a diffusion of the atoms into the crystals. The atoms could decrease their energies by migrating into the grain boundaries. The inclusion of the excess atoms in grain boundaries results in an average compressive stress. The compressive stress increases the energies of the atoms in the grain boundaries. The driving force for the atoms to migrate into the grain boundaries decreases with an increase in the compressive stress magnitude which results in a steady state behaviour. A schematic sketch of adatoms flowing into the grain boundaries is shown in Figure 2.6.



Figure 2.5: Schematic sketch of the island coalescence: (I) shape of the island before coalescence (Stage I) (II) shape of island after coalescence (Stage II)



Figure 2.6: Schematic sketch of adatoms flowing into the grain boundary (Stage III)

Structure Zone Model

A variety of Structure Zone Models (SZM) were developed to demonstrate the influence of the deposition parameters on the film microstructure. By considering evaporation processes the important process parameter is the homologous temperature which is defined as the relation between the substrate temperature and the melting temperature of the target material. For sputtering processes a zone model developed by Thornton [21] was introduced which considers the working gas pressure as a further parameter, shown in Figure 2.7. The different zones are described briefly below.

Zone 1: At a low substrate temperature T the mobility of the impinging atoms is low. Therefore the film is expected to be less dense and shows a columnar growth structure with voided grain boundaries.

Zone T: For sputtering, where a low working gas pressure is used, the atoms reach the surface with high energies. This leads to a high atom mobility which results in a fine grained and dense microstructure. This zone almost vanishes by high working gas pressures

Zone 2: As the temperature increases the columns increase in width and the higher surface mobility and diffusion of atoms lead to a dense columnar grained microstructure.

Zone 3: The high temperature leads to a bright surface and large grains.

As can be seen from Figure 2.7, the transition between the different zones is shifted by varying the working gas pressure. This model clearly demonstrates that the microstructure of a polycrystalline film changes by the influence of the process parameters.



Figure 2.7: Structure Zone Model (SZM) of Thornton [21]

2.3.3 Energetic deposition effects

Besides the stresses due to the mismatch in CTEs and grain growth other stress generation mechanism occur in multilayer systems. In sputter-deposited films, described in Section 2.1.1, atoms with high kinetic energies arrive at the growth surface. The energetic atoms bombard the surface of the growth film and lead to a more dense configuration or create stress-inducing defects in the near-surface region reffered to as energetic deposition effects. This modification of the stress is referred to as "atomic peening". The damage on the surface depends on both the energy of the arriving atoms and on the pressure of the inert gas. The stresses which arises from growth effects (Section 2.3.2) act independently from those from high-energy bombardment. Consequently, the resulting residual stresses can be assumed to be a superposition of intrinsic growth stress and energetic bombardment stress [3].

2.4 Typical failure modes

It is very difficult to avoid the appearance of high residual stresses in multilayer systems. The residual stress state can induce a large variety of effects which highly influence the performance of the multilayer system. When the stresses in the multilayer systems are too high failure is induced. Typical failure modes are illustrated in Figure 2.8. The dominant failure mode under tensile conditions is the appearance of cracks in the layers. Under compressive stress the two typical failure modes are edge delamination and buckling driven delamination [20].



Figure 2.8: Failure modes of a thin coating under residual stress (a) edge delamination (b) microcracking (c) buckling driven delamination [20]

2.5 Techniques for stress measurement

Several techniques have been developed for measuring residual stress distributions in multilayer systems. Two non-destructive methods will be presented in this chapter. The first method is based on measuring the deflection of a cantilever and the second uses X-ray diffraction (XRD) to measure the lattice spacing.

Laser beam deflection method

Looking at the Stoney equation, Equation (1.1), the curvature κ is the only free variable allowing to balance the film stress. Figure 2.9 shows a schematic sketch of the laser beam deflection method for measuring this curvature. A beam of length L is clamped at one end and is held horizontally. The deflection of the cantilever is δ and the angle of the curved cantilever is denoted as θ . A position-sensing photodetector (PSD) is fixed at a distance d to the beam. The reflected laser beam hits the PSD at a distance Δb with respect to the incoming beam. The distance Δb is recorded by the PSD and θ can be calculated by the following equation

$$\tan(2\theta) \sim 2\theta = \frac{\Delta b}{d-\delta} \sim \frac{\Delta b}{d}$$
(2.2)

with the assumption

$$\Rightarrow \sin(\theta) = \theta \tag{2.3}$$

$$\theta \ll 1 \qquad \Rightarrow \cos(\theta) = 1 \tag{2.4}$$

$$\Rightarrow \tan(\theta) = \theta \tag{2.5}$$

In Equation (2.2) the reduction of d due to a change of δ is neglected and a small θ is assumed. The radius of curvature ρ , the beam length L and the angle of deflection

 θ are depicted in Figure 2.10 [24]. The radius of curvature ρ , or the curvature κ , of the beam can be derived, according to Figure 2.10, as



Figure 2.9: Schematic of a laser beam deflection measurement [24]



Figure 2.10: Relationship between the length of the beam L, the angle of deflection θ and the radius of curvature ρ

(2.6)

X-ray diffraction (XRD)

X-ray diffraction techniques (so called $\sin^2 \psi$ methods) are used to measure lattice spacings for unstressed and stressed lattices. The methods are based on the relation

$$n\lambda = 2d\sin(\beta) \tag{2.7}$$

between the wavelength λ of the incident X-ray, the diffraction order n, the lattice spacing d within the polycrystalline material and the Bragg angle β . Equation (2.7) is often referred to as Bragg's Law. A change in the lattice spacing Δd will cause a corresponding change $\Delta\beta$ in the Bragg angle, such that the lattice strain ε can be estimated as:

$$\varepsilon = \frac{\Delta d}{d_0} \tag{2.8}$$

where d_0 is the unstrained lattice spacing. The residual stresses can than be calculated by assuming a linear elastic distortion of the crystal lattice [26].



Figure 2.11: Relationship between the Bragg angle β and the lattice spacing d to obtain Bragg's Law [26]

Chapter 3

Modelling Approach

An analytical approach has been developed to predict the residual stress distribution in multilayer systems, such as those produced by the physical vapor deposition technique. The model considers thermal stress due to differential thermal contraction during a cool down process, discussed in Chapter 2.3.1, and growth-induced stress explained in Chapter 2.3.2. It is assumed that there are no external constraints influencing the deformation of the multilayer system, so that it is free to bend due to a residual stress distribution. Various loading conditions are considered in the following sections to give insight into the effects of residual stress on the mechanical behaviour of a multilayer. First, the residual stress state due to different CTEs during cooling down from the manufacturing temperature to room temperature is considered. Second, the residual stress distribution related to growth induced stress generated from physical vapor deposition is estimated. The influence of growth induced stress is obtained by gradually adding prestressed layers onto the substrate. Finally, the stress distributions arising from the cooling and growth processes are superimposed to give the overall residual stress distribution in the system. For the implementation of the analytical approach the PYTHON [13] programming language was chosen. The validity of the analytical model is assessed qualitatively by comparison with the results of the various load cases with a Finite Element (FE) model presented in Section 3.2. The FE simulations are conducted using the commercial software package ABAQUS [5].

3.1 Analytical Methods

In the first chapter some general assumptions for the analytical approach are made. Furthermore, a solution for elastic deformation of multilayers due to thermal stresses according to Hsueh [11] is presented in Section 3.1.2. The approach developed in the present thesis to predict residual stresses in multilayers is explained in detail in Section 3.1.3. The main difference between these two approaches lies in the definition of the normal strain.

3.1.1 General considerations

The analytical approach is based on Euler-Bernoulli beam theory where a uni-axial linear elastic stress state is considered. It is assumed that the layers are bonded perfectly to each other and to the substrate. The following kinematic assumptions are known as the Euler-Bernoulli assumptions for beams:

Assumption 1: The cross section is rigid in its own plane.

Assumption 2: The cross section of a beam remains plane after deformation.

Assumption 3: The cross section remains normal to the deformed axis of the beam.

Experimental measurements show that these assumptions are only valid for long, slender beams made of isotropic materials with solid cross section. A further requirement is that the structure is subjected to uni-axial extension or bending deformation [2].

Within this framework near edge effects are neglected. Therefore the stress-strain

distributions obtained are only valid away from the boundaries of the structure.

Within this thesis the elastic material behaviour of the substrate and the layers is assumed to be isotropic. For the substrate this assumption can only be made if the material is of polycrystalline form. The layers are expected to be isotropic in-plane due to the fact that they consist of many crystals. The properties in the out-of-plane direction may be different and are neglected in the present approach. The elastic properties of an isotropic material can be defined with two parameters, the Young's Modulus E and the Poisson's ratio ν . Since only small deformations are considered, the first order theory can be applied. The balances are formulated for the undeformed system. Hence, a superposition of the thermal and growth stress is allowed.

An elastic multilayer beam of length l and width b is considered within the current study, schematically shown in Figure 3.1. The layers are added sequentially to the substrate. The system consists of a substrate with a thickness t_s and of *n*-layers with individual thickness, $t_j (j = 1, 2, ..., n)$. The coordinate system x - z is defined in such a way that the reference plane is located at the free surface of the substrate at z = 0. The thermoelastic properties of the substrate and the film are E_s , α_s and E_j , α_j , respectively, where α denotes the coefficient of thermal expansion.



Figure 3.1: Schematics showing the multilayer beam and the considered coordinate system

For all considered eigenstress models the equilibrium is estimated by the force and moment balances for a beam in the absence of external forces and moments, represented by the formula

$$\sum_{j=1}^{n} F_j + F_s = \sum_{j=1}^{n} \int_{h_j}^{h_{j+1}} \sigma_{\mathbf{x},j}(z) b dz + \int_0^{h_s} \sigma_{\mathbf{x},s}(z) b dz = 0$$
(3.1)

$$\sum_{j=1}^{n} M_j + M_s = \sum_{j=1}^{n} \int_{h_j}^{h_{j+1}} \sigma_{\mathbf{x},j}(z) \cdot zbdz + \int_0^{h_s} \sigma_{\mathbf{x},s}(z) \cdot zbdz = 0$$
(3.2)

where F_j and F_s denote the resulting force in each layer and in the substrate, respectively. M_j and M_s denote the resulting moments in each layer and in the substrate with reference to z equals zero. $\sigma_{x,s}(z)$ and $\sigma_{x,j}(z)$ denote the stress distribution in the substrate and each layer, respectively. For an isotropic material the relation between the stress and strain, at every position in thickness direction z, can be written as

$$\sigma_{\mathbf{x}}(z) = E\varepsilon_{\mathbf{x}}(z) \tag{3.3}$$

The relationship between the normal strain $\varepsilon_x(z)$, the radius of curvature ρ and the position of the neutral axis z_0 is illustrated in Figure 3.2. The neutral axis is defined in beam theory as the line in the cross section of an isotropic beam where the normal stress vanishes. If z_0 is the distance from the reference plane at z = 0 to the location of the neutral axis, the normal strain at location z is:

$$\varepsilon_x(z) = \frac{ds(z) - ds}{ds} = \frac{(\rho + (z - z_0)d\varphi) - \rho d\varphi}{\rho d\varphi} = \frac{z - z_0}{\rho}$$
(3.4)



Figure 3.2: Schematic sketch of the relationship between the radius of curvature ρ , the position of the neutral axis z_0 and the normal strain $\varepsilon_x(z)$

3.1.2 Modelling Approach of Hsueh

The definition of the neutral axis in Equation (3.4) cannot be used in solving the bending problem of a multilayer system when residual stresses are included. Hsuch [11] developed an analytical approach for analysing thermal stresses in elastic multilayer systems where the strain distribution is decomposed into a uniform strain component c and a bending strain component $\varepsilon_{\rm b}$. The uniform strain component results from the uniform tensile/compressive stress which is imposed on the individual layers to achieve displacement compatibility described in Figure 2.3c. The bending component results from the logic outlined in Figure 2.3d and hence corresponds to ε_x in Equation (3.4).

Therefore, the total strain $\varepsilon'_{\mathbf{x}}(z)$ at position z can be formulated as:

$$\varepsilon_{\mathbf{x}}'(z) = c + \frac{z' - z_0}{\rho} \tag{3.5}$$

The calculations are based on the multilayer system illustrated in Figure 3.1 except that the coordinate system x' - z' is used whereby z' = 0 is located at the interface between substrate and layer 1 and the substrate's free surface is located at $z' = -t_s$. The strain/stress distribution in the systems is determined by using the following three equations to calculate the three unknown parameters c, ρ and z_0 . First, the resultant force per unit area due to the uniform strain component c is zero:

$$E_{\rm s}(c-\alpha_{\rm s}\Delta T)t_{\rm s} + \sum_{j=1}^{n} E_i(c-\alpha_j\Delta T)t_j = 0$$
(3.6)

Furthermore the resultant force due to bending is zero:

$$\int_{-t_{\rm s}}^{0} \frac{E_{\rm s}(z'-z_0)}{\rho} dz' + \sum_{j=1}^{n} \int_{h_j}^{h_{j+1}} \frac{E_j(z'-z_0)}{\rho} dz' = 0$$
(3.7)

Finally the sum of the bending moments with respect to the bending axis is zero:

$$\int_{-t_{\rm s}}^{0} \sigma_{\rm x,s}(z'-z_0)dz' + \sum_{j=1}^{n} \int_{h_j}^{h_{j+1}} \sigma_{\rm x,j}(z'-z_0)dz = 0$$
(3.8)

With the three equillibrium conditions, Equations (3.6)-(3.8), the solutions for the three unknowns are:

$$c = \frac{(E_{\rm s}t_{\rm s}\alpha_{\rm s} + \sum_{i=j}^{n} E_j t_j \alpha_j)\Delta_T}{E_{\rm s}t_{\rm s} + \sum_{j=1}^{n} E_j t_j}$$
(3.9)

$$z_0 = \frac{-E_{\rm s}t_{\rm s}^2 + \sum_{j=1}^n E_j t_j (2h_j + t_j)}{2(E_{\rm s}t_{\rm s} + \sum_{j=1}^n E_j t_j)}$$
(3.10)

$$\frac{1}{\rho} = \frac{3\left[E_{\rm s}(c-\alpha_{\rm s}\Delta T)t_{\rm s}^2 - \sum_{j=1}^n E_j t_j (c-\alpha_j\Delta T)(2h_j + t_j)\right]}{E_{\rm s}t_{\rm s}^2(2t_{\rm s} + 3z_0) + \sum_{j=1}^n E_j t_j \left[6h_j^2 + 6h_j t_j + 2t_j^2 - 3z_0(2h_j + t_j)\right]}$$
(3.11)

The stress distribution in the system can be obtained based on the above approximations. By inserting Equations (3.9)-(3.11) into Equation (3.5) the strain distribution $\varepsilon_{\rm x}(z)$ can be obtained. In combination with Equation (3.3) the corresponding stress distribution can be evaluated.

3.1.3 Analytical approach for the simulation of residual stresses in multilayer systems

In this section the developed analytical approach for the following Load cases is extensively described:

- Load case 1: Thermal mismatch stress
- Load case 2: Film growth stress
- Load case 3: Superposition of thermal mismatch stress and film growth stress

The elastic multilayer system and the x - z coordinate system, shown in Figure 3.1, are applied in the following calculations. In contrast to the approach of Hsueh, the neutral axis z_0 is replaced by z_e , which defines the line in the cross section of the beam where the total strain contribution $\varepsilon_{\mathbf{x}}(z)$ is zero. The uniform strain component c is set to zero. By means of this approach the uniform stain c and the bending strain $\varepsilon_{\mathbf{b}}$ are already included in the $\varepsilon_{\mathbf{x}}(z)$. Therefore, the total strain of the system can be formulated as:

$$\varepsilon_{\rm x}(z) = \frac{z - z_{\rm e}}{\rho} \tag{3.12}$$

As a result of this transformation the uniform strain component c is already accounted for. There remain two unknowns ρ and $z_{\rm e}$ for which two equations are required.

Load case 1: Influence of thermal mismatch stress

Thermal stresses due to different coefficients of thermal expansion, that is introduced by a temperature change, will be discussed in this section. The thermal stress can be calculated from the temperature change ΔT , the Youngs moduli E, the CTE α and the dimensions of the substrate and the layers, respectively. The equilibrium for a beam in the absence of external forces and moments is estimated by the force and moment balances given as

$$\int_{0}^{h_{\rm s}} \sigma_{\rm x,s}^{\rm th}(z) \, b \, dz + \sum_{j=1}^{n} \int_{h_j}^{h_{j+1}} \sigma_{\rm x,j}^{\rm th}(z) \, b \, dz = 0 \tag{3.13}$$

$$\int_{0}^{h_{\rm s}} \sigma_{\rm x,s}^{\rm th}(z) \cdot z \, b \, dz + \sum_{j=1}^{n} \int_{h_j}^{h_{j+1}} \sigma_{\rm x,j}^{\rm th}(z) \cdot z \, b \, dz = 0 \tag{3.14}$$

 $\sigma_{\mathbf{x},\mathbf{s}}^{\mathrm{th}}(z)$ denotes the stress distribution in the substrate and $\sigma_{\mathbf{x},j}^{\mathrm{th}}(z)$ denotes the stress distribution in the *j*-th layer in thickness direction. bdz defines the integration area. The relation between h_j and t_j can be described as follows:

$$h_j = \sum_{i=1}^{k=j-1} t_i + t_s$$
 (j=1,...n) (3.15)

It should be noted that j = 1 implies k = 0 and therefore $h_1 = t_s$. The thermoelastic constitutive relation between stress $\sigma_x(z)$ and strain $\varepsilon_x(z)$ is given as

$$\sigma_{\mathbf{x}}(z) = E(z)(\varepsilon_{\mathbf{x}}(z) - \alpha \Delta T)$$
(3.16)

Substituting Equations (3.12) and (3.16) into Equations (3.13) and (3.14) yields

$$\int_{0}^{h_{\rm s}} E_{\rm s} \left(\frac{z - z_{\rm e}}{\rho} - \alpha_{\rm s} \Delta T \right) \, b \, dz + \sum_{j=1}^{n} \int_{h_j}^{h_{j+1}} E_j \left(\frac{z - z_{\rm e}}{\rho} - \alpha_j \Delta T \right) \, b \, dz = 0 \quad (3.17)$$

$$\int_{0}^{h_{\rm s}} E_{\rm s}\left(\frac{z-z_{\rm e}}{\rho}-\alpha_{\rm s}\Delta T\right) \cdot z \, b \, dz + \sum_{j=1}^{n} \int_{h_{j}}^{h_{j+1}} E_{j}\left(\frac{z-z_{\rm e}}{\rho}-\alpha_{j}\Delta T\right) \cdot z \, b \, dz = 0 \quad (3.18)$$

Equations (3.17) and (3.18) can be transformed so that the two unknowns, the radius of curvature ρ and the position of zero strain, $z_{\rm e}$, can be determined as follows

$$\rho = \frac{AA - BC}{AD - BE} \qquad (3.19) \qquad \qquad z_{\rm e} = \frac{A - D\rho}{B} \qquad (3.20)$$

in which

$$A = E_{s}A_{s}z_{s} + \sum_{j=1}^{n} E_{j}A_{j}z_{j} \qquad B = E_{s}A_{s} + \sum_{j=1}^{n} E_{j}A_{j}$$
(3.21)

$$C = E_{\rm s}I_{\rm s} + \sum_{j=1}^{n} E_j I_j$$
(3.22)

$$D = E_{\rm s}\alpha_{\rm s}\Delta T A_{\rm s} + \sum_{j=1}^{n} E_j \alpha_j \Delta T A_j$$
(3.23)

$$E = E_{\rm s}\alpha_{\rm s}\Delta T z_{\rm s}A_{\rm s} + \sum_{j=1}^{n} E_j\alpha_j\Delta T z_jA_j$$
(3.24)

where z_j , z_s denote the distance from the reference plane to the center of gravity of each layer and the substrate, compare Figure 3.1. A_s and A_j , respectively, are the cross section areas of the substrate and the film. I_s and I_j are, respectively, the second moment of area of the substrate and the layers and can be estimated as

$$I_{\rm s} = \frac{bt_{\rm s}^3}{12} + \left(\frac{t_{\rm s}}{2}\right)^2 bt_{\rm s} \tag{3.25}$$

$$I_j = \frac{bt_j^3}{12} + \left(t_s + \frac{t_j}{2} + \sum_{i=1}^{k=j-1} t_i\right)^2 bt_j$$
(3.26)

The approximate stress distributions, in the substrate and the layers, due to a temperature change ΔT can be obtained based on the above approximations by inserting the resulting curvature ρ and the location of zero strain $z_{\rm e}$ into Equations (3.27) and (3.28) leading to

$$\sigma_{\mathbf{x},\mathbf{s}}^{\mathrm{th}}(z) = E_{\mathbf{s}} \left(\frac{z - z_{\mathbf{e}}}{\rho} - \alpha_{\mathbf{s}} \Delta T \right) \qquad (0 < z < h_{\mathbf{s}})$$
(3.27)

$$\sigma_{\mathbf{x},j}^{\mathrm{th}}(z) = E_j \left(\frac{z - z_{\mathrm{e}}}{\rho} - \alpha_j \Delta T \right) \qquad (h_j < z < h_{j+1}) \qquad (j = 1, \dots n)$$
(3.28)

Due to the fact that the neutral axis of zero stress is defined as the axis where the normal stress vanishes, the following condition can be used to calculate the position of the neutral axis

$$\sigma_{\mathbf{x},\mathbf{s}}^{\mathrm{th}}(z_0) = 0 \qquad \sigma_{\mathbf{x},j}^{\mathrm{th}}(z_0) = 0$$
(3.29)

Load case 2: Influence of film growth stress

The influence of growth induced stress is estimated by adding a prestressed layer to a system consisting of a substrate and of n layers that is self equillibrated, but not stress free. The prestressed layers are added onto the system one after the other. The entire deposition process is divided into three steps, (i) deposition of the first layer; (ii) deposition of the second layer and superimposition with the results of adding the first layer (iii) extension to the deposition of the n-th layer, as described in the following section.
Deposition of the first layer

At the beginning the deposition of the first layer onto the stress free substrate is considered. The equilibrium is estimated by the force and moment balances, Equations (3.30) and (3.31). The layer is deposited with a prestress $\sigma_{\rm g}$ which accounts for the stress state arising from the growth process.

$$\int_{0}^{h_{\rm s}} \sigma_{\rm x,s}^{(1)}(z) \, b \, dz + \int_{h_1}^{h_2} \sigma_{\rm x,1}^{(1)}(z) \, b \, dz + \int_{h_1}^{h_2} \sigma_{\rm g}^{(1)} \, b \, dz = 0 \tag{3.30}$$

$$\int_{0}^{h_{\rm s}} \sigma_{\rm x,s}^{(1)}(z) \cdot z \, b \, dz + \int_{h_{1}}^{h_{2}} \sigma_{\rm x,1}^{(1)}(z) \cdot z \, b \, dz + \int_{h_{1}}^{h_{2}} \sigma_{\rm g}^{(1)} \cdot z \, b \, dz = 0 \tag{3.31}$$

The subscript denotes the considered layer and the superscript denotes the current prestressed layer. $\sigma_{\rm x,s}^{(1)}$ and $\sigma_{\rm x,1}^{(1)}$ denote the resulting stress distribution in the substrate and the first deposited layer on the basis of the prestress, respectively. To obtain the curvature $\rho^{(1)}$ and the axis of zero strain $z_{\rm e}^{(1)}$, Equations (3.3) and (3.12) are substituted into Equations (3.30) and (3.31). The approximate stress distribution in the form

$$\sigma_{\mathbf{x},\mathbf{s}}^{(1)}(z) = E_{\mathbf{s}}\left(\frac{z - z_{\mathbf{e}}^{(1)}}{\rho^{1}}\right) \qquad (0 < z < h_{S})$$
(3.32)

$$\sigma_{\mathbf{x},1}^{(1)}(z) = E_1\left(\frac{z - z_{\mathrm{e}}^{(1)}}{\rho^{(1)}}\right) \qquad (h_1 < z < h_2) \tag{3.33}$$

Deposition of the second layer

Consider the next (second) layer added to the already coated substrate. Initially the prestress from the first deposited layer is not taken into account. The initial contribution considers a system consisting of the substrate and the first layer, both stress free, and a prestressed second layer. The moment and force balances are expressed as

$$\int_{0}^{h_{\rm s}} \sigma_{\rm x,s}^{(2)}(z) \, b \, dz + \sum_{j=1}^{2} \int_{h_j}^{h_{j+1}} \sigma_{\rm x,j}^{(2)}(z) \, b \, dz + \int_{h_2}^{h_3} \sigma_{\rm g}^{(2)}(z) \, b \, dz = 0 \tag{3.34}$$

$$\int_{0}^{h_{\rm s}} \sigma_{\rm x,s}^{(2)}(z) \cdot z \, b \, dz + \sum_{j=1}^{2} \int_{h_j}^{h_{j+1}} \sigma_{\rm x,j}^{(2)}(z) \cdot z \, b \, dz + \int_{h_2}^{h_3} \sigma_{\rm g}^{(2)}(z) \cdot z \, b \, dz = 0 \qquad (3.35)$$

Inserting $\rho^{(2)}$ and $z_{\rm e}^{(2)}$ obtained from Equations (3.34) and (3.35) into Equations (3.36) to (3.38) leads to the stress distribution of the substrate and the layers.

$$\sigma_{\rm x,s}^{(2)}(z) = E_{\rm s}\left(\frac{z - z_{\rm e}^{(2)}}{\rho^2}\right) \qquad (0 < z < h_S) \tag{3.36}$$

$$\sigma_{\mathbf{x},1}^{(2)}(z) = E_1\left(\frac{z - z_{\mathbf{e}}^{(2)}}{\rho^{(2)}}\right) \qquad (h_1 < z < h_2) \tag{3.37}$$

$$\sigma_{\mathbf{x},2}^{(2)}(z) = E_2\left(\frac{z - z_{\rm e}^{(2)}}{\rho^{(2)}}\right) \qquad (h_2 < z < h_3) \tag{3.38}$$

To calculate the final stress distribution, after the deposition of two prestressed layers, the principle of superposition is applied. The stress distributions obtained from the deposition of the first and the second layers are superimposed

$$\sigma_{\rm x,s}^{\rm p}(z) = \sigma_{\rm x,s}^{(1)} + \sigma_{\rm x,s}^{(2)}$$
(3.39)

$$\sigma_{\mathbf{x},1}^{\mathbf{p}}(z) = \sigma_{\mathbf{x},1}^{(1)} + \sigma_{\mathbf{x},1}^{(2)} + \sigma_{\mathbf{g}}^{(1)}$$
(3.40)

$$\sigma_{\rm x,2}^{\rm p}(z) = \sigma_{\rm s,2}^{(2)} + \sigma_{\rm g}^{(2)} \tag{3.41}$$

where $\sigma_{\mathbf{x},\mathbf{s}}^{\mathbf{p}}(z)$ is the resulting stress distribution of the substrate, $\sigma_{\mathbf{x},1}^{\mathbf{p}}(z)$ is the final stress distribution of the first layer and $\sigma_{\mathbf{x},2}^{\mathbf{p}}(z)$ denotes the final stress distribution of the second layer, after the deposition of two prestressed layers.

To obtain the final curvature $\rho^{\rm p}$ and the position of zero strain $z_{\rm e}^{\rm p}$ Equation (3.42) is considered. By inserting Equations (3.43) into (3.42) and using the average values of $\sigma_{\rm x,1}^{\rm p}(z)$ and $\sigma_{\rm x,2}^{\rm p}(z)$ calculated over the height of the individual layers the two unknowns $\rho^{\rm p}$ and $z_{\rm e}^{\rm p}$ can be evaluated.

$$\int_{0}^{h_{\rm s}} \sigma_{\rm x,s}^{\rm p}(z) \, b \, dz + \int_{h_1}^{h_2} \sigma_{\rm x,1}^{\rm p}(z) \, b \, dz + \int_{h_2}^{h_3} \sigma_{\rm x,2}^{\rm p}(z) \, b \, dz = 0 \tag{3.42}$$

$$\sigma_{\mathbf{x},\mathbf{s}}^{\mathbf{p}}(z) = E_{\mathbf{s}} \frac{z_{\mathbf{s}} - z_{\mathbf{e}}^{\mathbf{p}}}{\rho^{\mathbf{p}}}$$
(3.43)

Deposition of the *n*-th layer

The above process is readily extended to the deposition process of n layers. The calculation is executed as for the deposition of two layers, shown above, only that the superposition process is performed over all deposited layers.

$$\sigma_{\mathbf{x},j}^{\mathbf{p}} = \sum_{i=1}^{n} \sigma_{\mathbf{x},j}^{i} + \sigma_{\mathbf{g}}^{j}$$
(3.44)

Load case 3: Superposition of Load case 1 and 2

To give the stress distribution due to growth stress in conjunction with a temperature change the stress states from Load case 1 can be superimposed on those calculated in Load case 2 to give

$$\sigma_{\mathbf{x},\mathbf{s}}(z) = \sigma_{\mathbf{x},\mathbf{s}}^{\mathrm{th}}(z) + \sigma_{\mathbf{x},\mathbf{s}}^{\mathrm{p}}(z) \tag{3.45}$$

$$\sigma_{\mathbf{x},j}(z) = \sigma_{\mathbf{x},j}^{\mathrm{th}}(z) + \sigma_{\mathbf{x},j}^{\mathrm{p}}(z) \tag{3.46}$$

3.2 Finite Element Model

The goal of the finite element analysis is to verify the analytical approach for the cooling process numerically. For this purpose it is necessary to develop an FE model which is able to handle a temperature change process. The FE model generation and specification are discussed briefly in the following section.

3.2.1 Modelling Approach

The used three-dimensional FE model is shown in Figure 3.3. Some simplifications are applied to this model: (i) a substrate with only two deposited layers is taken into account; (ii) the dimensions of the three parts are chosen to lie within the same range and (iii) the geometric symmetry of the model is exploited. Consequently one quarter of the whole structure is modelled. The symmetry planes and the quarter model are shown in Figure 3.3. The bilayer system is modelled with 20-node three dimensional continuum elements with second order interpolation and reduced integration (Type: C3D20R). Furthermore, perfect bonding is assumed between the substrate and the first layer and between the two layers. The temperature load is defined via a predefined field. For a better presentation the boundary conditions are illustrated schematically in Figure 3.4. Point P is fixed ($u_1 = u_2 = u_3 = 0$), face W is constrained in x-direction ($u_1 = 0$) and face S is constrained in y-direction ($u_2 = 0$)



Figure 3.3: Finite Element model with the planes of symmetry and the quarter model used for the calculation



Figure 3.4: quarter model with boundary conditions for face W and face S

Chapter 4

Results and Discussion

In the present chapter results obtained for the different Load cases are analyzed, interpreted and explained. The first section provides a short overview of the considered material properties. A verification of the analytical approach for residual stresses generated due to a temperature change and for film growth stresses is executed in Section 4.2. Finally, in Section 4.3 a parameter study is carried out to get an overview of how material and process parameters in multilayer systems influence the final residual stress state.

4.1 Material Properties

The coating consists of two different layer materials alternately deposited on an austenitic stainless steel substrate. The data sheet of Austenite can be found in Appendix A. The material properties were provided by the Institute of Materials Science and Technology for the substrates and the layers used in this study. Different materials are studied for both, the substrate and the layers. The isotropic Young's moduli E_s and E_j and the Poisson's ratios ν_s and ν_j for the substrate and the layers are listed in Table 4.1.

Substrate material	$E_{\rm s}$ [MPa]	$ u_{ m s}$
Austenite	200000	0.3
Ti6Al4V	110000	0.3
WC-CO	600000	0.22
	1	
Layer material	E_j [MPa]	$ u_j $
CrN	363000	0.257
TiN	450000	0.216
AlN	505000	0.166

 Table 4.1: Elastic material properties of the layers and the substrate

Within the present framework the thermal mismatch stress generated from a cooling process plays an important role, therefore the CTEs of the materials are of great importance. The CTEs were provided as instantaneous values $\alpha'(T)$ as functions of the temperature. Abaques requires CTEs $\alpha(T)$ that define the total value of the thermal strain with respect to a reference temperature T^0 as a function of the temperature, see Figure 4.1. To obtain the total values $\alpha(T)$, the instantaneous values $\alpha'(T)$ are integrated as follows

$$\varepsilon^{\rm th} = \int_{T^0}^T \alpha' dT \qquad \Rightarrow \qquad \alpha(T) = \frac{1}{T - T^0} \int_{T^0}^T \alpha' dT$$
(4.1)



Figure 4.1: Definition of the thermal expansion coefficient in instantaneous form α' and total form α

Figure 4.2a shows the instantaneous form of the CTE for different layer materials used for the analytical calculations in PYTHON. Figure 4.2b depicts the total value of the CTE required by ABAQUS. Furthermore, the reference temperature is chosen to be $T^0 = 293,15$ K which is taken into account during the analysis.



Figure 4.2: Temperature dependent CTE for the different layer materials as (a) instantaneous values and (b) total values for the implementation in PYTHON and ABAQUS

For the substrate materials the CTE is chosen to be constant so that $\alpha(T)$ and $\alpha'(T)$ are coincide. The parameter values are listed in Table 4.2.

 Table 4.2:
 CTE for the different substrate materials

	WC-Co	Ti6Al4V	Austenite
CTE $\left[\frac{1}{K}\right]$	$5.5 \times 10^{-6} [2]$	$9.7 \times 10^{-6} [12]$	16.5 [7]

4.2 Verification of the analytical approach

This section is dedicated to ensuring that the analytical model is working correctly. As a first step the thermal process and the film growth process are considered separately and compared to the results of the 3D Finite Element models, discussed in Section 3.2. The results of the thermal mismatch stress are additionally compared with the approach of Hsueh, explained in Section 3.1.2. To check if the equilibrium conditions in Equations (3.1) and (3.2) are satisfied the stress state in z-direction is integrated over the cross section of the substrate and over each individual deposited layer.

4.2.1 Load case 1: Thermal mismatch stress

Verification with Finite Element simulations

The FE-model explained in Section 3.2 is used to verify the residual stress state generated by a cooling process. To keep the FE model simple the thicknesses of the substrate and the two layers are chosen to lie within the same range. To illustrate the plausibility of the analytical model, specific results are calculated for a CrN/AlN coating deposited on an austenitic stainless steel substrate. The deposition temperature of the multilayer system is assumed to be $T_{dep} = 500^{\circ}$ C. The thermal stresses are generated due to cooling from the deposition temperature to room temperature $T_{end} = 20^{\circ}$ C. The architecture of the substrate and the layers is shown in the Table 4.3

	material	thickness $t \text{ [mm]}$
Substrate	Austenite	20
Layer a	CrN	10
Layer b	AlN	5

Table 4.3: Elastic properties of the substrate and the layers for the verification ofthe thermal mismatch stress with a Finite Element model

Fig. 4.3a shows the distribution of thermal stresses calculated with the above approximations. The stress distribution in both approaches is linear. The FE - model predicts a membrane stress exceeding the analytical results by about 24%. However, the FE - model is based on a three-axial stress state, whereas the analytical model is essentially biaxial. Accordingly, for the latter model the Young's moduli are replaced by the biaxial modulus $E_{\rm b} = \frac{E}{1-\nu}$ [11]. The stress distribution of the bilayer system, by considering biaxial moduli, is depicted in Figure 4.3b. A good agreement between the analytical and FE-model is obtained by applying the biaxial Young's moduli. This configuration leads to a maximum difference of 2.4% in terms of the membrane stress. Due to the better results obtained with the biaxial Young's modulus it is used in the following calculations. Both models show good agreement of the position of the neutral axis.



Figure 4.3: analytical and numerical thermal stress state in the multilayer system using (a) a axial Young's modulus and (b) a biaxial Young's modulus in the analytical model

Comparison with the approach of Hsueh

The calculations are based on the multilayer system illustrated in Fig. 3.1 where the coordinate system x' - z' is used. A total number of 4 layers is applied alternatingly. A temperature change of $\Delta T = -480$ K is applied. The architecture of the substrate and the layers is listed in Table 4.4

Table 4.4: Geometrical data of the substrate and the layers for the verification of
the thermal mismatch stress with the approach of Hsueh

	material	thickness $t \text{ [mm]}$
Substrate	Austenite	0.38
Layer a	CrN	5×10^{-6}
Layer b	AlN	5×10^{-6}

Comparing the results of the developed analytical approach Equations (3.13) and (3.14) and the approach of Hsueh, Equations (3.6) to (3.8), identical predictions for the stress distribution in substrate and layers are obtained see Fig. 4.4. This confirms that the parameter c used in the model of Hsueh is already considered in $z_{\rm e}$, compare Equations (3.12) and (3.5).



Figure 4.4: Comparison of the thermal stress state in (a) the substrate and (b) the coating between the developed analytical approach and the approach of Hsueh. $\sigma_{\rm x,c}$ denotes the coating membrane stress in *x*-direction over the total coating thickness.

Equilibrium conditions

The resultant forces and moments arising in the system, obtained from thermal mismatch stress, must be equal to zero to reach a static state of equilibrium, described as follows

$$\sum F = F_{\rm s} + \sum_{j=1}^{n} F_j = 0 \tag{4.2}$$

$$\sum M = M_{\rm s} + \sum_{j=1}^{n} M_j = 0 \tag{4.3}$$

whereby $F_{\rm s}$ denotes the resulting force in the substrate and F_j denotes the resulting force in each layer. Due to the assumption that the stress distribution in each constituent is linear the residual stress state of the substrate can be described as

$$\sigma_{\mathbf{x},\mathbf{s}}(z) = \frac{\sigma_{\mathbf{x},\mathbf{s}}(h_1) - \sigma_{\mathbf{x},\mathbf{s}}(0)}{h_1} z + \sigma_{\mathbf{x},\mathbf{s}}(0)$$
(4.4)

and that of the j-th layer as

$$\sigma_{\mathbf{x},j}(z) = \frac{\sigma_{\mathbf{x},j}(h_{j+1}) - d}{h_{j+1}} z + d$$
(4.5)

where

$$d = \frac{\sigma_{\mathbf{x},j}(h_j)h_j - \sigma_{\mathbf{x},j}(h_{j+1})h_{j+1}}{h_{j+1} - h_j}$$
(4.6)

To obtain the resultant forces and moments the stress distribution must be integrated over the thickness of each constituent. The equilibrium verification is executed with a 20-bilayer system. For the verification the following parameters are used

Table 4.5:	Geometrical	data	of the	substrate	and	the	layers	for	the	verification	of
	the equilibriu	ım co	nditio	n							

	material	thickness $t \text{ [mm]}$
Substrate	Austenite	0.38
Layer a	CrN	1×10^{-6}
Layer b	TiN	1×10^{-6}

The residual stress states of the substrate and the layers is depicted in Fig. 4.5 and 4.6, respectively. $F_{\rm s}^+$ and $F_{\rm s}^-$ denote the resulting substrate force corresponding to the tensile and compressive state. The calculated resulting forces and moments for the described configuration are read

$$\sum F = -1.714 \times 10^{-13} [\text{N}] \tag{4.7}$$

$$\sum M = -6.12843109593 \times 10^{-13} [\text{Nmm}]$$
(4.8)

and therefore, the equilibrium conditions are satisfied.



Figure 4.5: Thermal stress distribution in the substrate with the resulting substrate forces



Figure 4.6: Thermal stress distribution in the coating over (a) the entire coating thickness (b) the first four deposited layers including the resulting layer forces

4.2.2 Load case 2: Film growth stress

Verification with a Finite Element Model

In order to verify the film growth stress results the analytical approach is compared with an efficient 3D Finite Element model developed by Wagner [23]. A 20-bilayer system is formed by alternating deposition of CrN and TiN on a Austenite substrate. The compressive preload generated from the deposition process is assumed to be 3GPa. The architecture of the substrate and the layers is listed Table 4.6

 Table 4.6: Geometrical data of the substrate and the layers for the verification of the film growth stress

	material	thickness $t \text{ [mm]}$
Substrate	Austenite	0.38
Layer a	CrN	2×10^{-4}
Layer b	TiN	3×10^{-4}

In Fig. 4.7a the stress distribution in the layers obtained with the analytical and numercial models is depicted. Fig. 4.7b provides a more detailed presentation of the first four layers. There is a slight difference between the solutions of the two approaches. The values of the numerical and analytical approach differ by about of 4%. Due to the same assumptions regarding the material behaviour the difference can be seen as a result of the numerical error generated in the Finite Element model.



Figure 4.7: Film growth stress in the coating (a) over the entire coating thickness and (b) over the first four deposited layers

Homogenized Properties

Since only geometrically and physically linear behaviour is considered one might assume that modelling one layer with homogenized properties instead of a layerwise modelling would provide a good approximation. To asses this assumptions, three different modelling approaches are compared with each other. The first approach considers the introduction of the deposition stress as the coating is formed layer-bylayer. For the second approach elastic properties of the layers are homogenized with a rule of mixture by a weighted mean of the Young's moduli

$$E_{\rm h} = \xi_{\rm a} E_{\rm a} + \xi_{\rm b} E_{\rm b} \tag{4.9}$$

where $E_{\rm a}$ and $E_{\rm b}$ are the Young's moduli of layer material a and b, respectively. $\xi_{\rm a}$ and $\xi_{\rm b}$ represent the volume fractions of the layer materials. For the third approach the coating is modelled with the homogenized material properties represented by one single layer. The three different models are shown in Fig. 4.8.



Figure 4.8: Different modelling approaches: inhomogeneous layer-by-layer modelling (left), layer-by-layer modelling with homogenized properties (middle), homogenized single layer (right)

The considered mulitlayer system is formed by alternating deposition of CrN and TiN with equal thickness of 0.00001mm deposited on an austenite substrate. The entire thickness of the coating is chosen to be 0.001mm. A compressive prestress of 1GPa is taken into account. The elastic properties calculated with Equation (4.9) lead to a

homogenized Young's modulus of 406.5 GPa. The Poisson's ratio is also calculated with a rules of mixture

$$\nu_{\rm h} = \xi_{\rm a} \nu_{\rm a} + \xi_{\rm b} \nu_{\rm b} \tag{4.10}$$

which leads to a value of 0.2365.

The film growth stress state of the coating is shown in Figure 4.9. Both layer-bylayer modelling techniques are carried out with 50-bilayers. By comparing the three approaches it is easy to see that the homogenized single layer model gives different results compared to the layer-by-layer modelling approaches. This is attributed to the fact that the overall stiffness and the position of the neutral axis of the entire system change in every deposition step. Therefore the system has to find a state of equilibrium after each layer deposition. Bending of the system occurs and leads to a tensile stress component in previously deposited layers. This is not necessary for the deposition of one single layer, which results in a different stress state in the coating. The good agreement of the two layer-by-layer models suggest that not the homogenization of the layer properties but the difference in the deposition sequence leads to the significant deviation of the single homogenized layer.

To give a fairly accurate indication how many homogenized layers are necessary for obtaining correct results compared to the layer wise deposition for the stress distribution, the single thick homogenized layer is divided into various numbers of thin layers. The maximum membrane stress of the top and bottom layer, after the deposition of the various layers, is plotted in Figure 4.10a. The average magnitude of the membrane stress of the top layer converges towards the applied prestress with increasing number of layers. The maximum stress value of the bottom layer stays nearly constant over the number of layers. In summary it can be said that when applying a total coating thickness of 0.001mm at least 100 layers are necessary to obtain accurate results. Figure 4.10b illustrates the maximum in-plane stress in top and bottom layers after every deposited layer until the entire coating reaches a thickness of 0.001mm . The compressive stress of the bottom layer decreases with further deposition steps. The compressive stress of the top layer stays constantly at the same magnitude as the applied stress.



Figure 4.9: Film growth stress distribution obtained for layerwise and homogenized modelling



Figure 4.10: Local residual stress in the coating (a) by division of the homogenized layer into a certain number of individual homogenized layers and (b) after every deposition step until the system reaches the entire coating thickness by applying 500 bilayers

4.3 Film growth stresses in conjunction with thermal mismatch stresses

In this chapter the results of the computational simulations based on an reference configuration are visualised and discussed. In a parameter study the effect of the following varying parameters on the total residual stress state is discussed: (i) influence of the manufacturing temperature; (ii) influence of the coating height; (iii) influence of material properties of the substrate and the layers; (iv) influence of the prestress; (v) influence of the layer architecture.

4.3.1 Reference configuration

To execute an efficient parameter study an reference configuration of the multilayer system is defined. A 500-bilayer system is formed by alternating deposition of TiN and CrN on an Austenite substrate. The sample is cooled down from a manufacturing temperature $T_{dep} = 500^{\circ}$ C to room temperature $T_{end} = 20^{\circ}$ C. Each layer is deposited with a compressive preload of $\sigma_{g} = 8$ GPa. The architecture of the substrate and the layers is listed in Table 4.7

 Table 4.7: Geometrical data of the substrate and the layers in the reference configuration

_		material	thickness $t \text{ [mm]}$
-	Substrate	Austenite	0.50
	Layer a	TiN	16×10^{-6}
	Layer b	CrN	8×10^{-6}

In this section the total residual stress state is described in terms of thermal mismatch stress $\sigma_x^{\text{th}}(z)$, film growth stress $\sigma_x^{\text{p}}(z)$ and total residual stress $\sigma_x^{\text{total}}(z)$ for the substrate and the coating as can be seen in Figure 4.11 and 4.12. First, the residual stress distributions in the substrate are considered. On the basis of the fact that the CTE of Austenite is higher than the CTEs of TiN and CrN, the substrate contracts more strongly compared to the layers. Therefore, after the applied temperature change the substrate is subjected to tensile stress near the first layer and to compressive stress on the opposite side, as can be seen in Figure 4.11. The same trend of the stress distribution is observed by applying a prestress onto each layer. Both Load cases result in the same sign of the curvature of the system. Since only linear effects are considered a superposition of the two Load cases can be applied.

In the case of a high residual stress distribution the substrate may be beyond its elastic deformation range. The yield strength of Austenite (1.4301) at manufacturing temperature $T_{dep} = 500^{\circ}$ C is approximately 92MPa, see Appendix ??appendix. By considering the total residual stress distribution in Figure 4.11 one can suggest that the yield strength is already exceeded and plastic deformation takes place.

The average membrane stress in each layer is calculated and furthermore interpolated between the layers. The stress distributions in the layers, for the three Load cases, is depicted in Figure 4.12. When a compressive prestress is applied to the layers, the film growth stress appears as a compressive stress in layer a and b. The magnitude of the film growth stress in the layers increases with an increase in the z-position. This is substantiated by the fact that, in a progressive deposition process, the compressive stress component in each layer is progressively reduced by deposition of subsequent layers on top of it. The layer material with the higher Young's modulus (TiN) exhibits a smaller film growth stress. The applied prestress can be reduced to a higher degree by using a layer material with a higher Young's modulus compared to a layer material with a smaller Young's modulus. When considering the exact values of the average thermal stress, one can see that the magnitude of the thermal stress slightly decreases by an increasing z-position. This is because the curvature of the system induces a higher magnitude of tensile stress with a greater radius of curvature. Figure 4.13 depicts the stress states for each Load case in the first four deposited layers. For the thermal mismatch stress can be said that the layer material with a higher Young's modulus exhibits a higher compressive stress value. Another general comment is that a layer material with a CTE closer to the substrate's CTE result in a smaller compressive stress. In this case the CTE of TiN is closer to that of the substrate.

Since the equilibrium of the system must be fulfilled, the total residual stress in the substrate is significantly smaller than in the coating. This is due to the large thickness ratio between the coating and the substrate.

For each Load case the position of the neutral axis is located at the same z-position in the substrate, as can be seen in Figure 4.11. The position of the neutral axis as a function of the numbers of deposited layers is depicted in Figure 4.14. As one can see, the neutral axis is located in the substrate and doesn't change its position significantly. This is due to the fact that the position of the neutral axis is controlled by the geometry of the cross-section and is independent of the applied loads. For the considered system the cross-sectional area is dominated by the thick substrate compared to the thin coating which has only a minor influence on the position of the neutral axis. Figure 4.15 plots the radius of curvature as a function of the numbers of deposited layers. The radius of curvature decreases with an increasing number of deposited layers for the considered reference configuration.



Figure 4.11: Superposition of the residual stress distributions including film growth stresses and thermal mismatch stresses in the substrate after deposition of 500 bilayers



Figure 4.12: Superposition of the residual stress distributions including film growth stresses and thermal mismatch stresses in the coating after all layers have been deposited



Figure 4.13: Residual stress distributions including (a) the total residual stresses and the film growth stresses and (b) the thermal mismatch stresses in the coating over the first four deposited layers



Figure 4.14: Position of the neutral axis depending on the number of deposited layers



Figure 4.15: Radius of curvature ρ depending on the number of deposited layers

4.3.2 Influence of the coating height

Furthermore the influence of the total coating thickness on the total residual stress state is considered. The number of deposited layers increases until it reaches the number of deposited layers, defined in the reference configuration (500 bilayers). The stress magnitude is evaluated at the top and bottom of the substrate and the coating, respectively.



Figure 4.16: Local residual stress at top and bottom in the substrate depending on the number of deposited layers

Figure 4.16 shows the stress magnitude in the top and bottom of the substrate as a function of the numbers of deposited layers. The absolute values at the top and bottom increase with an increasing number of deposited layers. Furthermore the yield strength of Austenite is shown in Figure 4.16. One can see that the substrate material reaches the yield strength by a number of about 100 deposited layers. This corresponds to a coating height of 0.0012mm. Plastic deformation will appear in the substrate close to the interface to the coating.



(a) Influence of number of deposited layers(b) Influence of number of deposited layerson thermal stresson fiml growth stress



on total residual stress

Figure 4.17: Local residual stress at top and bottom in the coating depending on the numbers of deposited layers

The average stress magnitude in the top and bottom layers of the coating, for each Load case, is depicted in Figure 4.17. The average thermal stress of the top and bottom layers decreases with a further increase of the thickness of the coating, shown in Figure 4.17a. As can be seen in Figure 4.17b the average film growth stress of the top layer remains nearly constant in the range of the applied prestress of $\sigma_p = 8$ GPa. As the coating gets thicker the average stress magnitude of the bottom layer decreases. In summary it can be said to fulfil the force and moment equilibria a higher number of deposited layers leads to an increase of the residual stress level in the substrate and to an decrease of the stress level in the layers.

4.3.3 Influence of the manufacturing temperature

In order to investigate how the total residual stress state in the system changes due to the deposition temperature, the manufacturing temperature is varied and the system is cooled down to room temperature. The stress magnitude in the top and bottom of the substrate and the coating as a function of the manufacturing temperature is depicted in Figure 4.18 and 4.19. The membrane stress in the top and bottom of the substrate increases with an increasing deposition temperature. Figure 4.19 shows that the value of the compressive residual stress in the bottom and top layers increases with increasing deposition temperature. This indicates that the manufacturing temperature plays a considerable role on residual stress.

In summary it can be said that, for the considered reference configuration, the manufacturing temperature should be chosen as low as possible to minimize the total residual stress state in the substrate and the layers.



Figure 4.18: Local residual stress at top and bottom of the substrate as a function of the manufacturing temperature



Figure 4.19: Local residual stress at top and bottom of the coating as a function of the manufacturing temperature

4.3.4 Influence of the material properties

Influence of the substrate material

In this section the influence of the properties of the substrate material on the total residual stress state in the substrate and the coating is studied. The considered substrate materials are WC-Co, Austenite and Ti6Al4V. For a better representation the resulting stress states of the three Load cases are depicted separately for the substrate and the layers in Figs. 4.20 and 4.21, respectively.

First the effect on the substrate is studied. From Figure 4.20a it can be clearly seen that WC-Co causes the highest value of residual stress due to the film growth process on top and bottom of the substrate. From this it can be said that the substrate material with the highest Young's modulus exhibits the highest film growth stress state in the substrate. Figure 4.20b shows the effect of different substrate materials on the thermal residual stress. Due to the fact that the CTE of Ti6Al4V and Austenite is greater than that of the layer materials, the substrate is subjected to compression at the free surface and to tension at the interface between coating and substrate. The CTE of WC-Co is smaller compared to that of the layer materials, consequently the layers contract more than the substrate. Therefore, the top of the substrate is subjected to compressive normal stress and the bottom is subjected to tensile normal stress. This results in a different sign of the curvature. If the CTE of the substrate material lies in the same range as the CTE of the layer materials a low stress level in the substrate is achieved. This can be obtained by using Ti6Al4V. As can be seen in Figure 4.20c WC-Co and Ti6Al4V as substrate material cause the smallest stress magnitude on top and bottom of the substrate by superposition of thermal and film growth stress. The high stress magnitude of WC-Co is reduced since the sign of the thermal stress and film growth stress is different.

Figure 4.21 presents the stress distributions in the coating for the three Load cases. Considering WC-Co as a substrate material the highest film growth stress between the substrate and the coating is achieved. A high Young's modulus of the substrate leads to a higher bending stiffness and an increase of the substrates resistance against deformation. Therefore WC-Co causes a less degradation of the applied film growth stress in the coating. Due to the smaller CTE of WC-Co compared to the coating, the layers are subjected to tension by thermal loading, depicted in Figure 4.21b. By a superposition of thermal and growth stresses, the high growth stresses of WC-Co are reduced due to the signs of the thermal stress contribution. The equal signs of the stress contributions by using Austenite or Ti6Al4V as substrate material, leads to a higher total residual stress state.



Figure 4.20: Residual stress distributions in the substrate due to different substrate materials including (a) film growth stresses, (b) thermal mismatch stresses and (c) total residual stresses

Furthermore, the maximum difference in stress magnitude between the bottom and the top layer and between the substrate and the bottom layer is presented in Figure 4.22. The smallest difference in stress magnitude between bottom and top layer is achieved by using WC-Co as substrate material. It is also demonstrated that Ti6Al4V causes the smallest stress difference at the interface between the substrate and the

bottom layer.

In summary it can be said that the level of total residual stress of the substrate and the layers can be reduced by using a substrate material with a small Young's modulus. Furthermore the total residual stress state can be decreased by using a substrate material with a CTE which lies in the approximately same range as the CTE of the layers. A higher CTE of the substrate leads to an accumulation of the film growth stress and thermal mismatch stress.



Figure 4.21: Residual stress distributions in the coating due to different substrate materials including (a) film growth stresses, (b) thermal mismatch stresses and (c) total residual stresses



Figure 4.22: Difference in stress magnitude $\Delta \sigma$ between the top and bottom layer and between the substrate and the bottom layer for different substrate materials

Influence of the layer materials

The influence of the layer materials on the total residual stress state in the substrate and layers is investigated in Figure 4.23 and 4.24. Two different layer combinations are discussed: TiN/CrN and AlN/CrN.

For the film growth stress in the substrate hardly any difference is observed between the two layer combinations, depicted in Figure 4.23a. Only a small reduction of the stress magnitude in AlN/CrN can be observed. This is because the Young's moduli of TiN and AlN do not differ significantly and hence it does not have a great influence on the thick substrate. Using of AlN/CrN compared to TiN/CrN leads to a smaller thermal stress magnitude in the substrate. This i because AlN/CrN leads to a smaller mismatch of thermal strain between the substrate and the coating. A superposition of the two Load cases shows that the change of the layer material has no strong influence on the total residual stress state in the substrate.



Figure 4.23: Residual stress distributions in the substrate due to different layer materials including (a) film growth stresses, (b) thermal mismatch stresses and (c) total residual stresses

In Figure 4.24 the effect of different layer materials on the residual stress state in the layers is presented. A higher Young's modulus of layer AlN leads to a slightly smaller magnitude of film growth stress in the layers close to the substrate, whereas hardly any difference is observed at the top of the coating. The bending stiffness of AlN is higher compared to TiN, which leads to a higher degradation of the applied prestress.

Considering the thermal stress state in Figure 4.24b, one can see that AlN exhibits a lower stress value. This is due to the fact the the CTE of AlN is closer to the CTE of the substrate (Austenite). Additionally the higher Young's modulus of AlN would lead to higher thermal stresses compared to TiN. All in all it can be said that the smaller CTE of AlN has a stronger influence on the thermal residual stress distribution as its higher elastic modulus.

The third diagram shows the total residual stress state in the coating, obtained by a superposition of the two Load cases. In summary it can be said, that a CTE of the layers being closer to the substrates CTE reduce the total residual stress state in the layers.



Figure 4.24: Residual stress distributions in the coating due to different substrate materials including (a) film growth stresses, (b) thermal mismatch stresses and (c) total residual stresses

4.3.5 Influence of the prestress

The influence of a variation of the applied coating prestress is investigated in this section. A comparison between the resulting residual stress values for the substrate and the coating for compressive preloads of 6-10GPa shows a residual stress increase by growth of the intrinsic film stress as expected.



Figure 4.25: Total residual stress distribution in the substrate (left) and the coating (right) depending on the compressive preload



Figure 4.26: Local residual stress at the top and bottom of the (a) substrate and (b) coating as a function of the applied prestress

In Figure 4.26 the local residual stress at the top and bottom of the substrate and the coating as a function of the applied prestress can be seen. One can realize by this illustration, that a linear relation between the applied prestress and the local residual stress at the top and bottom of the substrate can be obtained. For the coating the relation is almost linear.

4.3.6 Influence of the layer architecture

The influence of the individual layer thicknesses on the total residual stress state in the layers investigated in this section. The total coating thickness being kept constant. The results for the top and bottom layer for different combinations of thickness parameter for layer a and layer b are plotted in Figure 4.27 and 4.28. In Figure 4.27 the thickness of layer a stays constant. The thickness of layer b and therefore the number of deposited layers varies. As can be seen the magnitude of the residual stress in the bottom layer stays constant. In the top layer the magnitude of the total residual stress increases with an increase of the thickness parameter. The same trend is observed by varying the thickness of layer b while layer a stays constant, as can be seen in Figure 4.28.



Figure 4.27: Local residual stress at the top and bottom in the substrate by using a relative layer thickness t_b/t_a



Figure 4.28: Local residual stress at the top and bottom in the substrate by using a relative layer thickness t_a/t_b

4.3.7 Conclusions - parameter study

In principle it can be said that the material properties strongly influence the residual stress distribution in multilayer systems. As outlined in Section 4.3.4 the most favourable results for the stress evolution are obtained by using WC-Co as substrate material and AlN/CrN as layer material. By applying this material combination with equal prestress, thickness parameter and temperature change, as defined in the reference configuration, the resulting residual stress state is compared to the reference configuration in Figure 4.29. σ^{initial} denotes the total residual stress distribution due to the configuration defined in section 4.3.1. One has to be careful by changing the process parameters such as the temperature or the pressure in the chamber. As outlined in section 2.3.2 a change of the process parameters can have a strong influence on the microstructure of a polycrystalline film.


Figure 4.29: Stress distribution in the substrate (left) and the coating (right) for the reference configuration and the modified configuration

Chapter 5

Summary and Outlook

In the present work an analytical model is developed for predicting residual stress distributions in multilayer systems. After the manufacturing process such systems are in a stresses state. The developed model takes into account the two main residual stress generation mechanism, thermal mismatch stress and film growth stress. The model provides an illustration of how the total residual stress state in the substrate and in each layer is generated. The residual stress state can be directly determined from the elastic material properties, the architecture of the multilayer system and the film growth stress. Within this thesis only linear effects are taken into account. The model is able to simulate systems comprising of several hundreds of layers. The analytical approach is based on Euler - Bernoulli beam theory. With a force and moment balance the stress distribution in the multilayer system can be obtained. No external forces and moments are applied.

The effects of varying the different parameters can be predicted easily, so the analytical approach provides an efficient tool for assessing total residual stress states in multilayer systems. Due to its low computation time the model allows simulating various configurations within seconds and provides a powerful tool for comparing residual stress distributions of different configurations.

While the developed approach is a valid tool for estimating residual stress states in

multilayer systems, they are still quite simplified regarding to the actual nature of such multilayer systems. Further work can be done in taking plasticity and edge effects into account. Additionally, the developed script can be combined with a Graphic User Interface where different results can be compared more easily.

Appendix A

Material properties of Austenite

Figure A.1 shows a product information about austenitic stainless steel according to EN 1.4301. The mechanical properties, according to EN 10088-2, are used in Section 4.3.2. The yield strengths of austenitic stainless steel, at elevated temperatures, are listed in the data sheet. They are used to calculate the maximum number of deposited layers when plasticity will occur, compare Figure 4.16.

EN 1.4301, AISI 304 EN 1.4307, AISI 304L

Austenitic stainless steel

Type X5CrNi18-10 stainless steels EN 1.4301, AISI 304 EN 1.4307, AISI 304L, low carbon

Applications

• These are the most commonly used stainless steels, those resistant against corrosion is utilized e.g. in chemical, paper and food industry. These steels are also popular in household wares, architecture and transportation.

 $\bullet\,$ Can be used at low temperatures down to -196°C even as welded structures.

- Moderate strengths can be reached at elevated temperatures (~550°C). Temperatures for excessive scaling are close to $850^\circ\text{C}.$

Welding

• Weldability is good. The thermal expansion is 1,5-times larger compared with carbon steels.

• Chromium and nickel contents of the filler metal have to match or to be higher than the composition of the base metal, e.g. type 19-9.

 In welded plates with wall thickness exceeding 6 mm, steels with low carbon content (1.4307, AISI 304L) or (1.4541, AISI 321) are recommended.

 Cleaning the weld seam has a significant importance for corrosion resistance. Pickling is recommended.

Forming and machining

• Formability is good, thus forces needed and the elastic return is bigger compared with carbon steels.

 Because of a high ductility and a strong work hardening it is recommended to use sharp tools, an effective cooling

and adequate feed of tool.
Higher austenite stability and a lower work hardening rate can be achieved by an increase of nickel and some other alloying elements.

Corrosion resistance

 Resistance to atmospheric corrosion is adequate for several applications. Special attention should be paid on surface finish and regular cleaning procedures in marine and industrial environments.

 These steels have a good resistance against oxidizing acids. Corrosion resistance in non-oxidazing acids like sulphuric acid, hydrofluoric acid and hydrochloride acid is limited.

• Can be used e.g. in the following chemically pure, boiling solutions: acetic acid (\leq 5%), acetone, ammonia, ammonia sulphate, benzene, benzene, citric acid (\leq 10%), copper sulphate, ethanol, ethylic ether, formaldehyde, fruit juice, HNO₃ (\leq 45%), lactic acid (\leq 10%), NaOH (\leq 30%), Na₂SO₃ (\leq 50%), oil, phosphoric acid (\leq 10%), toluene, wine and sodium-carbonate, tartaric acid (\leq 15%), toluene, wine

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Product Information April, 2009

(when SO_2 used for preservation grade 1.4404, AISI 316L or 1.4432 is recommended), xylene and yeast.

 In chloride containing solutions pitting and crevice corrosion is possible depending on various parameters like chloride concentration, temperature, pH value, redox potential, crevice geometry and others. For instance in drinking water supply systems chloride concentration up to 200 mg/l are usually tolerable.

• When the temperature of chloride containing solutions exceeds 50°C and the construction is loaded, stress corrosion cracking is possible.

• The best material performance is reached usually with the help of adequate design, correct post-weld treatment and regular cleaning during use (if applicable).

Physical properties

Austenitic crystal structure, non-magnetic as soft

annealed.
Density: 7,9 g/cm³

Coefficient of thermal expansion: 16x10⁻⁶1/K

- T=20...100°C • Thermal conductivity at 20°C: 15 W/(m x K)
 - Mechanical properties

• According to EN 10088-2:2005

EN	AISI	Proof strength R _{p0,2} (N/mm ²)	Tensile strength R _m (N/mm ²)	Elongation after fracture A (%)	
1.4301	304	min. 230	540750	min. 45	
1.4307	304L	min. 220	520670	min. 45	

 Minimum values of 0,2 % proof strength (R_{p0,2}, N/mm²) at elevated temperatures, EN 10088-2:2005

EN	100	150	200	250	300	350	400	450	500
1.4301	157	142	127	118	110	104	98	95	92
1.4307	147	132	118	108	100	94	89	85	81

Chemical composition (typical)

EN	C wt-%	Cr wt-%	Ni wt-%	Fe wt-%
1.4301	Max. 0,07	18,1	8,2	Bal.
1.4307	Max. 0,030	18,1	8,2	Bal.

Further information

- Standard Specification EN 10088-2:2005
- Standard Specification ASTM A-240-06c
- Corrosion Handbook, Outokumpu
 Technical Customer Service

Disclaimer

Information given in this document may be amended without notice. Care has been taken to ensure that the contents are accurate but Outokumpu and its affiliated companies makes no warranty underrating and have no liability for the anything in this document unless explicitly agreed in writing.

Figure A.1: Product Information about austenitic stainless steel according to EN 1.4301

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