EFFICIENT NUMERICAL MODELLING OF MULTILAYER SYSTEMS

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INTRODUCTION

The multilayer systems considered in this study consist of a substrate and a coating formed by several hundred bi-layers with a thickness of a few nanometers each, deposited via PVD (physical vapor deposition), see Fig.1. After the manufacturing process residual stresses in the range of GPa can be observed in the multilayers [1]. These stresses are induced primarily by two effects. When cooling down the multilayer system from deposition to room temperature a bending moment is induced due to the mismatch between the thermal expansion coefficients of the substrate and the bi-layers. Furthermore stresses originating from the film growth process contribute to the overall residual stress state. The aim of the present study is to develop an efficient finite element model (FEM) allowing to estimate the residual stresses in such multilayer systems and to gain further insight into experimental results and facilitate interpretation. Compared to analytical approaches the FEM simulation provides details on the three-dimensional behaviour of multilayer systems and enables implementing plastic yielding in the layers as well as damage in the interfaces between the layers.

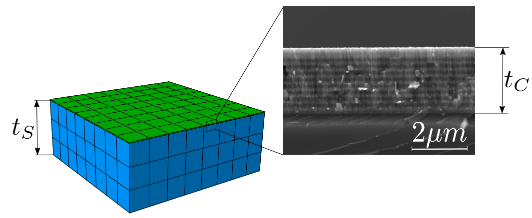

Figure 1: FEM-model and scanning electron microscopy image of a multilayer system

MODELLING APPROACH

The modelling of the multilayer system is realized using the FEM software package ABAQUS. Due to the fact that the layers are only a few nanometers thick and thus much thinner than the substrate (Fig.1), modelling both, the substrate and the bi-layers, with FEM using standard continuum elements leads to a high number of degrees of freedom (DOF). This results in excessive simulation times. To overcome this limitation the layers are discretized by conventional shell elements. The modelling of the substrate material is done with continuum elements. The connection between the substrate material and the individual layers is realised with cohesive zone elements. To further increase computational efficiency when considering a system with up to hundreds of bi-layers a unit cell is modelled and 2D-periodic boundary conditions (PBC) are applied. In finite element models the PBCs can be implemented by means of equations relating the displacement of the corner, edge and surface nodes to initially defined master nodes. Unlike standard PBCs which describe periodicity in all directions, for the present purpose the top and bottom faces are allowed to deform freely. With these boundary conditions a representative unit cell of an infinite plate with periodicity in two dimensions is simulated. Since the interfaces between the layers do not intersect a free surface, damage in the interfaces is not considered in the current model. When applying periodic boundary conditions to an FE-model consisting of a combination of continuum and shell elements, the difference in formulation has to be considered. Whereas continuum elements have only the three translational DOFs, for the shell elements the rotational DOFs have to be restricted additionally.

APPLICATION EXAMPLE

To demonstrate the present modelling approach the compressive residual stress originating from the film growth process is treated in the following. For testing the algorithm, the coating, which is actually deposited layer by layer, is modelled as a homogenized coating represented by one single layer. The considered bilayer system consists of TiN and CrN of equal thickness. For the simplified model the elastic properties are calculated with the rule of mixture. For the substrate a thickness t_s of 380 μm is chosen and four different materials are considered: Ti6Al4V, Si (100), Austenite and WC-Co (in ascending order of their Young's moduli). With this model a parameter study is carried out by varying the thickness of the coating t_c ranging from 0.5 to 5 μm in order to investigate its effect on the residual stresses. Moreover the influence of different substrate materials can be observed by changing the elastic properties. To simulate the compressive growth stresses, the shell elements representing the layers are removed in the first step of the FE-analysis. Then a compressive stress is applied to the coating and the shell elements are added in a second step. The equilibrium which is restored by stress redistribution returns the results for the residual stresses of the substrate and the coating, see Fig.2.

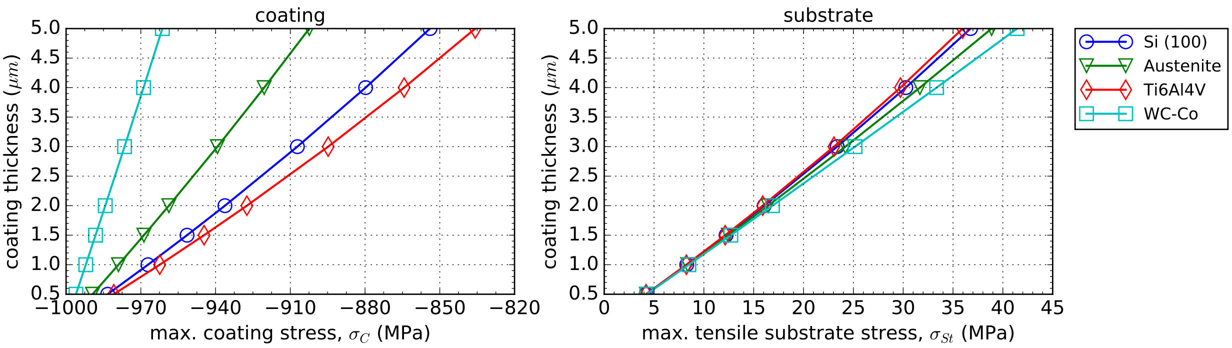

Figure 2: Maximum in-plane residual stresses of the homogenized coating and maximum residual stresses of the substrate as a function of coating thickness and substrate material for a coating preload of 1GPa

The side of the substrate closer to the coating is subjected to compression and the opposite to tensile stress. The coating is exposed to compressive stress over the entire thickness. Extending the coating thickness reduces the magnitude of the compressive stress in the coating, but increases the maximum tensile stress in the substrate as shown in Fig.2. Using a substrate material with a high Young's modulus leads to an increase of the total value of maximum stress in the coating and the substrate.

CONCLUSION AND OUTLOOK

In this study an efficient FE-model for a multilayer system with hundreds of bi-layers was developed by means of implementing periodic boundary conditions and choosing shell elements to discretize the individual layers. The next step of this work is to simulate the cooling down from deposition temperature of a multilayer arrangement and to consider the influence of damage in the interfaces. To do so the boundary conditions of the model have to be modified such that one of the lateral surfaces is left free to deform. An accurate prediction of the residual stresses in a multilayer coating obtained from the FEM model will be used to provide initial conditions for further simulations and can consequently improve the final results.

REFERENCES

[1] F.Lomello,Temperature dependence of the residual stresses and mechanical properties in TiN/CrN nanolayered coatings processed by cathodic arc deposition, Surf.Coat.Technol. 238(2014) 216-222