ANALYTICAL TREATMENT OF RESIDUAL STRESSES IN MULTILAYER COATINGS

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INTRODUCTION

Multilayers on substrates have extensive applications in optical, microelectronic and structural components as well as for protective coatings [1]. The multilayer systems are strongly influenced by residual stresses (in range of GPa [2]) which directly affect the mechanical behaviour of the substrate and the coating. These stresses occur because of 1) different coefficients of thermal expansions (CTEs) when the multilayer system is cooled down from its production temperature to room temperature and 2) film growth stresses (e.g., atomic and ionic peening during film growth generating lattice defects). The multilayer system which is considered in this study consists of a substrate and a few hundred nanometer-thick bi-layers deposited by PVD (physical vapor deposition), see Fig. 1. The aim of the present study is to develop an analytical approach for predicting residual stresses in multilayer systems. The advantage of an analytical model, in contrast to the Finite Element approach, lies in providing for efficient parameter studies.

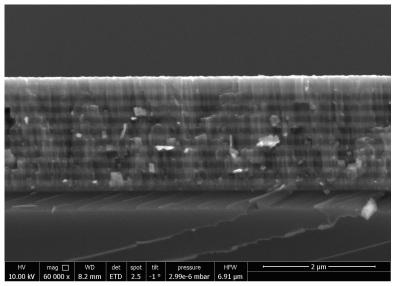

Figure 1: Cross-section of a PVD nitride multilayer system

MODELING CONCEPT

The analytical approach is based on Euler-Bernoulli beam theory where a one dimensional linear elastic stress state is considered. The influence of growth-induced stresses is estimated by adding a prestressed layer to a system consisting of a substrate of n layers that is self equilibrated, but not stress free. The equilibrium of this modified system is estimated by the force and moment balances for a beam in the absence of external forces and moments using:

$$N = \int_0^{t_S} \sigma_{x,S}(z)dA + \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} \sigma_{x,j}(z)dA + \int_{t_n}^{t_{n+1}} \sigma_{D,n}(z)dA = 0 \qquad (1)$$

$$M = \int_0^{t_S} \sigma_{x,S}(z) \cdot zdA + \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} \sigma_{x,j}(z) \cdot zdA + \int_{t_n}^{t_{n+1}} \sigma_{D,n}(z) \cdot zdA = 0 \qquad (2)$$

In Eqs. (1) and (2) $\sigma_{x,S}(z)$ denotes the stress distribution in thickness direction in the substrate, $\sigma_{x,C}(z)$ denotes the stress distribution in the coating consisting of an compressive prestress $\sigma_D(z)$ in the layer $n+1$ because of growth stresses. A is the integration area, t_S is the thickness of the substrate and t_j denotes the thickness of the j-th layer.

APPLICATION EXAMPLE

As a test case a configuration is considered that consists of a substrate and a coating with the smeared-out properties of multiple CrN and TiN layers of identical thickness. The elastic properties of the

simplified coating are calculated via the rules of mixture.
With this approach a parametric study of the multilayer system is carried out with regard to the influence of different substrate materials. Furthermore different thickness parameters of the coating and a varying compressive preload in layer $n+1$ of 1, 3 and 5GPa are taken into account. For the substrate two different materials are considered: Si(100) and WC-Co, which has a four times greater Young's modulus. The substrate thickness t_S is chosen to be $380\mu m$. The thickness of the coating t_C ranges from $0.5\mu m$ to $5\mu m$.

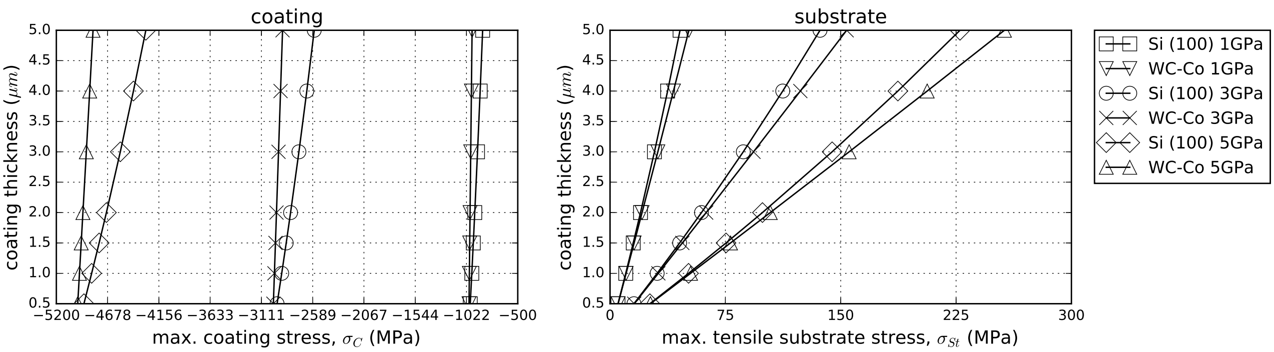

Figure 2: Maximum residual stress in the homogenized coating (left) and substrate (right) depending on substrate materials, coating thickness and compressive preload

When a compressive preload is applied to the coating, the residual stress in the coating appears as a compressive stress, see Fig. 2. The substrate is subjected to compressive stress near the film and to tensile stress on the opposite side. Due to the fact that the maximum tensile stress is greater than the maximum compressive stress in the substrate, only the tensile stress in the substrate is depicted in Fig.2. Increasing the total coating thickness leads to a reduction of the magnitude of the residual stress in the coating. Furthermore the magnitude of the stress increases in the substrate and the coating with an increasing Young's modulus of the substrate. Additionally the influence of a variation of the applied coating prestress can be observed. A comparison between the resulting residual stress values for the substrate and the coating for compressive preloads of 1, 3 and 5GPa shows a stress increase by a factor of five in the coating and the substrate.

CONCLUSION

Within this work an analytical approach to determining residual film growth stresses in an elastic multilayer system was presented. The advantage of an analytical model is the low computational effort when a parametric study is executed. The next stage of the project should include a cooling process after the deposition of the pre-stressed coating on the substrate. Instead of a homogenized coating a multi-layer arrangement, with alternating pre-stressed bi-layers will be considered. Consequently the thickness, the material data and the compressive preload of each single layer can be adjusted.

REFERENCES

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