Numerical analysis of crack evolution in PVD-deposited TiN-coated steel sheets under loading conditions

Konrad Perzynski[1*], *Lukasz* Madej[1]

[1]Faculty of Metals Engineering and Industrial Computer Science, AGH University of Krakow, Krakow, Poland

Abstract. Titanium nitride (TiN) coated steel sheets are widely utilized across various industries, offering tailored solutions for diverse applications. Manufacturers appreciate its adaptability and precision, utilizing it to create intricate components for electronics, packaging, and specialized industrial equipment. In construction and design, TiN coated sheet enables crafting detailed architectural elements and custom fixtures, providing strength and corrosion resistance. One of the methods used for the production of such coated films is the PVD (Physical Vapour Deposition) process. However, electron and scanning electron microscopy analysis reveals the frequent occurrence of a complex columnar nanostructure of the deposited TiN film resulting from the specific nature of the PVD process. The morphology of such nanostructure is one of the main reasons for uncontrolled delamination and fracture observed in films during, e.g., stamping processes. Accurate investigation of film behavior during forming and exploitation conditions requires a series of very sophisticated laboratory experiments, which are time-consuming and expensive. Therefore, in this work, a new approach to the numerical analysis of the crack evolution of deposited films based on the digital material representation concept is proposed. A series of microstamping simulations were carried out as a case study to evaluate the model capabilities. The study proved that the model based on digital material representation can be used for reliable predictions of the local material behaviour of sheets with deposited complex films.

Keywords: Titanium nitride (TiN) coated sheet; finite element modeling; stamping; Physical Vapour Deposition

1 Introduction

The deposition process is one of the methods based on the idea that two different conventional materials can be combined together to improve the mechanical, strength, thermal, biocompatibility or visual parameters of the final product. One of the representatives is the physical vapor deposition (PVD) method. PVD is characterised by a process in which the material goes from a condensed phase to a vapour phase and then back to a coating condensed phase. One of the widely used materials for PVD coating is TiN.

The TiN is a hard coatings with the longest (around 30 years) history. The first patent for this kind of thin film structure was published in 1988. The rationale for using TiN as a wear-resistant coating is its high hardness (about HV 2600), high scratch resistance and low friction coefficient. However, the brittleness of this coating is a major problem, which negatively affects the quality and durability of its applicability. The adhesion of coating on metal alloys mainly depends on the coating properties (thickness, morphology) and substrate properties (type of material, surface quality, hardness).

Experimental procedures for investigating thin film properties are highly expensive because of the specialised equipment that has to be used. Microscale materials do not allow the use of typically available equipment for macroscale investigation; instead, state-of-the-art equipment, such as nano/picoindenters, atomic force microscopes, electron microscopes, etc., has to be considered. As a result, performing a series of investigations related to their fracture behavior under various forming conditions is also time-consuming.

Therefore, the creation of an advanced numerical model to assess the state of the coating during various forming operations of the final component with deposited layer is extremely important. Standard FEM models that do not take into account the columnar structure of the TiN films do not allow correct modelling of the fracture phenomenon. Therefore, in this study, multiscale simulation of microforming of the sheet coated with a thin film was developed. The concept of the numerical model is based on the digital representation of the material that allows detection of crack initiation and propagation in TiN coatings including various micro scale heterogeneities.

2 Digital Material Representation

The DMR concept initiated by the micro-scale polycrystalline materials research [1] was adapted here to the microscale coating investigation. The main objective of the DMR is to create a digital representation of microstructure with its features (i.e. grains, columns, grain orientations, inclusions, fractures, different phases, etc.) represented explicitly [2,3]. Such exact digital morphology after discretisation with, e.g., finite elements and, after providing required local materials properties, is further used in numerical simulations of material behaviour under processing or exploitation conditions. That is why the more accurate the digital representation is in the case of morphology and properties, the more accurate the results can be obtained.

In this research, cellular automata and the Monte Carlo approach [4] to 3D DMR generation were

* Corresponding author: kperzyns@agh.edu.pl

developed to recreate the microstructure morphologies of coating for subsequent numerical modeling of their in-use behavior. Material properties of the coating were calculated based on the nanoindentation test and inverse analysis approach. To differentiate the hardening behaviour of subsequent columns, slightly different flow stress model parameters were assigned to each of them. The diversification was introduced by the random Gauss distribution with the spread of approx. 10% (Fig. 1).

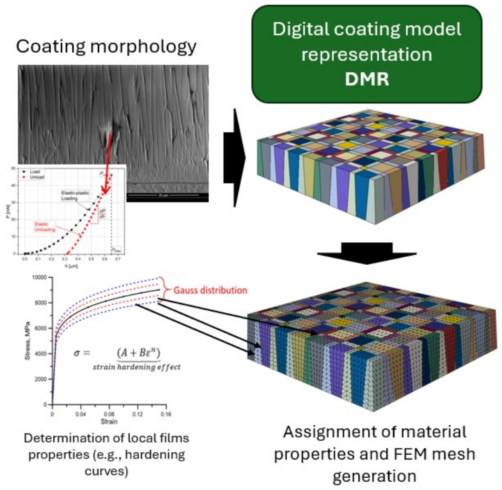

Fig. 1 Digital material representation model of the coating.

3 Multiscale microstamping model

The generated DMR coating model was used in this work to create a multiscale simulation of the microstamping process. Models were developed using commercial ABAQUS software. In this approach, the partially coupled concurrent multiscale methodology was used due to a significant length scale difference between the macroscopic model of the microstamping test and the microscale model based on the digital material representation. Thus, a certain area of interest from the macroscale model is selected and recalculated with a refined mesh to obtain a more detailed solution. The microscale model contains information on the microstamping test's sample geometry and boundary conditions. A schematic description of this multiscale technique applied for the microstamping test is presented in Fig. 2.

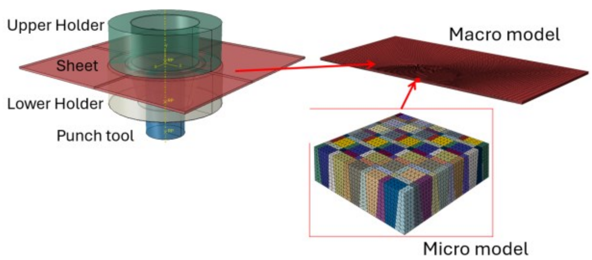

Fig. 2 Schematic description of multiscale technique applied for the microstamping.

The two main fracture mechanisms are involved in a substrate/coating system, namely the propagation of fracture between the columns and delamination of the columns from the substrate [5]. Therefore, both mechanisms are incorporated into the developed full-field model. All column boundaries inside the thin film and the interface between the thin film and the substrate are connected by cohesive regions using a traction-separation law [6].

Examples of results obtained from the macro and micro model of stamping operation indicating crack formation are shown in Fig. 3.

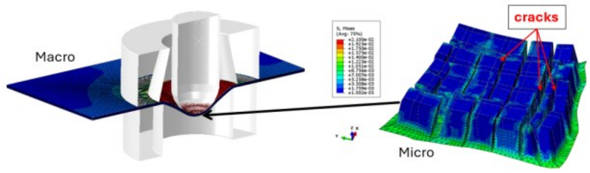

Fig. 3 Equivalent stress distribution within the DMR model after microstamping.

4 Conclusions

It can be concluded that the developed approach allows a preliminary estimation of the quality of the applied coating and its resistance to loading conditions. As a result, it is possible to select the optimal coating thickness and morphology that allows to achieve the required degree of deformation without causing cracks or delamination within the material.

Acknowledgements

Research project supported by program „Excellence initiative – research university" for the AGH University of Krakow. We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017298.

References

1. L. Madej, P. Cybulka, K. Perzynski, L. Rauch, Comp. Meth. in Mater. Sci. **11**, 375 (2011)
2. M. Bernacki, Y. Chastel, H. Digonnet, H. Resk, T. Coupez, R. Logé, Comp. Meth. in Mater. Sci. **7**, 142 (2007)
3. K. Perzynski, R. Wiatr, L. Madej, Mater Sci. Pol. **33**, (2015)
4. K. Perzynski, Comp. Mater. Sci. **251**, 113745 (2025)
5. J. Jian, J.H. Lee, Y. Liu, F. Khatkhatay, K. Yu, Q. Su, X. Zhang, L. Jiao, H. Wang: Mater. Sci. and Eng. A. **650**, 445 (2016)
6. S. Rezaei, M. Arghavani, S. Wulfinghoff, N.C. Kruppe, T. Brögelmann, S. Reese, K. Bobzin, Mech. of Mater. **117**, 192 (2018)