Numerical analysis of substrate influence on fracture mechanisms in PVD deposited TiN coatings

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Abstract: *Coatings of titanium nitride (TiN) are widely used due to their high hardness and wear resistance, making them suitable for protective, decorative, and semiconductor applications. However, their tendency toward brittle cracking and low fracture toughness limits their performance in demanding environments. Understanding and accurately modelling fracture behaviour in TiN is therefore essential to improving reliability in microelectronics, protective coatings, or biomedical devices. This work presents a first approach to modelling fractures in TiN films by explicitly representing their columnar morphology. A procedure for generating statistically representative digital microstructures and incorporating them into finite element simulations is described. The approach uses a hybrid cohesive–XFEM fracture model to capture crack initiation and propagation under complex deformation states, particularly during nanoindentation. The numerical results are validated with results from a scanning electron microscopy (SEM) investigation.*
KEYWORDS: COATINGS, CZM, XFEM, FRACTURE MECHANISMS, OPENCV

1. Introduction

Nowadays, there is a growing demand for new methods to extend the functionality of devices used across key industrial areas. Therefore, composites comprising multiple thin films of conventional materials are increasingly used to improve the properties of the final product. One of the most popular techniques for creating these composites is the PVD (Physical Vapor Deposition) method. It consists of the material's target evaporation and its synthesis with the substrate, characterized by nanoscale accuracy in the creation of thin films and coatings [1]. Another technique used in this work is the PLD (Pulsed Laser Deposition), schematically shown in Fig. 1a. This method is based on laser ablation, which involves local evaporation of the target material using a laser beam. The plasma containing the material atoms is then transported to the substrate, where it condenses to form the thin film structure (Fig. 1b).

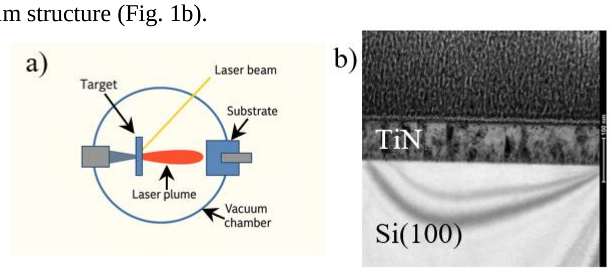

Fig. 1. a) Concept of PLD, b) TEM image of TiN film on Si(100) substrate.

2. Thin films morphology

Since the deposition process involves transporting plasma onto the substrate, the resulting morphology often depends on the chamber's operating parameters. Thornton's model has extensively described the possible film morphologies. This model is one of the basic diagrams illustrating the possible growth of the polycrystalline microstructure of thin films deposited physically from the gas phase [2]. The growth of the columns is represented as a map with four distinct zones, each corresponding to different column density and composition characteristics as shown on Fig. 2. The horizontal axis represents the ratio between the substrate temperature and the melting temperature of the deposited material.

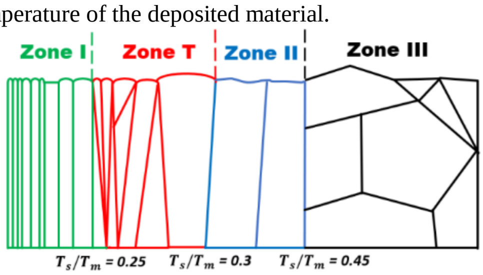

Fig. 2 Schematical illustration of Thorton's model.

Film behaviour under loading conditions is often evaluated using the nanoindentation technique. Since it probes extremely small volumes, nanoindentation is especially valuable for thin films and coatings where conventional mechanical testing is not feasible.

3. Numerical model of the nanoindentation test

As mentioned, nanoindentation is used to analyse the mechanical properties of films and coatings. It involves inserting a diamond tip of a specific shape into the material's surface while simultaneously monitoring the applied force and the corresponding displacement. From this data, information on the material's mechanical response can be extracted [3].

In this work, a numerical model for this test was created using a plug-in implemented in Abaqus CAE software, which automated the process of creating models ready for nanoindentation analyses. Based on this plug-in, a 2D planar model was created, including:

- Conical indenter with a spherical tip with a radius of 1μm, which was considered as an analytical rigid shell.
- Thin film 0.1μm thick and 15μm wide, consisting of 100 funnel-shaped columns representing film morphology, defined as a deformable shell.
- Substrate of the selected material, defined as a deformable shell with dimensions of 30×50μm.

Additionally, the concentrated force was applied to the indenter, with a value of 1 gf (0.0098 N). Fig. 3 illustrates the developed 2D model used to conduct numerical simulations of the nanoindentation process.

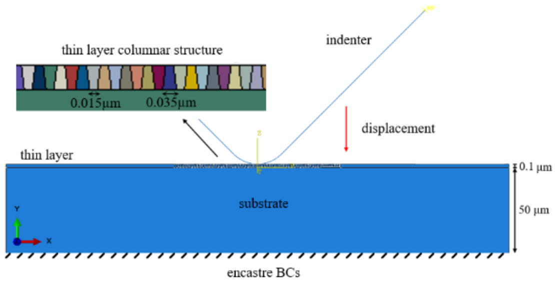

Fig. 3. 2D Numerical model of the nanoindentation process.

The aim of this work was to determine the crack characteristics of the Titanium Nitride (TiN) thin film deposited on 2 different material hardness bases: stainless steel (SS316L) and aluminum (Al 1050). Material data were derived from literature[4, 5]. A simplified rheological model of Swift-type hardening was used (1) $\sigma = (A + B \cdot \varepsilon^n)$).

(1) $$\sigma = (A + B \cdot \varepsilon^n)$$

where: σ – yield stress, A – initial yield strength, B – strain hardening constant, ε – plastic strain, n – strain hardening exponent.

In the presented model, two numerical methods were used to model fracture mechanisms: the cohesion zone method (CZM) and the extended finite element method (XFEM). The CZM method is based on a traction-separation law that represents the fracture mechanism at the boundary of TiN microstructure columns (Fig. 4a) and at the delamination between the thin film and the substrate (Fig.

4b). The XFEM model depends on the maximum nominal stress at the crack tip and can predict fractures within the columns (Fig. 4c).

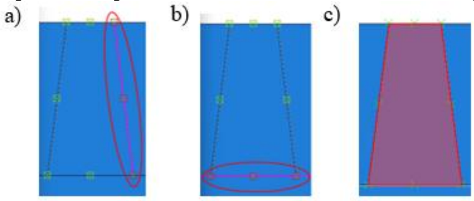

Fig. 4. Assignment of the CZM to a) intercolumn boundary, b) column-substrate boundary and XFEM to c) intracolumn area.

These models assume initial linear-elastic behaviour, followed by crack formation and propagation. To simulate fracture development, it is necessary to define a crack initialization and propagation criteria, in which the maximum nominal stresses (σ_{max}) and total displacement (δ_c) can be specified. These parameters were analytically determined using the critical stress-intensity K_{IC} factor calculated according to the formula (2) $K_{IC} = \sqrt{\frac{1}{2}\sigma_{\max}\,\delta_c E}$) [4]. Values for crack initialization and propagation are listed in Table 1.

(2)
$$K_{IC} = \sqrt{\frac{1}{2}\sigma_{\max}\,\delta_c E}$$

where: E – Young modulus, $\sigma_{\max}$ – maximal nominal stress, δ_c – total displacement.

Table 1. Fracture parameters for crack nucleation and growth for CZM (intercolumn, delamination) and XFEM (intracolumn).

	CZM		XFEM
criterion	intercolumn	delamination	intracolumn
σ_{max} [GPa]	5	10	5.5
δ_c [μm]	1E-05	1E-05	1E-05

4. Simulation results

Numerical simulations were conducted using a hybrid (CZM, XFEM) method, which resulted in the formation of numerous cracks in thin TiN films on all base materials. Fig. 5 presents the result of combining both CZM and XFEM methods, where all three fracture mechanisms: intercolumnar, intracolumnar, and delamination are simultaneously visible.

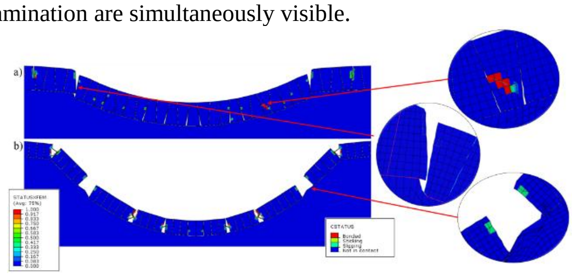

Fig. 5 Hybrid CZM and XFEM fracture model of a thin TiN film on a) SS316L and b) Al 1050.

The OpenCV library was used to develop a script that automates the verification of the dimensions of structures formed in a thin TiN film deposited on an Al1050 substrate after the nanoindentation simulation as presented in Fig. 6.

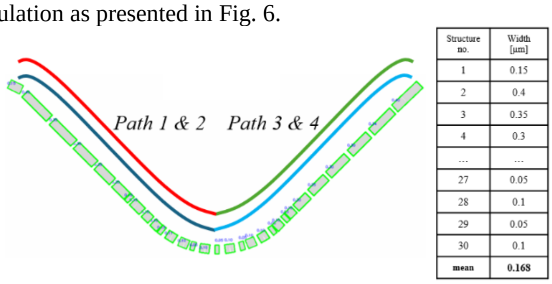

Fig. 6 Calculated widths of the structures after numerical simulation.

The average structure sizes in individual simulations were then compared with the average structure sizes obtained from 4 different paths, determined from SEM imaging of the sample surface after nanoindentation, as shown in Fig. 7.

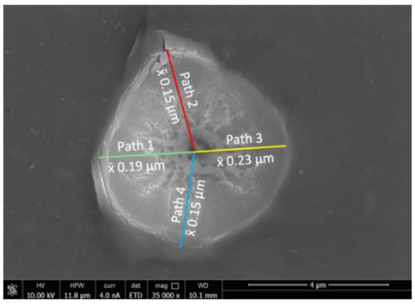

Fig. 7 Average TiN-Al 1050 structure sizes of 4 paths from [3].

Table 2 shows the accuracy of the simulation results compared to the laboratory results, calculated as the relative error.

Table 2. Calculated relative error of the mean structure sizes.

	Simulation 1	Simulation 2	Simulation 3	Simulation 4
Path 1	88.13%	96.86%	89.75%	69.72%
Path 2	87.78%	76.67%	85.71%	88.77%
Path 3	88.52%	77.48%	86.47%	88.18%
Path 4	71.94%	79.06%	73.26%	56.91%

5. Conclusion

The aim of this work was to demonstrate the potential of finite element method calculations in conjunction with OpenCV image analysis techniques to predict fracture in thin films.

The key factor enabling the observation of cracking was the development of a model representing the columnar morphological structure of a thin TiN film, in which cracks were modelled using CZM and XFEM methods.

The presented numerical method can be widely used in the virtual testing of thin films. Numerical simulations enable the prediction of the impact of various parameters, such as the thickness of deposited films, the properties of the base material, or the film's morphology, saving time and resources that would otherwise be required to conduct a series of costly laboratory experiments.

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6. References

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