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R. MAJOR[*], P. LACKI[**]

FINITE-ELEMENT MODELING OF THIN FILMS DEPOSITED ON THE POLYURETHANE SUBSTRATE

MODELOWANIE METODĄ ELEMENTÓW SKOŃCZONYCH ZACHOWANIA WARSTW NA PODŁOŻU POLIURETANOWYM

Segmented polyurethane (PU) is seen as a critical bio-material for clinical applications. This is due to the excellent combination of mechanical and elastic properties with bio-compatibility. However, the reported tendency to form micro-thrombuses as well as control of wettability makes it possible to apply the processes of surface engineering to modify the surface of implants. Pulsed laser deposition (PLD) has been selected to deposit titanium nitride (TiN) on PU due to possible deposition without PU substrate heating, leading to thermal degradation. The formation of the hard and brittle ceramic TiN coating can influence the rigid properties of the bulk material and the physico-chemical properties. They are related to the thickness of the deposited layer. It is necessary to apply an optimal thickness which does not diminish the rigidity of the device but enhances its behavior in the biological environment.

The work presents a computer simulation realized with the ADINA program. The contribution of the TiN coating thickness to the implant rigid properties was simulated. Generally, three types of extortion conditions could be considered, namely short contact with surgery tool; long continuous contact with natural tissue; long cyclic contact with natural tissue. The authors focused in this work on the first type: short contact with surgery tool.

Poliuretan segmentowany (PU) znajduje szerokie zastosowanie w medycynie. Stwierdzono jednakże tendencję do formowania się mikrozakrzepów i kontrolowaną zwilżalność. Stwarza to konieczność modyfikacji powierzchni poprzez naniesienie warstw. Do tego celu wybrano metodę osadzania laserem impulsowym (metoda PLD) do naniesienia azotku tytanu TiN na podłoże poliuretanowe (PU). Ze względu na to, że jest to proces niskotemperaturowy, możliwe było uzyskanie wysokiej jakości warstw bez degradacji podłoża. Wzrost grubości ceramicznej warstwy TiN może wpłynąć na zmianę sztywności i właściwości

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[*] INSTYTUT METALURGII I INŻYNIERII MATERIAOWEJ IM. A. KRUPKOWSKIEGO, POLSKA AKADEMIA NAUK, 30- 059 KRAKÓW, UL. REYMONTA 25

[**] POLITECHNIKA CZĘSTOCHOWSKA, 42-200 CZĘSTOCHOWA, UL. ARMII KRAJOWEJ 21

fizykochemicznych. Te zmiany ściśle zależą od grubości osadzanej warstwy. Niezbędnym jest zastosowanie takiej grubości warstwy, która nie wpłynie na obniżenie właściwości mechanicznych i biologicznych elementu pokrywanego.

W pracy przedstawiono symulację komputerową zachowania.warstw w teście nanotwardości. W tym celu zastosowano program komputerowy ADINA. Przeprowadzono obliczenia dla różnych penetratorów, które w normalnych warunkach miałyby symulować kontakt z narzędziem.

1. Introduction

The finite-element method has gained a growing popularity among the numerical techniques in engineering [1]. This is firstly because the engineering design of modern products requires an engineer to predict accurately the performance and produce the optimal object, which requires an integrated use of the finite-element analysis software in CAD. Secondly, fast progress in hardware performance and a great decrease in the price of computers offer the possibility of using finite-element analysis software. Another important factor is that the analysis functions of the finite-elements program themselves develop rapidly, offering a user-friendly interface and CAD software transor [2].

In recent years, nanoidentation techniques have been used to determine the hardness and Young's modulus of thin films [3]. Identation hardness measurements are now extensively used for characterization and ranking of coated systems for mechanical applications because they are simple, cheap and reproducible [4]. However, the presence of the underlying substrate — including the interface — of material, may complicate the interpretation of measurement results. Owing to a gradually increasing influence of the substrate, the hardness of composite systems possibly depends not only on coating material, but also on the applied load, coating thickness and substrate hardness. The impact of the substrate on the hardness of composite systems is also transferred by an interaction that occurs at the interface. While discussing the interface influence, it is difficult to experimentally obtain detailed information, such as deformation behavior and a stress and strain distribution inside the coated systems, especially near the interface. Up to now, not much work has been done dealing with the influence of the interface strength between coating and substrate on the indentation process of the coated systems. It is well known that the finite-element method can handle the infinite continuum problem as a discrete approximation and give a dynamic insight into a deformation process as well as yield important values which are difficult to obtain in experiments. The goal of this work was to simulate the thin layer properties established by different nanoindenter treatments.

2. Numerical model

Thin layers of TiN with the Ti interface deposited on the elastic polyurethane substrate were selected for theoretical investigations. The parameters of the materials are given in Table.

TABLE

Material parameters used in the FEM calculations

Material	Yong's modulus	Poisons ratio	Material law
TiN (deposited layer)	616 [GPa]	0.25	elastic-plastic bilinear Initial Yield Stress σ = 5000 [MPa] Strain Hardening Modulus E_H = 5000 [MPa]
Ti (deposited interlayer)	116	0.3	elastic
Polyurethane (substrate)	$4.420*10^{-3}$	0.49	elastic
Nanoindenter	—	—	rigid structure

Different nanoindenters were considered and their influence on the stress and strain distribution was calculated. The distance of the indenter movements was established to be 10nm. Titanium nitride (70 nm thick) with the titanium interface (16nm thick) deposited on the polyurethane substrate was taken for FEM. Two cases of nanoindentation were considered: a round-shaped indenter and an edge indenter. The influence of the radius indenter on the properties of the layer were examined. The analyzed variants are presented schematically in Fig. 1.

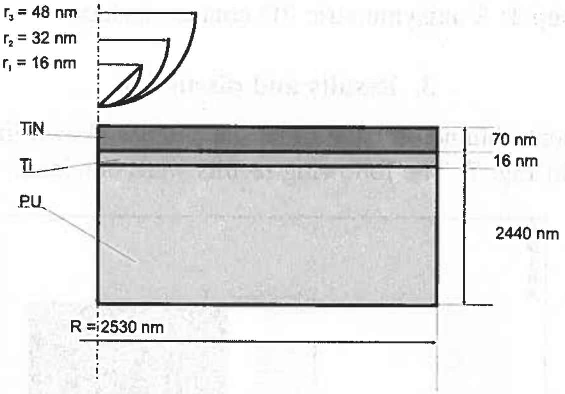

Fig. 1. Geometry of the analysed variants

The indentation process was simulated with ADINA program, which allows one to perform an analysis of solids, structures, fluids and fluid flow with structural interactions [5]. Two- dimensional calculations were chosen as a much more efficient than three-dimensional ones because of the lower mesh complexity. The calculated layer consisted of TiN external layer, and Ti interlayer. The mesh near the indenter and the interface layer has to be very fine, if one is to be able to describe the deformation and stress distribution with sufficient accuracy. The specimen was represented by four node elements connected with each other, Fig. 2.

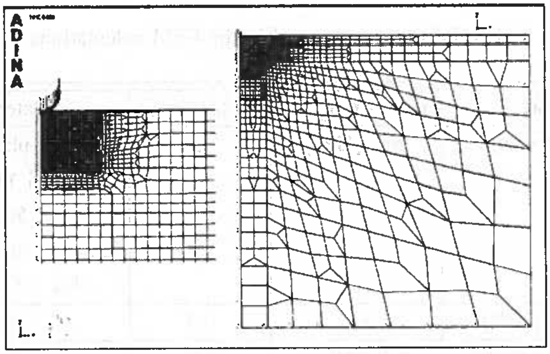

Fig. 2. FE mesh drawing of the TiN layer with the Ti interlayer on PU substrate

Main structure information:

- FEM model: axisymmetric, 4195 nodes, the total of 4142 elements in the main structure.
- 3 element groups:
  Element group 1: 1020 axisymmetric solid elements. (PU)
  Element group 2: 90 axisymmetric solid elements. (Ti)
  Element group 3: 3032 axisymmetric solid elements. (TiN
  1 contact surface groups:
- Contact group 1: 2 axisymmetric 2D contact surfaces.

3. Results and discussion

The displacement obtained for the round indenter is shown in Fig. 3., and for the sharp indenter — in Fig. 7. The following results were obtained:

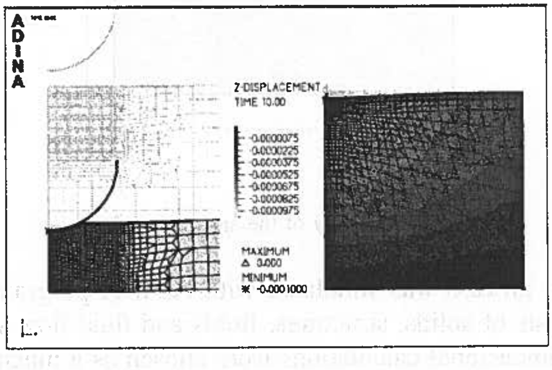

Fig. 3. Displacement [mm] of the indenter into the layer for the round indenter r_3 = 48nm

- Strain distribution: Fig. 4 for the round indenter, Fig. 8 for the sharp one
- Stress distribution: Fig. 5 for the round indenter, Fig. 9 for the sharp one
- The area of plastic flag: Fig. 6 for the round indenter, Fig. 10 for the sharp one

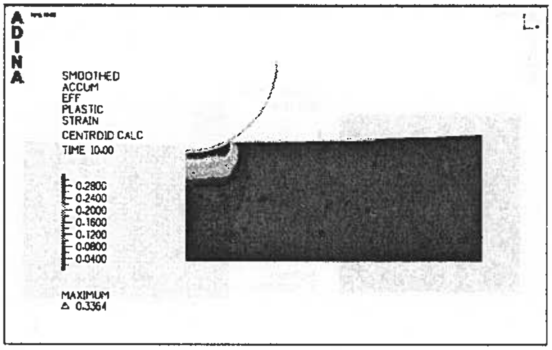

Fig. 4. Plastic strain distribution in the TiN layer for the round indenter r_3 = 48nm

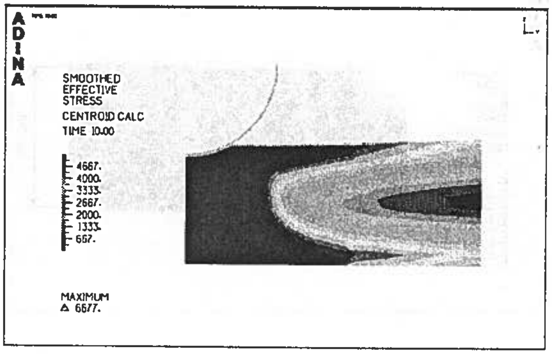

Fig. 5. Effective stress distribution [MPa] in the TiN layer for the round indenter r_3 = 48nm

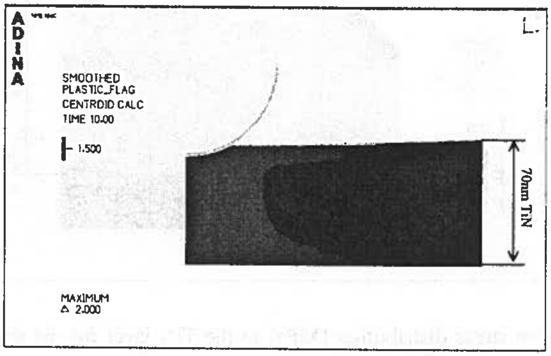

Fig. 6. Area of the crack formation for the round indebter r_3 = 48nm

The differences of the material behavior were observed in the case of stress and strain distribution as well. The application of the round-shaped indenter resulted in

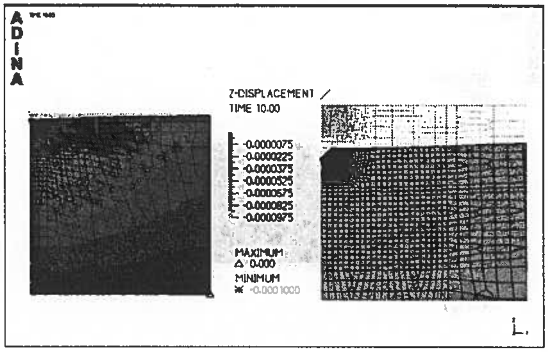

Fig. 7. Displacement [mm] of the sharp indenter into the layer

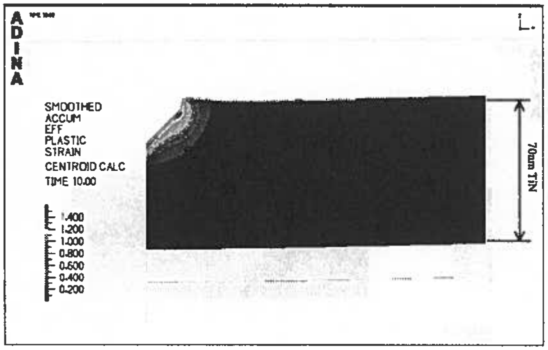

Fig. 8. Strain distribution in the TiN layer for the sharp indenter

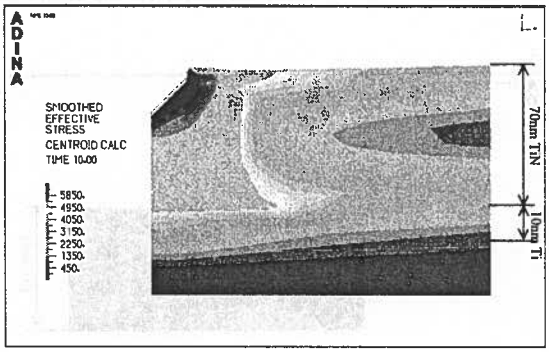

Fig. 9. Effective stress distribution [MPa] in the TiN layer for the sharp indenter

lower values of the plastic deformation and a bigger reaction area than in the case of the sharp indenter. The typical edge for the plastic flow was calculated for the layer the parameters of which were simulated under the sharp indenter conditions. The strongest stress occurred near the indentation area as well as the plastic flow edge area. Fig. 6

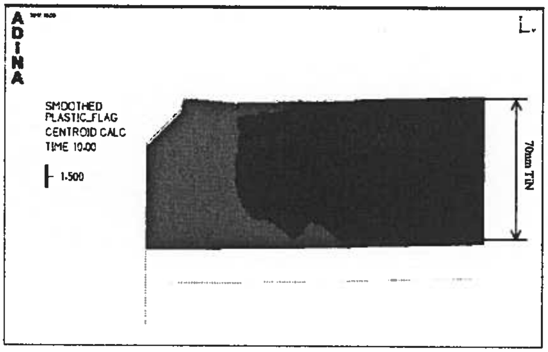

Fig. 10. Area of the crack formation for the sharp indenter

and Fig. 10 present the results of the crack formation in the endangered areas. They seemed to be similar to each other, and thus, the influence of both indenters on the crack appearance was similar as well.

4. Concluding remarks

The finite element modeling presented in the paper does not reveal any reactions of molecules. In the thin layers — less than 100 nm — it could influence layer properties.

Differences were observed in the stress as well as strain distribution. They were dependent on the shape of the indenter. The formation of the elastic edge in the case sharp indenter was right. Similar phenomenon was observed in a practical experiment.

Acknowledgements

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