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ANALYSIS OF THE STRESS CONCENTRATION IN THE NANOMULTILAYER COATINGS BASED ON DIGITAL REPRESENTATION OF THE STRUCTURE

NUMERYCZNA ANALIZA KONCENTRACJI NAPRĘŻEŃ W WIELOWARSTWOWYCH NANOPOWŁOKACH NA BAZIE CYFROWEJ REPREZENTACJI MATERIAŁU

Investigation of the stress concentration in the nanomultilayer materials under exploitation conditions is the main objective of the work. During loading a failure can initiate and propagate, which have important impact on material strength and reliability. This is of importance when materials for biological applications are considered. Special features of the investigated material, including irregular shape of the boundaries and columnar structure of these layers lead to growth of local stresses in the material and may be responsible for mentioned instabilities. To capture this behavior during numerical modeling an innovative solutions are required.

Authors propose numerical simulation, which combines algorithms of the deposition process for realistic digital material representation of coatings and finite element (FE) approach for modeling of material behavior under loading. Algorithm of the deposition process is implemented using the cellular automata (CA) approach. Based on the developed model, a simple plastometric compression tests are simulated to analyze stress distribution in the material and possibility of failure initiation. These results are compared qualitatively with experimental data, including ball-on-test and transmission electron microscope (TEM) observation. Obtained results are the basis for development of a numerical model for fracture propagation with adopted extended finite element method (XFEM).

Keywords: CA, TEM, layers depositions, nanomaterials, XFEM

Głównym celem pracy jest zaproponowanie podejścia numerycznego umożliwiającego analizę koncentracji naprężeń w materiałach o strukturze nanowarstwowej przeznaczonych dla bioinżynierii. Jest to szczególnie istotne w przypadku prowadzenia analizy zachowania się materiałów w warunkach eksploatacji ponieważ umożliwia zlokalizowanie miejsc szczególnie narażonych na uszkodzenia. Do przeprowadzenia szczegółowej analizy numerycznej konieczne jest uwzględnienie typowych cech nanowarstwowego materiału np. nieregularnego kształtu granicy pomiędzy warstwami. W tym celu Autorzy zastosowali model MES sprzężony z jawną reprezentacją mikrostruktury i automatami komórkowym (CA). Model na bazie CA uwzględnia wspomniane specyficzne cechy analizowanych materiałów.

W pracy przedstawiono algorytm generowania cyfrowej reprezentacji nanowarstw oraz wyniki symulacji z wykorzystaniem opracowanego modelu numerycznego dla warstw bez uwzględnienia chropowatości granicy międzywarstwowej, jak i z jej uwzględnieniem. Uzyskane wyniki w formie rozkładów naprężeń stały się podstawą do opracowania modelu procesu pękania w analizowanych materiałach z wykorzystaniem metody eXtended Finite Element Method (XFEM). Przykłady uzyskanych wyników również zamieszczono w niniejszej pracy.

1. Introduction

To ensure required properties of parts used in bioengineering applications like artificial heart valves, it is of importance to use a reliable materials. Long exploitation time of medical elements requires two major properties: good ductility combined with high hardness. Multilayer materials created in the processes of coating deposition fulfill both these demands [1]. The goal of the deposition is to obtain as many coating layers as possible. In the investigated deposition process the hard and soft layers are imposed periodically as seen in Figure 1. Usually an experimental approaches are involved to analyze behavior of these layers under loading conditions. However, there is strong demand to support experimental investigation with a series of numerical models

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that can qualitatively and quantitatively replicate material behavior. In the conventional finite element approaches available in literature [2] the flat boundaries between the layers are assumed (Figure 1) during investigation.

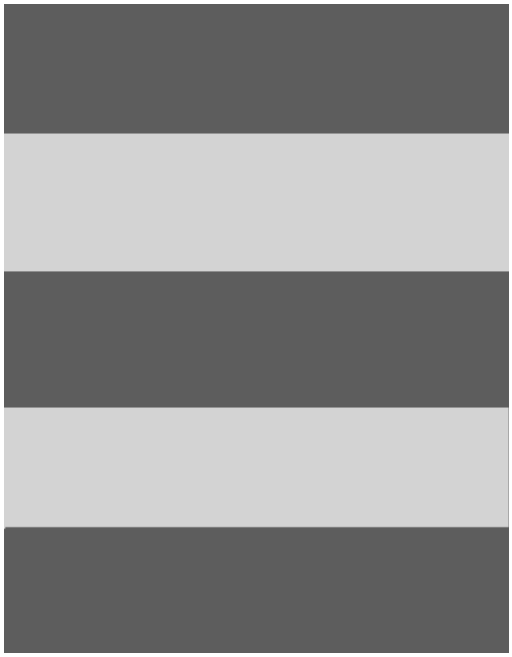


Fig. 1. Five layers of nanomaterials with simple boundary connections

This assumption significantly simplifies the calculations, however it do not properly reflect the reality. Experimental findings presented in [3,4] and briefly summarized below, clearly show how inhomogeneous these boundaries can be and how these inhomogeneities influence material behavior under loading.

The mechanical ball-on-test was performed to investigate material behavior under loading. Sample was deformed by a round tool and after that the microstructure of material was analyzed by TEM technique. The layers geometry and zones where the fracture occurs are clearly visible in Figure 2. Failure usually occurs through TiN layers, which are brittle in comparison to plastic Ti layers. Metallic Ti layers accumulate fracture energy and promotes it to the adjacent ceramic TiN layer.

All the inhomogeneities such as irregular shape of the layer boundaries should be taken into account during numerical modeling to accurately predict zones with maximum stress concentrations pretending to fracture. Application of the digital material representation [5] to develop such a model is the objective of the present work. It is expected that this model can meet mentioned requirements and provide reliable description of nanolayers materials under loading. The second goal is to use the model and extend it capabilities to simulate not only stress concentration zones but also subsequent failure initiation and propagation.

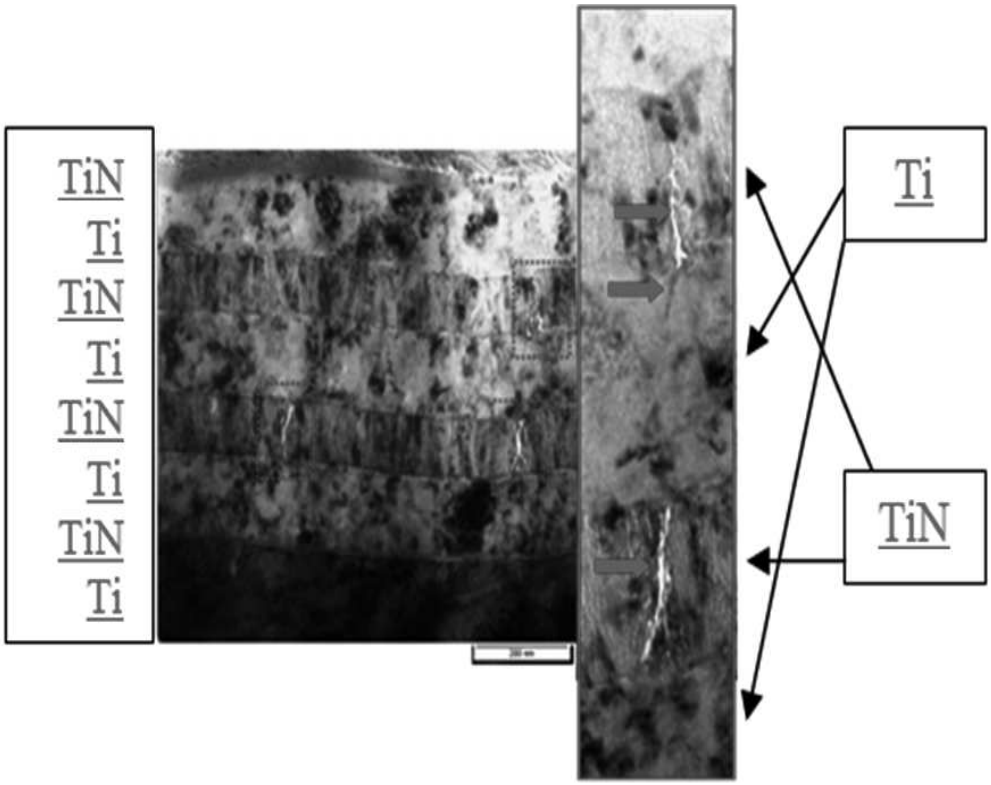


Fig. 2. The TEM image of the Ti/TiN 8 layered coating after mechanical test and cross-section of the coating

2. Digital representation of the nanolayer materials

There are various deposition processes of nanolayer materials that are investigated in research laboratories [3,6]. Most of them are fully understood from the experimental point of view what facilitates creation of a numerical model of such a deposition process. The deposition model is crucial to obtain statistically representative digital representation of material that is an input for the subsequent FE calculations. The digital material representation puts a lot of attention to correctly replicate geometry and properties of material after deposition process. Authors decided to use a numerical model of the molecular beam epitaxy (MBE) deposition method to create a digital representation [3,7] of a multilayer material.

In the MBE method material is heated to high temperature under pressure. These conditions build the phase of gas cloud, which is fired into the rotating substrate, where the new layer starts to grow. This physical process is simulated in the present work using the discrete cellular automata approach [3,5]. The model simulates both the deposition process as well as surface diffusion along deposited layers. Major assumptions of the deposition model are summarized further in the paper.

The algorithm [7] consists of three main steps: deposition of particles on the growing surface, migration of mobile particles along the surface and eventually desorption of particles from the surface.

In the first step particle randomly chose location where they are going to be deposited on the surface. This position determined by the r_i parameter:

$$r_i = (x_i, y_i) \tag{1}$$

Next every particle creates connection between neighbors to find out the total energy in the particular location. Total energy is calculated for every particle using the equation:

$$E_i = n_x^i J_x + n_y^i J_y \tag{2}$$

where: $n_{x,y}$- number of bonds between particles, $J_{x,y}$- energy of singular bond, i- number of a particle neighbors.

In the second step of the algorithm the Boltzmann factor P_i is calculated:

$$P_i \infty \exp(-E_i/k_B T) \tag{3}$$

where: k_B- Boltzman constant, T- temperature of the particle.

The P_i is a probability value for every particle r_i. This approach is used to apply local relaxation in the model leading to migrate of a particle along the surface. The probability P_i can be additionally reduced by the direction of diffusion calculated by equations $\exp(-V_x/k_B T)$ and $\exp(-V_y/k_B T)$. Parameter V is a energy barrier of diffusion along the surface. After probability reduction that particle selects the next position and a relaxation move is performed.

The digital material obtained by the described algorithm is presented in Figure 3 and is further used as an input for the simulation of a simple plastometric compression test. This test is used to evaluate how the geometry of the boundaries influences stress concentration.

Due to the fact that only part of the sample is replicated during numerical simulation to ensure the space continuity the periodic boundary conditions are taken into account. Schematic representation of the periodic boundary conditions is shown in Figure 4.

However, to create a periodic FE model a specific FE mesh have to be used. The OOF2 mesh generator was used in the present research to obtain a required mesh [8]. In that case the same number of nodes on both sides of the sample have to be ensured. Nodes from one side of material are then connected with the nodes on the opposite side [9]. In the ABAQUS application periodic

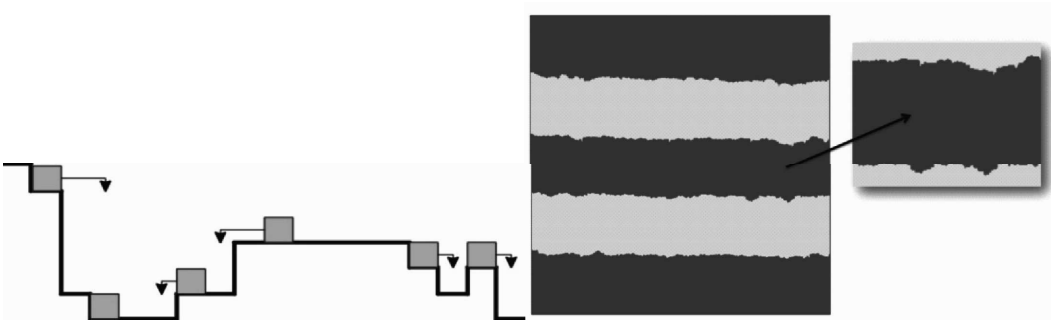


Fig. 3. The process of random deposition of particles with relaxation and multilayer material obtained from the algorithm

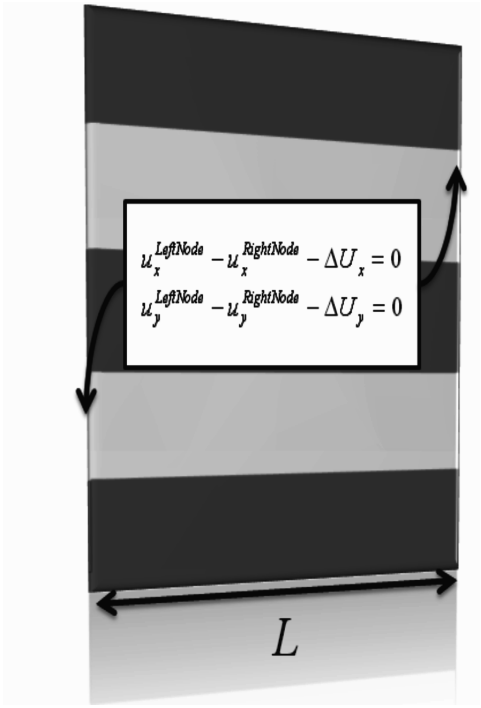


Fig. 4. Periodic boundary conditions applied for the two edges

boundary conditions can be applied by *EQUATION and *BOUNDARY definitions inserted into the input file.

Equations which have to be used are described as:

$$\begin{aligned} u_x^{LeftNode} - u_x^{RightNode} - \Delta U_x = 0 \\ u_y^{LeftNode} - u_y^{RightNode} - \Delta U_y = 0 \end{aligned} \tag{4}$$

where: $u_{x,y}^{LeftNode,RightNode}$ – displacements calculated in the particular node, $\Delta U_{x,y}$ – the difference of displacement for both directories.

2.1. Numerical simulation on the basis of DMR model

To highlight how important is to use an explicit representation of surface geometry Authors decided to perform a simple plastometric compression test using simplified approach with flat boundaries and with the geometry obtained from the deposition model. Obtained results in case of strain and stress distribution are significantly different as presented in Figure 5. When simplified model is applied the stress and strain distribution is in general uniform along subsequent layers and do not provide any valuable information. Contrary, when surface roughness is taken in to account the stress and strain distribution along the layers are highly inhomogeneous. Zones with high stress concentrations can be easily identified. Additionally relations between subsequent layers can also be investigated in the sense of e.g. transferring of strain.

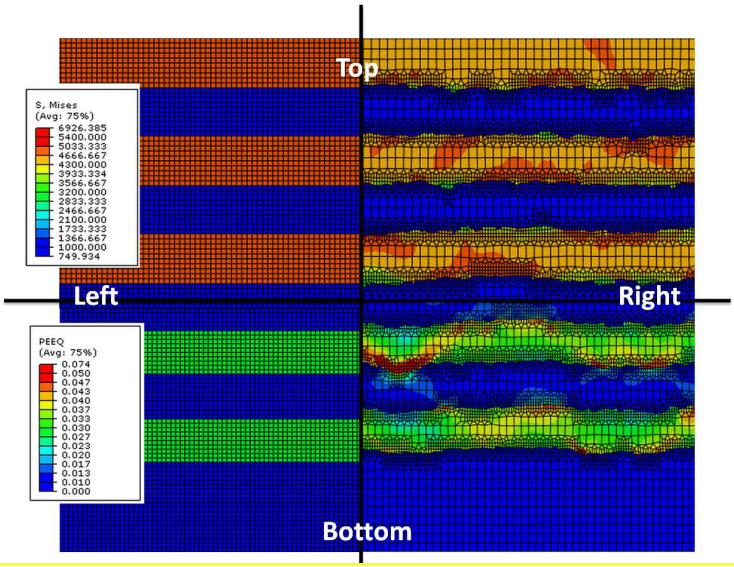
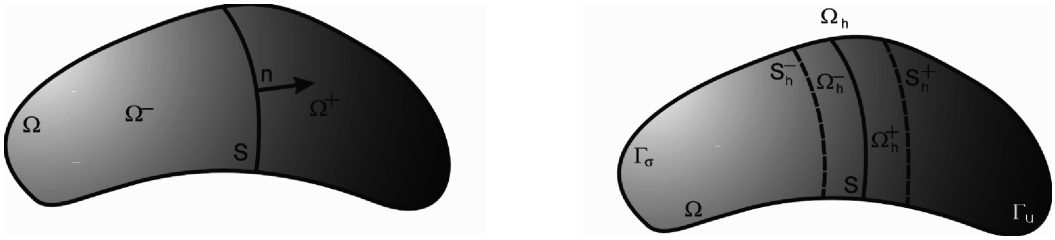


Fig. 5. The comparison of effective stress (top) and equivalent plastic strain (bottom) distribution between model obtained by an algorithm with relaxation TiN/Ti/TiN/Ti/TiN (right) and standard FE model (left)



a) b)

Fig. 6. Discontinuity path (a) and domains (b) created in [6]

As seen, accounting for a specific distribution of layers and shape of boundaries is essential to properly describe inhomogeneous material deformation. These zones with high stress concentrations are usually a precursor of material failure. When simplified model is applied this behavior can not be predicted.

To investigate not only location of the stress concentration zones but also actual failure initiation and propagation Authors decided to go a step further and combine developed model with the extended finite element method (XFEM).

The XFEM is used for numerical modeling of processes where strong discontinuity can be found. That is why this method is widely used for simulation of materials fracture [10-12].

The major assumption is to consider the existence of a body Ω subjected to strong discontinuity conditions along the discontinuity path S. This discontinuity path is fixed at the reference configuration and characterized by the normal vector $\mathbf{n}$. The S path is introduced in a way that it divides the Ω domain into Ω^+ and Ω^- parts (Figure 6).

Additionally a Heaviside function $H_s(x)$ is defined on Ω:

$$H_S(x) = \begin{cases} 1 \forall x \in \Omega^- \\ 0 \forall x \in \Omega^+ \end{cases} \tag{5}$$

Discontinuity path S is presented in Figure 6 where Γ_u and Γ_σ are the Ω boundaries subjected to the usual essential and natural boundary conditions, respectively, and they obey three conditions:

$$\Gamma_u \cup \Gamma_\sigma = \partial\Omega, \Gamma_u \cap \Gamma_\sigma = 0, \Gamma_u \cap \Omega^h = 0 \tag{6}$$

andare the two boundaries of the and subdomains, which surround the S path. It is also assumed that a function $\varphi^h(x)$ is defined as:

$$\varphi^h(x) = \begin{cases} 0 \forall x \in \Omega^- \backslash \Omega_h^- \\ 1 \forall x \in \Omega^+ \backslash \Omega_h^+ \end{cases} \tag{7}$$

Additionally a unit jump function, which takes the zero value everywhere in Ω excluding Ω_h, is introduced:

$$M_S^h(x) = H_S(x) - \varphi^h(x) \tag{8}$$

Such a function exhibits a jump across the discontinuity path S. An expression for the displacement field $u(x, t)$ under a strong discontinuity condition on S is:

$$u(x,t) = \hat{u}(x,t) + M_S^h(x)\,[[u]](x,t) \tag{9}$$

where: $\hat{u}$- the conventional part of the displacement field, $[[u]](x, t)$ - displacement jump function.

A finite element approximation of the strong discontinuity problem is illustrated in Figure 7, where: l_e – length of a straight line in the element, n_e – the normal vector to S_e.

Finally the strain field is then calculated as it is shown in:

$$\varepsilon^h(x,t) = \\ = \left(\nabla \hat{u}^h\right)^S + \sum_{e=1}^{n_{el}} \left(\nabla M_{Se}^h \times [[u]]^h(t)\right)^S \Rightarrow regular + enhanced \tag{10}$$

Presented method allows to model the behavior of the material without re-creating the grid in the widening cracks. Crack initiation in the XFEM method is usually based on the maximum principal stress or strain value criterion. That is why an accurate stress distribution calculations in deforming material is extremely important. Also finding the appropriate density of finite element mesh is crucial for these calculations. Figure 8 shows influence of the mesh density on accuracy of the fracture process prediction with the XFEM method.

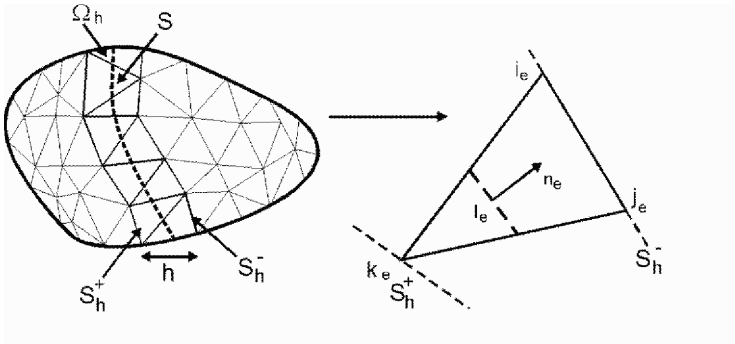


Fig. 7. Illustration of the finite element approximation of the discontinuity [6]

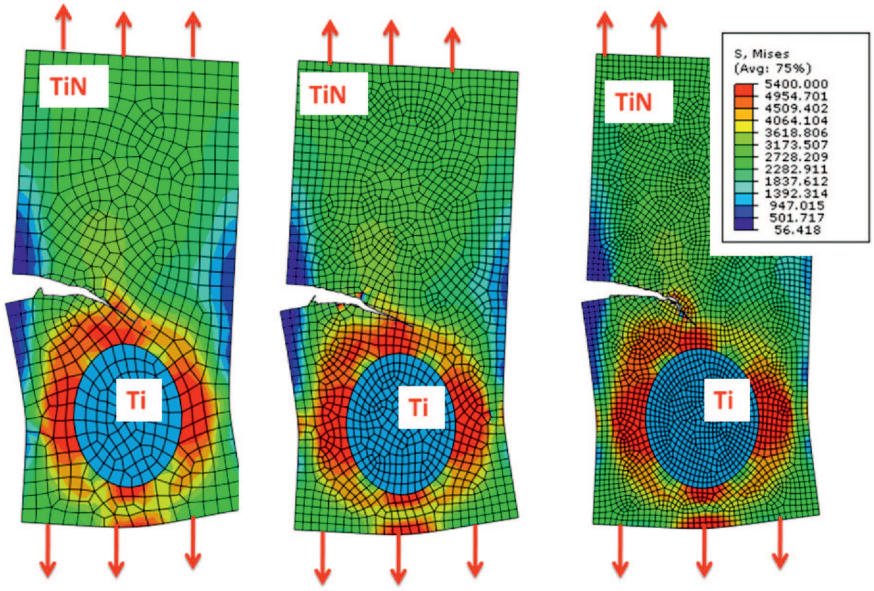


Fig. 8. Mesh sensitivity impact in the XFEM method

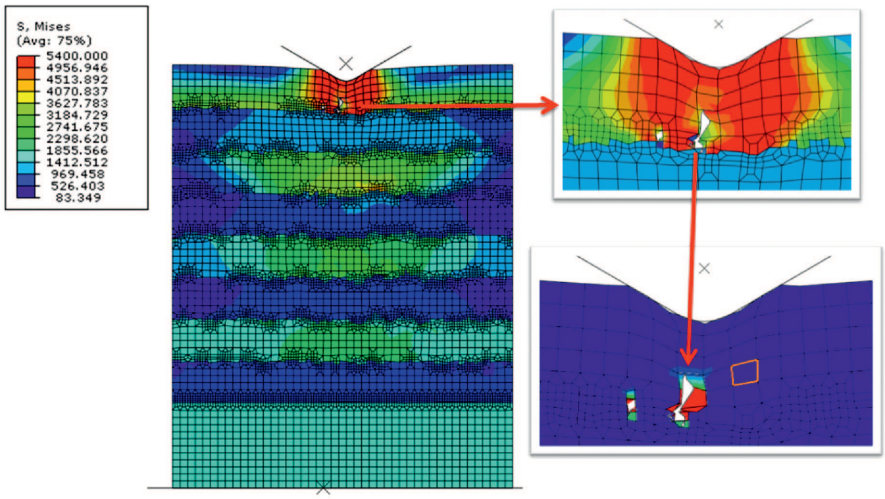


Fig. 9. XFEM fracture propagation in TiN/Ti material layers

As seen for the same deformation degree, obtained fracture behaves slightly different in investigated models. This differences have to be considered during numerical simulation of a real process in order to obtain reliable results.

Described approach, that is a combination of DMR model with the XFEM, is applied in the present paper to investigate fracture propagation in the nanolayers during simple nanoindentation test. This test is commonly used during investigation of material behavior under loading conditions.

Results presented in Figure 8 show that fractures occurs only in the TiN layer at the surfaces interface, what corresponds with the experimental observations. Fracture begins in the stress concentration zone and then propagates through the surface. Such an analysis was not possible with the assumption of perfectly flat interface between layers.

3. Conclusions and future work

Inhomogeneous stress distribution and fracture propagation in the multilayer coatings simulated on the basis of digital material representation was presented in the paper. The major conclusion from the research is that it is important to include representation of geometry of the material surface during numerical simulations. Replacing flat surface between boundaries in multilayered materials by a real shape of the surface, allows to predict inhomogenous stress distribution. The stress concentration zones pretend to be the locations failure initiation.

It can also be concluded that by application of the DMR with the XFEM approach it is possible to simulate not only stress concentration zones but also failure initiation and subsequent propagation.

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