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Computational investigation of the tensile behaviour of the hard coated Ti-6Al-4V alloy

W. Ziaja
Department of Materials Science, Rzeszow University of Technology,
ul. W. Pola 2, 35-959 Rzeszów, Poland
* Corresponding author: E-mail wziaja@prz.edu.pl

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Analysis and modelling

ABSTRACT

Purpose: Modification of the surface layer of the titanium alloys is frequently applied in order to improve their tribological properties. Various surface engineering techniques can be used to produce hard coatings, e.g. composed of metallic carbides, nitrides or more recently DLC. The coating and substrate materials possess significantly different stiffness and strength properties. This can lead to premature failure of the usually elastic coating in case of plastic deformation of the substrate when the high stresses are encountered. Cracking of the hard coating leads to stress concentration and localized plastic deformation of the substrate that can modify macroscopic deformation behaviour of the system. In the paper the influence of coating and substrate properties on local plastic deformation of substrate material was numerically investigated.

Design/methodology/approach: Two dimensional finite element analysis of the process of tensile deformation of titanium alloy with hard elastic coating was carried out. Two cases were analyzed, i.e. with and without diffusion strengthened layer underlying the coating.

Findings: The influence of the difference in Young's modulus between coating and substrate material, yield strength of substrate material, coating thickness and depth of the crack in the coating on local plastic deformation of substrate material was determined.

Research limitations/implications: Some extension of the numerical model should be pursued in order to take into account initiation of microcracks in surface layer of the coated material and process of coating delamination.

Practical implications: The results could be used in the element design process for selection of parameters of surface layer with complex structure for load bearing applications.

Originality/value: The mechanical behaviour of hard coated material was most frequently studied for indentation and friction conditions and much less investigations were carried out for coated systems under tension or compression.

Keywords: Computational material science; Titanium alloys; Surface layer

1. Introduction

Titanium alloys are very attractive materials for heavily loaded engineering components working in severe environment conditions. The main reason for that is favourable combination of properties like high specific strength, corrosion resistance and biocompatibility. However low resistance to oxidation at high temperature and poor tribological behaviour very often necessitate in surface treatment of elements made of titanium alloys in order to obtain surface layer having favourable properties [1,2]. PVD methods lead to formation of intermetallic or compound layers (e.g. TiN, Ti_2N, Ti(C,N), Ti_3Al, TiAl) with thickness of the order of several μm. As the result of thermochemical treatment (e.g. nitriding, carbonitriding) hardened diffusion layer is formed, at the top of which intermetallic or compound layer can also be present (e.g. TiN). These phases have high Young's modulus and exhibit brittle behaviour. Because of high value of elastic modulus and very low plastic deformability of the layer, when large tensile stresses are present, microcracks form in the layer. They induce stress concentration that leads to local plastic deformation of the substrate at the macroscopic tensile stress value well below its yield stress [3,4]. Plastic deformation of the substrate is an additional factor decreasing durability of the layer because of delamination and flaking [4,5]. Especially in the presence of tensile and compression stresses fatigue strength of the coated system can be significantly reduced [5-7]. The influence of many factors affecting coating performance and durability of coated elements can be effectively studied by finite element method in order to speed up the process of coating optimization [6-10]. The aim of this work was to study the influence of substrate and coating properties and effect of microcracks in the coating on the plastic deformation of the substrate under tensile loading in order to develop some guidelines for design of surface layers with complex microstructure.

2. FE model of the coated system

Tensile deformation of the flat specimen of the titanium alloy covered with hard elastic coating having crack of certain depth was analyzed (Fig. 1). The objective of this work was to determine the influence of the elastic coating thickness, elastic modulus of the coating, depth of the crack in the coating and yield properties of the substrate with and without hardened diffusion layer on the local yielding of the substrate in the area of stress concentration induced by the crack in elastic layer. The analysis was carried out using commercial finite element software ADINA [11].

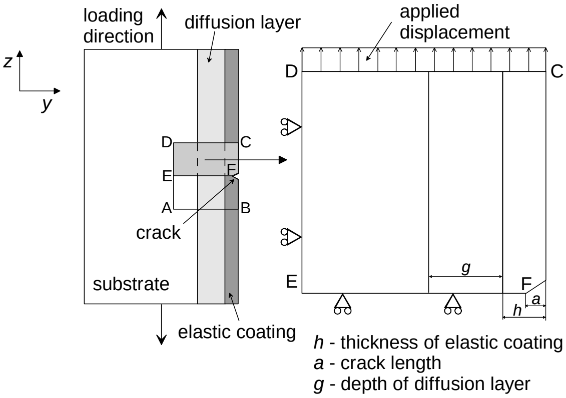

Fig. 1. FE model of the hard coated specimen segment

In order to increase calculation efficiency specimen segment containing crack in elastic coating was analyzed imposing proper boundary conditions. Because of symmetry only the half of the segment was modelled with the crack lying on the symmetry axis. On the symmetry plane EF all nodal displacements in the vertical direction was set to zero and the nodes were allowed to move horizontally. In the initial analyses the size of the segment was gradually increased until homogeneous, uniaxial tension boundary conditions imposed on CD and DE edges did not affect the strain distribution around the crack. Thus on the DE edge nodal displacements in the horizontal direction were set to zero and the nodes were allowed to move vertically. Tensile load was applied through the vertical displacement of the nodes on CD edge. For the segment size of 0.8×0.8 mm convergence of the results was reached enabling correct analysis of the distribution of the stresses and strains generated under tensile loading in the vicinity of the crack in the elastic coating.

The substrate was modelled as an isotropic, rate-independent elastic-plastic solid. Young's modulus of the titanium alloys varies between 98 and 125 GPa depending on their chemical composition and microstructure [1,12]. It was assumed that comparing with the significantly higher Young's modulus of the potential coating materials and wide range of these values, the influence of the possible differences in Young's modulus of titanium alloys on the deformation process is negligible. Because of that constant values of Young's modulus E=115 GPa and Poisson ratio ν=0.3 were assigned to the substrate in all analyses [13]. On the other hand the heat treatment applied, phase composition and microstructure of the alloy significantly affect its yield properties. Therefore the analyses were carried out for yield strength of the substrate ranging from 500 to 900 MPa. Two phase titanium alloys exhibit low strain hardening and are frequently modelled even as elastic-perfectly plastic material [13]. In current analysis low linear strain hardening was assumed for the substrate.

The coating was assumed to be isotropic, linear elastic material with Young's modulus in the range of 180-420 GPa, that covers values reported for several hard coatings phases like TiN, Ti(C,N), Ti_3Al, TiAl [14,15]. The coating thickness was set to 3, 5, 7 and 10 μm. The analysis was carried out for crack depth ranging from 0.4 to 0.9 of the coating thickness.

The influence of hardened diffusion layer underlying elastic coating on yielding of the substrate was also analyzed. For this case the yield strength of the substrate was set to 800 MPa. The depth of diffusion layer was varied between 50 and 100 μm. It was divided into several sublayers in order to account for variation in mechanical properties within the layer. Maximum value of yield strength in the diffusion layer ranged from 880 to 960 MPa.

Plane stress conditions were assumed in all analyses. Eight-node, isoparametric elements were used. The density of the finite element mesh was increased in the region around crack tip in order to capture the details of the stress and strain distribution in the area of high stress and strain gradients.

3. Results of the simulations

From the results of calculations distribution of z component of plastic strain in the substrate was determined. The crack in elastic coating acts like stress concentrator and high local stresses generates localized plastic deformation zones (*PDZ*) in the substrate which follow the direction of maximum shear stress (Fig. 2a). Local yielding of the substrate starts at the imposed macroscopic strain that would be in elastic range in case of the absence of elastic coating. The size of *PDZ* was compared for various cases at imposed macroscopic plastic strain of the substrate ε_z = 0.0005. The *PDZ* size was measured as a distance from coating/substrate interface to the point where plastic strain is ε_z = 0.003 (*d* Fig. 2a).

With increasing depth of the crack in elastic layer plastic strain in PDZ is raised, strain gradient is higher and the location of strain maximum is shifted towards coating/substrate interface increasing the possibility of coating delamination due to excessive strain at the interface (Fig. 2b).

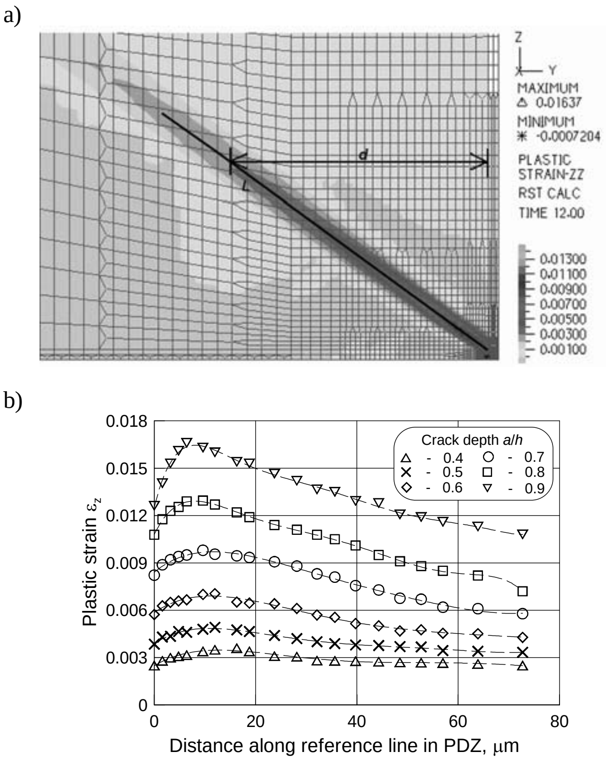

Fig. 2. Plastic strain distribution: (a) in the substrate for crack depth a/h=0.8 (b) along the reference line in the plastic deformation zone (*PDZ*); *d* – *PDZ* size, *L* – reference line; substrate: 0.2% yield strength σ_y=600 MPa; elastic coating: thickness *h*=10 μm, Young's modulus *E*=300 GPa

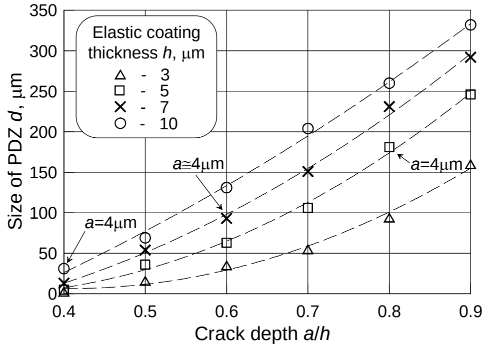

Fig. 3. The size of *PDZ* in the substrate as a function of coating thickness (*h*) and depth of the crack in the coating (*a*/*h*); 0.2% yield strength of the substrate σ_y=600 MPa, Young's modulus of the coating *E*=300 GPa

As the elastic coating thickness increases, larger *PDZ* develop for a given crack depth (Fig. 3). At the certain crack depth, absolute crack length in thicker coating is larger, what in turn raises maximum value of the stress in the crack tip vicinity. At the same crack length, the *PDZ* size increases with decreasing coating thickness (Fig. 3). This can be attributed to reduced distance between crack tip and coating/substrate interface and thus higher stresses generated in substrate in the stress concentration zone.

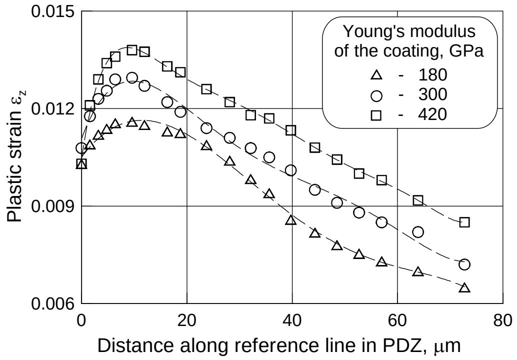

Fig. 4. The influence of Young's modulus of elastic coating on plastic strain distribution along the reference line in the *PDZ* (for crack depth *a*/*h*=0.8); 0.2% yield strength of the substrate σ_y=600 MPa, coating thickness *h*=10 μm

As the Young's modulus of the coating increases, there is a distinct shift in the maximum value of plastic strain in *PDZ*, caused by increase in stresses in whole elastic coating especially in the area of stress concentration around crack tip (Fig. 4).

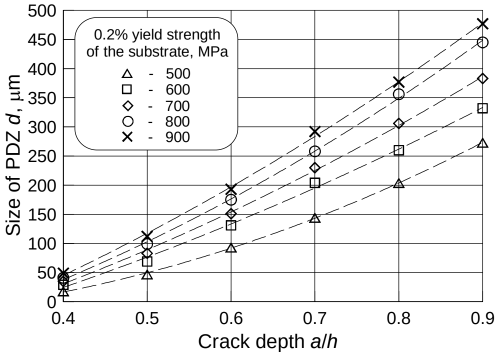

Fig. 5. The size of PDZ in the substrate as a function of 0.2% yield strength of the substrate and depth of the crack in the coating; Young's modulus of the coating *E*=300 GPa, the coating thickness *h*=10 μm

As the yield strength of the substrate increases larger *PDZ* develop for a given crack depth as indicated in Fig. 5. It should be reminded here that *PDZ* sizes are compared not at the same value of imposed macroscopic strain, but at the strain values corresponding to identical macroscopic plastic strain of the substrate. Reaching these conditions requires imposing larger displacement on the CD edge of the segment, for the substrate with higher yield strength. This in turn results in larger strain of the coating and consequently larger stresses in it. Naturally, assuming constant imposed displacement, the size of the *PDZ* in the substrate with higher yield strength would be smaller. However such analysis does not comply with real service conditions when loads acting on components made of material with higher strength properties are more severe. Thus the influence of the substrate yielding on life of the elastic coating is expected to be stronger for the substrate with higher yield strength.

It was found that hardened diffusion layer between elastic coating and the substrate substantially reduces development of the local plastic deformation of the substrate in the vicinity of the crack in the coating. Increase in diffusion layer depth and in maximum value of the yield strength in this layer resulted in decrease in the size of *PDZ* (Fig. 6a). The maximum yield strength in diffusion layer had decisive influence on the decrease in maximum plastic strain in *PDZ* (Fig. 6b).

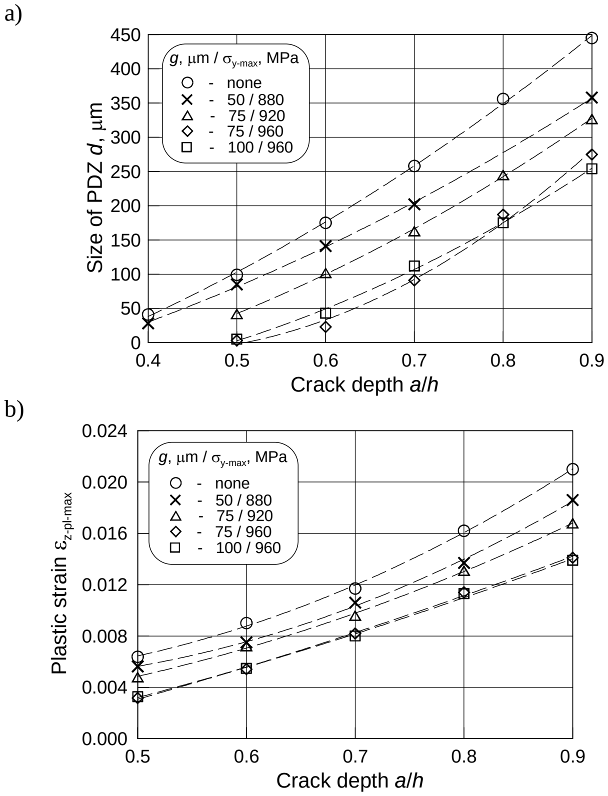

Fig. 6. Influence of the depth of diffusion layer *g*, maximum value of the 0.2% yield strength in this layer $\sigma_{y\text{-max}}$ and the depth of the crack in the coating a/h on the size of *PDZ* in the substrate (a) and max. plastic strain ($\varepsilon_{z\text{-pl-max}}$) in the *PDZ* (b); Young's modulus of the coating E=300 GPa, the coating thickness h=10 μm

4. Conclusions

Two dimensional finite element analysis of the unidirectional tensile deformation of the titanium alloy covered with the hard, elastic coating was performed. The presence of the crack in the coating was assumed. The distribution of plastic deformation in the substrate induced by stress concentration was determined. The size of plastic deformation zones (*PDZ*) was compared for various coating and substrate parameters. Following conclusions can be drawn on the basis of the results of the studies:

- Local plastic deformation of the substrate starts at the imposed macroscopic strain, which in the absence of the coating would be in elastic range,
- As the coating thickness increases, the *PDZ* in the substrate becomes larger for a given crack depth (*a*/*h*), however for a given crack length (*a*) larger *PDZ* develop in the case of thinner coatings,
- The higher is the value of Young's modulus of the elastic coating the larger is *PDZ* size and maximum plastic strain in *PDZ*,
- In the substrate with higher yield strength larger *PDZ* develop, because of larger "acceptable" macroscopic strain, generating higher stresses in the elastic coating,
- Hardened diffusion layer reduces local plastic deformation in the vicinity of the crack tip, leading to decrease in both *PDZ* size and maximum plastic strain in *PDZ.*

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