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Finite element modelling of the fracture behaviour of surface treated Ti-6Al-4V alloy

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ABSTRACT

Purpose: Surface treatments of the titanium alloys are frequently applied in order to modify the surface layer microstructure and to improve tribological properties or resistance to high temperature oxidation of the alloy. Various surface engineering techniques can be used to increase the surface hardness, e.g. deposition of the coatings composed of metallic carbides, nitrides or more recently DLC. The stiffness and strength properties of the coating and substrate materials differ significantly. Cracking of the usually brittle coating leads to stress concentration and localized plastic deformation of the substrate which can facilitate propagation of microcracks into the substrate. This can result in premature failure of the hard coated component. In the paper the crack penetrating hard coating was analysed and the influence of coating and substrate properties on crack driving force was numerically investigated.

Design/methodology/approach: Two dimensional finite element analysis of the four point bending test of surface modified titanium alloy with the crack penetrating hardened layer was carried out.

Findings: The effect of the coating thickness and stiffness, residual stresses in the coating, yield strength of substrate material and yield properties of diffusion hardened layer on crack driving force was determined.

Research limitations/implications: Some extension of the numerical model should be introduced in order to take into account the interactions of the crack with microstructure of the material.

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

Originality/value: The fracture behaviour of hard coated materials was most frequently studied for indentation and friction conditions and considerably less concern was devoted to coated systems under tension or compression.

Keywords: Titanium alloys; Surface layer; Analysis and modelling; Computational material science

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METHODS OF ANALYSIS AND MODELLING

1. Introduction

Surface treatment is widely used for elements made of titanium alloys in order to enhance their resistance to oxidation at high temperature, tribological properties and load bearing capacity [1]. For biomedical applications in which titanium alloys are used for hard tissue replacement critical properties that can be improved by surface treatment include wear and abrasion resistance, corrosion resistance and biocompatibility. The important issue is that the surface layer modification should not deteriorate fatigue behaviour of the material in the presence of tensile and compressive stresses resulting from bending [2].

The surface hardening of titanium alloy components is usually carried out by means of either coating deposition by techniques like CVD, PVD and plasma spray, or modification of surface layer by diffusion treatments, laser assisted treatments and ion implantation [3,4].

The result of certain surface treatment of titanium alloys, e.g. PVD methods, is 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. These phases usually have high Young's modulus and hardness and exhibit brittle behaviour [5,6,7].

They offer some advantages like low friction coefficient, high hardness and sliding wear resistance and also improved corrosion resistance. Despite the enhancement of tribological properties such hard, stiff coatings can cause some detrimental effects.

When the element is subjected to cyclic tensile and compression stresses, fatigue strength of the coated system can be significantly reduced [4,8,9]. This is due to very low plastic deformability of the elastic coatings that leads to formation of microcracks when large tensile stresses are present. Growth of these microcracks can lead to premature failure of the element. That is why the fracture behaviour of the coating–substrate system is often a major consideration.

Coating deposition technology is often joined with substrate surface pretreatment, such as the laser pretreatment of the steel substrate surface prior to plating a chromium coating [10] laser treatment of titanium alloy prior to plasma nitriding [11] or thermochemical treatment (e.g. nitriding, carbonitriding) of titanium alloys before PVD coating deposition [12]. This technology can greatly improve the mechanical properties of a coating–substrate system because the surface layer with structure modified by the pre-treatment changes the character of the interactions between the coating and substrate.

Better load bearing properties can be obtained by application of diffusion treatments, which take advantage of the high reactivity of titanium with carbon, nitrogen and oxygen to produce surface layers with high hardness and good adhesion to tough substrate. Diffusion treatments, e.g. glow discharge method, inherently produce the layer with complex, gradient structure i.e. hard elastic coating at the surface and diffusion strengthened layer underneath the coating in which chemical composition and thus mechanical properties vary continuously with the distance from the surface [13]. These changes affect stress state and modify the fracture behaviour of the coated material.

Important factor that controls interactions between coating and substrate and have pronounced effect on coating adhesion and durability of coated component is the level of residual stresses that are frequently present in the coating [14,15].

PVD and CVD coatings possess high hardness and may be in a state of tensile or compressive stress, depending on the choice of material and process used. In most cases a compressive stress acts in the coating. Such combination of hard surfaces and compressive stresses can be expected to have a profound influence on the fatigue properties of surface coated material system [16,17].

Large number of parameters that characterize the surface layer and have significant effect on its properties and performance make difficult the process of optimization of the microstructure and properties of surface layer. Beside the experimental *trial-and-error* methods some numerical tools like finite element method, can be effectively used to predict the particular properties of hard coatings, e.g. residual stresses resulting from the deposition process, and to analyze the effect of individual parameters of the surface layer on coating performance and durability of coated components [9,18,19,20,21,22].

Various coated system configurations containing cracks were previously analysed. They differ in some assumptions concerning substrate and coating properties, residual stress state, loading mode and crack geometry.

Smith [23] stated that the typical failure mode of the coating–substrate system is often a two stage process: at the first stage, when a coating–substrate system is under sufficient tensile stress, through-thickness cracks develop in the usually brittle coating. At the second stage, when the crack tip reaches the interface, the crack may stop at the interface or propagate along the interface or into the substrate. Whether the crack stops or propagates depends on many factors, such as the load conditions, mechanical properties of the coating and the substrate and interfacial adhesion properties between the coating and the substrate [24].

The behaviour of the crack perpendicular to the interface was studied by Romeo and Ballarini [25] and most relevant conclusions are:

- local stress intensity decreases and reaches zero at the interface when crack approaches the interface from an elastically weaker material to a stiffer one,
- local stress intensity increases and reaches infinity at the interface when crack approaches the interface from a stiffer material to a weaker one.

Chakravarthy [26] calculated energy release rate for the crack perpendicular to the interface between the coating and the substrate with its tip in the homogeneous substrate.

However in all that investigations both the coating and the substrate were assumed to be elastic which is not the case for ductile alloys with hardened surface layer.

Yang [10] studied the fracture behaviour of material system composed of laser prequenched steel substrate and elastic coating. The case of a crack perpendicular to the interface between the coating and the hardened layer, with the crack tip in the substrate was analysed and yield properties of the substrate were taken into account.

In the case when material undergoes both elastic and plastic deformation, *J*-integral can be used instead of stress intensity factor to characterize the fracture behaviour of the material containing crack of a certain length. The value of *J* integral is related to strain energy in the vicinity of the crack and can be used to predict stress and strain conditions for crack initiation under monotonic loading.

It has been shown previously that the effect of microcracks developing in the elastic coating on localization of plastic deformation in the substrate material is sensitive to certain properties of the coating and substrate materials, i.e. the ratio of elastic moduli of both coating and substrate materials, coating thickness and distribution of yield strength in the diffusion strengthened layer [27].

In the current work, based on elastic-plastic fracture mechanics theory, a two-dimensional mechanical model of the titanium alloy with modified surface layer was developed that enables quantification of the effects of various parameters on crack driving force in terms of *J*-integral.

A numerical example is presented to investigate how the thickness and Young's modulus of the coating, residual stress level in the coating, yield properties of the substrate and yield strength distribution in the diffusion layer influence the crack driving force for the crack penetrating the elastic coating and diffusion layer in the substrate.

2. Methodology of FE calculations

Four-point bending of the flat specimen of the titanium alloy with modified surface layer consisting of hard elastic coating and diffusion hardened layer was analyzed numerically. The crack penetrating the coating and having its tip in the substrate material was introduced to examine the effect of various parameters on the crack dricing force (Fig. 1). Two dimensional analysis was carried out using commercial finite element software package ADINA v. 6.4 [36].

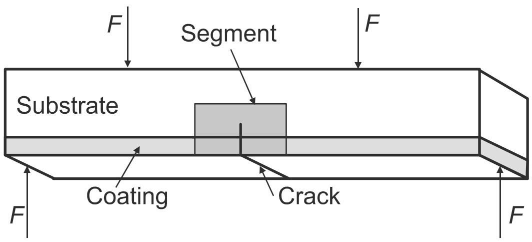

Fig. 1. Schematic diagram illustrating the four-point bending specimen with numerically analysed segment

After the surface treatment of titanium alloy, the treated layer is usually composed of several zones having different microstructure and properties [10]. Thus to analyze the sensitivity to fracture of the coated material a model was developed of a material composed of an elastic coating, and a substrate containing a diffusion hardened layer, as illustrated in Fig. 2, in which *h* and *d* denote the thickness of the coating and the total depth of the diffusion layer, respectively. The coating properties are characterized by the elastic constants E_c, υ_c and the substrate possesses elastic-plastic properties characterized by elastic constants E_s, υ_s and yield strength σ_s.

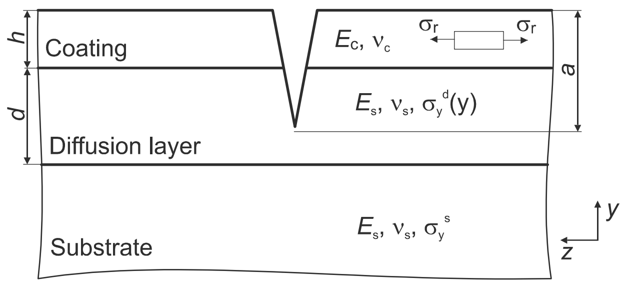

Fig. 2. The model of surface treated titanium alloy adopted for FE calculations

The system contains a crack of a length *a* penetrating the interface between the elastic coating and the ductile substrate with its tip lying in the diffusion hardened layer.

To examine the local interaction of the crack with surrounding material and to increase calculation efficiency only small specimen segment containing crack was analyzed imposing proper boundary conditions (Fig. 3). A substrate segment was large enough to avoid any artificial constraints or edge effects.

In the initial analyses the size of the segment was gradually increased until boundary conditions imposed on its edges did not affect the stress and strain distribution around the crack tip. Finally, the combined thickness of the substrate and the coating was set to 500 µm and the half width was 250 µm.

Because of symmetry only the half of the segment was modelled with the crack lying on the symmetry axis (Fig. 3). On the symmetry axis all nodal displacements in the vertical direction were set to zero and on the left-hand side nodal displacements in the horizontal direction were set to zero. These reflect the fact that, in reality, the region being simulated would be constrained by large sections of coating and substrate around and below it.

The four point bending load is applied sufficiently far from the crack (Fig. 1). Thus for the analyzed segment the loading was assumed in the form of tensile displacement changing linearly along the loaded edge (Fig. 3). The load was applied in 30 steps reaching the maximum displacement value corresponding to the total strain of 1%.

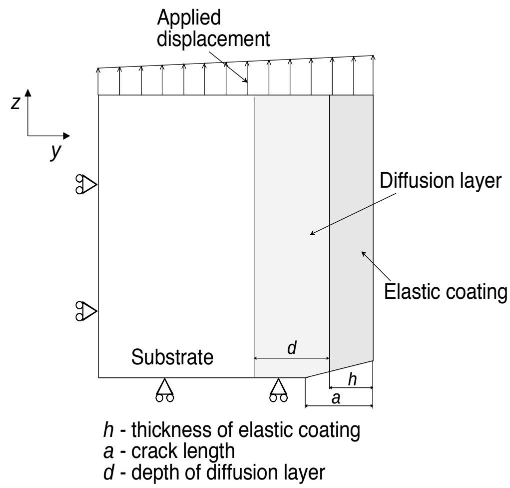

Fig. 3. Loading and boundary conditions of the FE model of the analyzed specimen segment

Plane stress conditions were assumed in all analyses which follow from the free boundary in y-direction of the very thin coating layer. Mesh with significant refinement around the crack region consisted of approximately 3500 isoparametric quadrilateral 9-node elements (Fig. 4). The ratio of largest to smallest element area was approximately 50. Further mesh refinement did not improve accuracy of calculations appreciably.

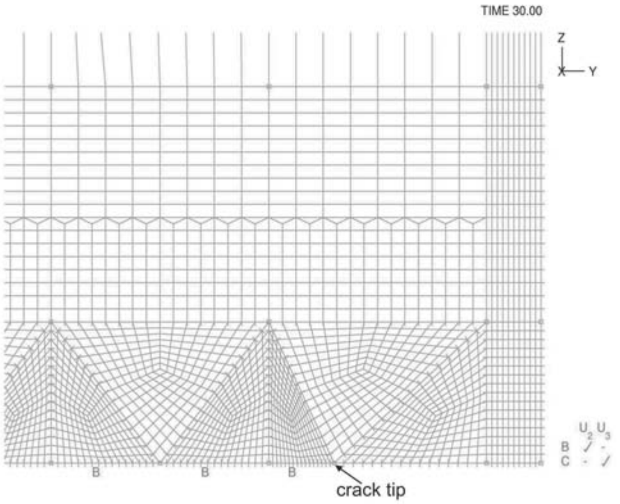

Fig. 4. FE mesh refinement in the vicinity of the crack tip

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 [28, 29]. The coating thickness was set to 3, 5, 7 and 10 µm. In this model the surface of the coating and the interface between the substrate and the coating were assumed to be ideally planar and free of defects.

The coating was subjected to an initial stress σ_r upon which the tensile stress resulting from the bending of the specimen was superimposed.

In TiN, and other types of hard coatings, compressive residual stresses can develop with magnitudes up to 6 GPa, resulting from both thermal expansion mismatch and deposition strains. These stresses depend on the thermal expansion mismatch between coating and substrate, and therefore differ between different substrate materials and deposition processes. Residual stresses in TiN coatings, which are significantly higher than the thermal stresses expected for typical processing temperatures, are largely attributable to growth strains that arise during the deposition process [30].

The measurements of the macro-stresses using the X-ray method carried out for the TiN phase produced by various deposition techniques show very big differences, both concerning their character and the magnitude [31]:

- glow discharge nitriding: -1500 to -2500 MPa;
- laser remelting by overlapping laser tracks using diode laser: +600 to +800 MPa;
- wide laser track using diode laser: -300 to -800 MPa;
- pulsed laser deposition: -5000 to -8000 MPa.

In the current model both compressive and tensile residual stresses were modelled and the values of the stresses ranged from -2500 to +500 MPa.

The ductile titanium alloy substrate was modelled as an isotropic, rate-independent solid with bilinear elastic–plastic constitutive relation, assuming kinematic strain-hardening and Von Mises yield criterion. It was assumed that comparing with the significantly higher Young's modulus of the potential coating materials and wide range of these values, the variation in Young's modulus of titanium alloys that depends on their chemical composition and microstructure on the deformation process is negligible [1,32]. Because of that, constant values of Young's modulus E=110 GPa and Poisson ratio ν=0.3 were assigned to the substrate in all analyses.

Values of Young's modulus $E_s = 110$ GPa and tangent (hardening) modulus $E_h = 1.25$ GPa assigned for analyses were determined on the basis of the tensile test result for Ti-6Al-4V alloy (Fig. 5).

For the substrate yield stress in the range of 800-1000 MPa was assumed in all analyses in which diffusion layer was not accounted for. The lower value is minimum yield stress required in case of Ti-6Al-4V ELI alloy (extra low interstitial) and the higher value reflects the possible effects of the heat treatment applied on phase composition, microstructure and thus on yield properties of the alloy.

Modelling of the properties of the material in the diffusion layer is a challenging task because the yield strength varies from the surface to the interior which was called the yield strength gradient effect by Kolednik [33]. Beside the surface treated and case hardened components this effect can also appear in welded structures, soldered joints and so on. Kolednik [33] analysed such a case and presented the yield stress gradient term of the crack driving force in terms of the J-integral.

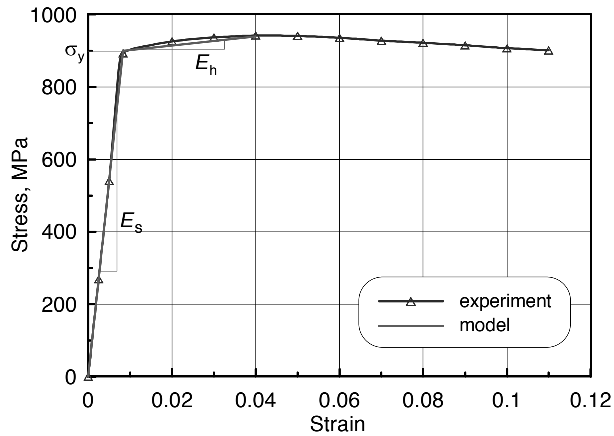

Fig. 5. Experimental stress-strain curve obtained for Ti-6Al-4V alloy and bilinear elastic-plastic relationship used in FE calculations (E_s – Young's modulus, E_h – hardening modulus)

It should be emphasized that, for materials with diffusion layer obtained by surface treatment, it is extremely difficult to measure the yield strength at the particular distance from the surface, as the chemical composition and thus material properties are changing continuously. One way to overcome this difficulty is to apply hardness measurement which is quick and easy to obtain hardness profile on the cross section of the surface layer and then use approximate relation between the hardness and the yield strength. Such a relation between the hardness and the yield strength has been developed using dimensional analysis and finite element calculations and discussed in detail by Cheng [34].

Hardness profile for titanium alloy after oxynitriding at the temperature of 1173 K showing typical character of hardness variation in the diffusion layer is presented in Fig. 6 [35].

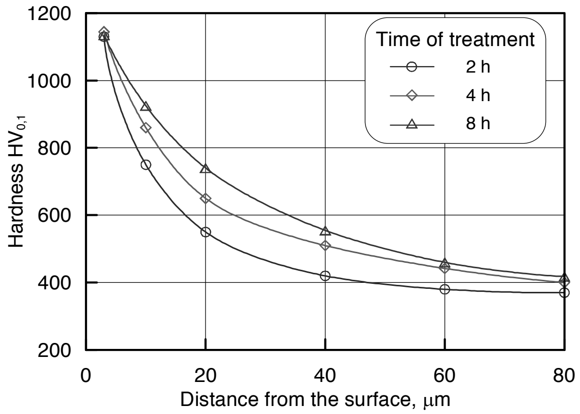

Fig. 6. Hardness profiles for the Ti-6Al-4V alloy oxynitrided at the temperature of 1173 K [35]

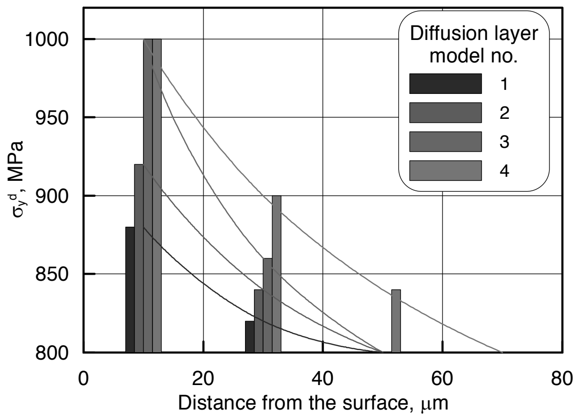

Fig. 7. Yield strength values assigned to individual sublayers in the diffusion layer; the curves represent corresponding yield strength profiles that are approximated in the models

Even if the yield strength could be estimated directly from the hardness measurement, another difficulty arises from the method of implementation of yield strength profile in the material model used for finite element calculations.

In the current model continuous variation of the yield strength in the diffusion layer with the distance from the surface was simplified by introducing gradual variation. The diffusion layer was divided into sublayers, each of them 20 μm thick, and various values of yield strength were assigned to each sublayer. Several cases were analysed. In the first case diffusion layer consisted of only one sublayer and the yield strength in it was varied between 840 and 1000 MPa. In the second case the diffusion layer with multi sublayer structure was analysed. The configuration of analysed models of diffusion layer is presented in Table 1. The values of yield strength assigned to each sublayer were chosen in such a manner to reproduce approximately character of the yield strength variation which in turn was assumed to correspond to the character of hardness variation (Fig. 7). In each case the yield strength of the substrate was set to 800 MPa.

Table 1.
Yield strength distribution in the diffusion hardened layer

Model no.	Yield strength, MPa		
	First sublayer	Second sublayer	Third sublayer
1	880	820	-
2	920	840	-
3	1000	860	-
4	1000	900	840

Values of J integral for particular model configuration calculated at the maximum loading applied were normalized with respect to the reference value J_{ref}, which denotes the J integral value obtained for the material system only with elastic coating, without the diffusion hardened layer and with an edge crack penetrating the coating and the substrate. Other parameters of the reference model configuration are presented in Table 2. This gives a comparative analysis of the effect of individual parameters, i.e. coating thickness and stiffness, level of residual stresses in the coating, substrate yield properties and distribution of yield properties in the diffusion layer on the crack driving force.

Table 2.
Model parameters for determination of the reference value of J integral

h_c (μm)	E_c (GPa)	a (μm)	σ_y^s	σ_r	diffusion layer
5	300	20	800	0	no

3. Results and discussion

The results of finite element simulations of the crack penetrating prestressed coating and going into the substrate are presented in this section. The parametric study performed presents the roles of various coating and substrate parameters on the crack driving force. Competing role between coating stiffness and residual stresses is highlighted.

The effect of the coating thickness on crack driving force is illustrated in the Figure 8. The results are given for fixed Young's modulus of the coating E_c = 300 GPa. Increasing the thickness of the stiff coating tends to raise the J integral value, which occurs due to an expansion of the zone of high tensile stresses in the system. In the case of less ductile substrate, crack driving force is lower for the same coating thickness but is more sensitive to the increase in coating thickness.

The effect of the coating stiffness on crack driving force is illustrated in the Figure 9. The results are given for fixed yield strength of the substrate σ_y^s = 800 MPa. As the Young's modulus of the coating increases, there is a distinct shift in the J integral value. It can be attributed to higher stress level in the whole elastic coating for a given deformation of the specimen. For a thicker coating the changes in the crack driving force with coating stiffness are more pronounced.

The influence of the yield strength of the substrate on crack driving force is shown in Figure 10. The results are given for fixed Young's modulus of the coating E_c = 300 GPa. As the yield strength of the substrate increases, crack driving force is lowered significantly. It can be related to the reduced level of plastic deformation in the vicinity of the crack tip. In the case of the thicker coating, the response of the system is less sensitive to the changes in the substrate properties.

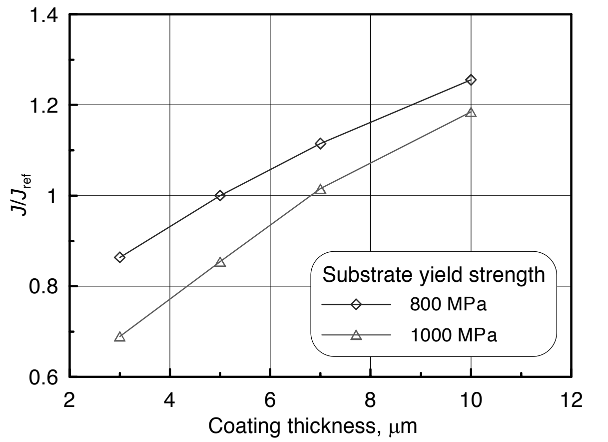

Fig. 8. The effect of coating thickness, *h*, on crack driving force for various yield strength of the substrate

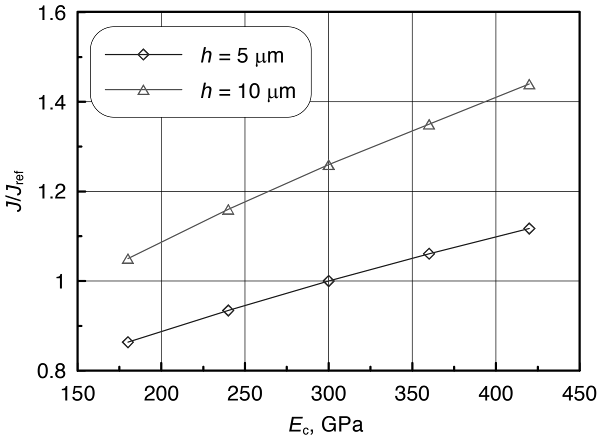

Fig. 9. The effect of coating Young's modulus, E_c, on crack driving force for various coating thickness, *h*

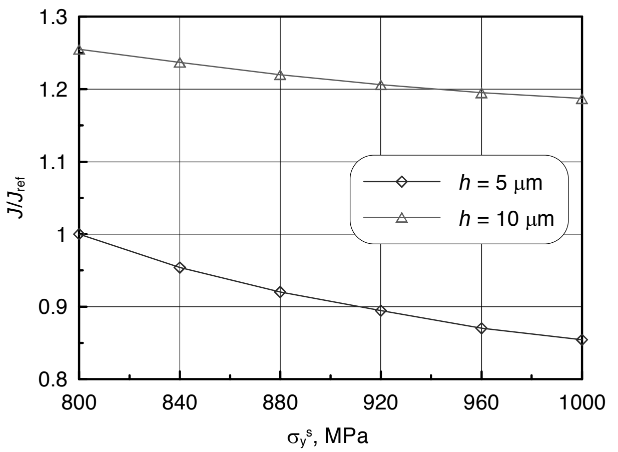

Fig. 10. The effect of substrate yield strength on crack driving force for various coating thickness

The influence of the residual stress level in the coating on crack driving force is shown in the Figure 11. The results are given for fixed Young's modulus of the coating E_c = 300 GPa and yield strength of the substrate σ_y^s = 800 MPa. It can be noticed that the crack driving force decreases significantly with increasing residual compressive stress in the coating. In contrast, if the residual stresses are tensile, the crack driving force will increase. Thus tensile residual stresses superimposed on the stresses generated by the external loading will adversely facilitate the crack propagation. The effect of the magnitude of residual stresses on crack driving force is stronger in case of the thicker coating.

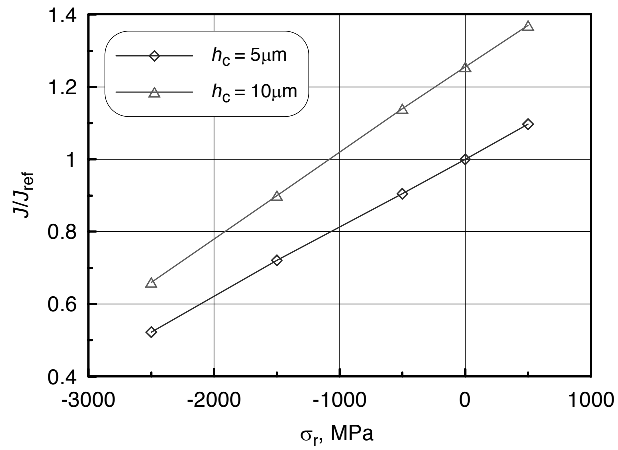

Fig. 11. The effect of coating residual stresses on crack driving force for various coating thickness

The influence of the diffusion layer properties on crack driving force is shown in the Figures 12-13. The results are given for fixed Young's modulus of the coating E_c = 300 GPa and various coating thickness. It can be seen that for thin diffusion layer, increase of the yield strength in that layer results in higher crack driving force. For certain deformation higher applied stresses arise in more hardened layer which cause more intense strains in the soft substrate, which is close to the crack tip. Thus the strengthening effect of the diffusion layer does not imply reduction of the crack driving force in that case. This effect is stronger with growing coating thickness due to the larger area of the high stresses.

In the case of the diffusion layer of higher thickness in which yield strength is decreasing gradually in consecutive sublayers, increase of hardening effect results in higher crack driving force values (Fig. 13, models no. 1-3). The crack driving force drops significantly when the diffusion layer thickness is further increased (model no. 4) even though the maximum yield strength in the layer is the same as in the model no. 3. This behaviour can be related to the change of the distance between crack tip and substrate/diffusion layer interface. It limits the interaction of the stress field generated in the vicinity of the crack tip with the more ductile material of the substrate.

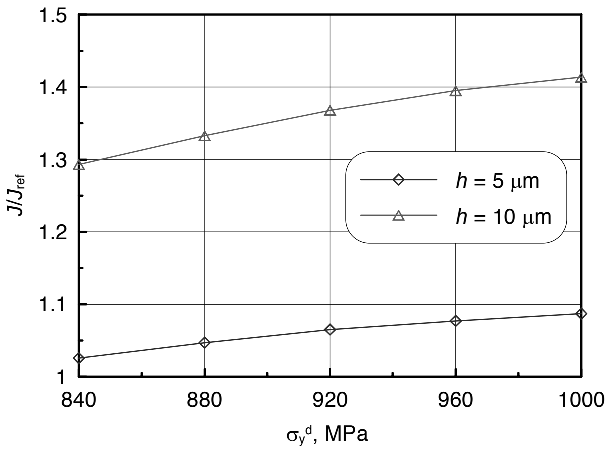

Fig. 12. The influence of the yield strength in thin diffusion layer, σ_y^d, on crack driving force for various coating thickness, *h*

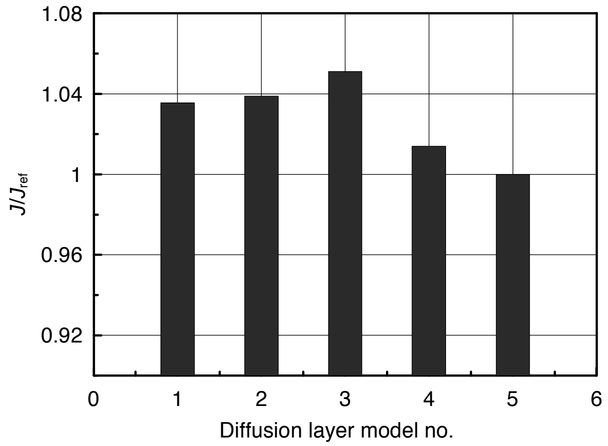

Fig. 13. The effect of yield strength distribution in diffusion layer on crack driving force; no. 5 – no diffusion layer

4. Conclusions

Two dimensional finite element analysis of the four point bending of surface hardened titanium alloy Ti-6Al-4V was carried out. Material system consisted of the stiff, elastic coating and diffusion hardened layer on top of the titanium alloy substrate. The presence of the crack penetrating the coating with its tip in the substrate was assumed. The effect of several parameters of the coating and the substrate on the crack driving force was determined in terms of *J* integral variation.

On the basis of the calculations results following conclusions can be drawn:

- Increase in the thickness and stiffness of the elastic coating leads to higher *J* integral values. The material system with lower ductility of the substrate is more sensitive to the increase in coating thickness. In turn when the coating thickness is larger its stiffness also have bigger impact on crack driving force.
- Increase in the yield strength of the substrate lowers crack driving force significantly. With growing coating thickness the response of the system is less sensitive to the changes in the substrate yield properties.
- The crack driving force decreases significantly with increasing residual compressive stress in the coating. Tensile residual stresses have the opposite effect. Thus compressive residual stresses in the coating can hinder the crack propagation in the substrate. This influence is more pronounced for the thicker coating.
- For the material with small depth of the diffusion layer crack, driving force increases with growing yield strength in that layer. This effect is further intensified by the increase of elastic coating thickness. Lowering of crack driving force for the same hardening level in the top sublayer can be obtained by increasing the diffusion layer thickness.
- Some extensions to the present model should be pursued in order to improve the accuracy of calculations. The important factor is the effect of the interactions between the short crack and microstructure of the material. Thus the strength properties of individual phases should be taken into account.

Acknowledgements

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