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THE EFFECT OF RESIDUAL STRESS ON THE LOAD BEARING CAPACITY OF PVD COATED SURFACES – PART 2

WPŁYW NAPRĘŻEŃ WŁASNYCH NA NOŚNOŚĆ POWIERZCHNI Z POWŁOKAMI PVD – CZĘŚĆ 2

Key words: PVD coatings, contact mechanics, residual stress, fracture toughness.

Abstract The article presents the results of modelling tests of the coating-substrate systems subjected to a contact load using a spherical diamond indenter with a 20 µm tip radius. Systems with 1 to 5 µm thick CrN coatings deposited on X5CrNi18-10 austenitic steel substrate were analysed. Systems without residual stress as well as with introduced 2 and 5 GPa compressive residual stresses were analysed. The article presents the effect of coating thickness on substrate deformations at load range up to 1 and 3 N. The evolution of maximum radial stress in the substrate and the range of substrate plastic deformation for the assumed coating thicknesses were also analysed. Modelling results showed a strong relation between maximum critical force and relative coating thickness. The maximum radial stresses in the substrate in a case of systems with a thin 1 µm coating are much smaller than for thicker 5 µm coating, referring to the relative coating thickness. However, the analysis of substrate yielding showed that, for thin 1 and 2 µm coatings, substrates deform plastically at 0.01 and 0.03 N, respectively, while the 5 µm coating prevent plastic deformations up to load 0.32N.

Słowa kluczowe: powłoki PVD, mechanika kontaktu, naprężenia własne, odporność na pękanie.

Streszczenie W artykule przedstawiono wyniki badań modelowania układów powłoka–podłoże poddanych obciążeniu działającego w styku skoncentrowanym przy użyciu diamentowego wgłębnika o promieniu zaokrąglenia 20 µm. Analizowano układy z powłokami CrN w zakresie od 1 do 5 µm nałożone na stal austenityczną X5CrNi18-10. Modelowano układy bez naprężeń własnych oraz układy z wprowadzonymi ściskającymi naprężeniami własnymi 2 i 5 GPa. W artykule przedstawiono ewolucje wpływu grubości powłok na deformacje podłoża w zakresie obciążenia do 1 i 3 N. Analizowano również przebieg maksymalnych naprężeń promieniowych w podłożu oraz zakres odkształceń plastycznych podłoża dla założonych grubości powłok i zakresu sił. Wyniki modelowania wykazały dużą zależność pomiędzy maksymalną siłą krytyczną, a względną grubością powłoki. Maksymalne naprężenia promieniowe w podłożu w układach z cienką powłoką 1 µm są znacznie mniejsze niż w przypadku układów z powłoką o grubości 5 µm, odnosząc wyniki do względnej grubości powłoki. Natomiast analiza odkształceń plastycznych podłoża badanych układów wykazała, że podłoże w układach z cienkimi powłokami 1 i 2 µm odkształcają się plastycznie już przy sile 0,01 i 0,03 N. Wzrost siły, przy której dochodzi do odkształceń plastycznych podłoża, widoczny jest w przypadku zmieniającej się grubości zastosowanej powłoki. I tak w przypadku układu z powłoką 5 µm pierwsze odkształcenia plastyczne zaczynają pojawiać się dopiero przy sile 0,32 N.

INTRODUCTION

The widespread use of coatings in almost all branches of industry, from tool to medical industry, prompted coating manufacturers to look for new materials to achieve their even greater hardness and wear resistance. Various properties, i.e. mechanical and tribological, are tested, which, in many applications, have a significant impact on the performance and durability of products. The interaction between the coating and the substrate

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is influenced by many factors, such as the coatings microstructure and parameters of the deposition process resulting residual stresses. These primarily affect wear processes of friction nodes in which coatings are applied to one or both surfaces. The choice of coating applied to the substrate, most often made of metal, should ensure small deformations of the whole system, which are determined by the properties of coating and substrate, contact geometry, residual stress, and load character. At small deformations, the risk of fracture and loss of adhesion of coating from the substrate is usually small. However, in practice, it is extremely difficult to predict critical loads due to the influence of many factors to which the coating-substrate system is subjected. In the XIX century, Hertz **[L. 1–4]** gave a method for calculating permissible loads and developed relationships for various geometries of contacting elements, but they are valid only for homogeneous materials. Unfortunately, Hertz's theory cannot be applied for coated systems. The existence of coating was taken into account by Liu **[L. 5, 6]** who extending Hertz's theory. Despite the introduction of additional assumptions, Liu did not take into account the residual stresses, the difference in the properties of the coating and the substrate leading to the sinking in or, in the case of thin, soft coatings, to the pile-up formation **[L. 7, 8]**. Hertz's theory and the extended theory by Liu are also limited to elastic deformations. They will not permit the plastic deformations of substrate with usually smaller Young's modulus and yield strength than the coating. Despite the works appearing in the literature **[L. 9]** that take into account the different properties of the coating and substrate and existing tangential forces, there are no further works that include residual stress and plastic deformation of the substrate. An effective tool that allows performing analyses related to contact mechanics is a finite element method (FEM). A numerical analyses makes it possible to model the coating-substrate system in which the spherical indenter is pressed, reflecting the experimental research technique which is indentation **[L. 1, 10–14]**. By combining experimental results with modelling results (FEM), it is possible to create failure maps of coating-substrate systems in t/R_i (coating thickness /indenter radius) and F/R^2 (critical force/indenter radius) coordinate system. The proposed coordinate system allows one to break free from coating thickness and contact geometry **[L. 15–18]**. So far, deformation maps have been created for the coating-substrate systems considering the place of contact of the coating with the indenter **[L. 1]**. For a complete analysis of the contact mechanics, coating and substrate interface is also important. Initially, under a small force at the interface, elastic deformations occur. When the sample contacts the indenter with a significantly larger tip radius than the coating thickness, the first permanent deformations appear in the substrate under the interface **(Fig. 1a)**. With increasing load, the plastic deformation zone increases **(Fig. 1b)**. A further process of load increase leads to the bending of the coating and the formation of tensile stresses on the surface of the coating just outside the contact area with indenter and in the axis of symmetry of the indenter at the coating-substrate interface **(Fig. 1c)**. By specifying the permissible loads, various forms of the wear of the coating-substrate system can be avoided by taking into account both stress concentration areas. Considering the intrinsic stresses arising during coating deposition, the question is whether, by calculating the permissible stresses, the intrinsic stresses can be deducted from the stresses derives from external loading. The solution to this problem is the main subject of this work.

RESEARCH METHODOLOGY

FEM numerical analysis was performed for all models using Ansys 14.5 software. Objects of modelling were coated systems: t = 1, 2, and 5μm coating thickness and bulk models (no coating) with the properties of the substrate and coating itself. The models were subjected to a simulation reflecting the indentation test, i.e.

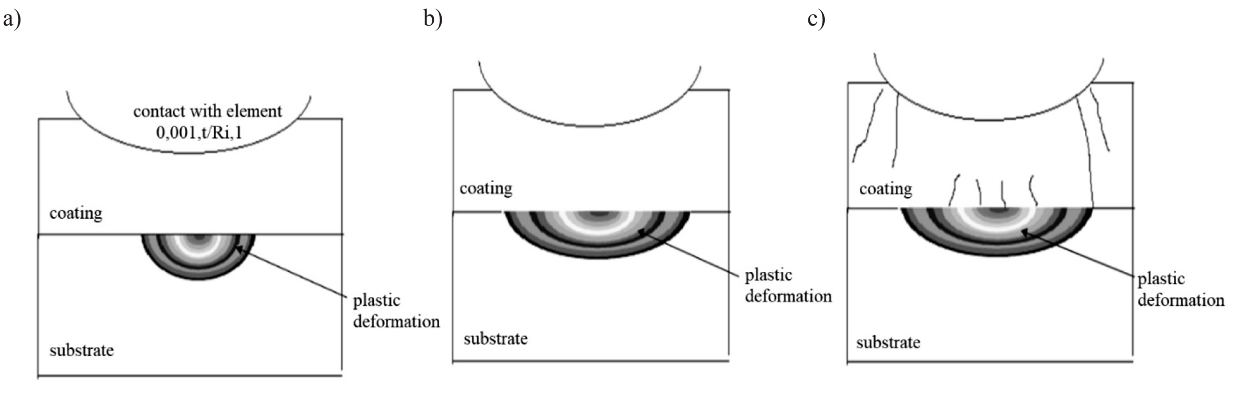

Fig. 1. Deformation of the coating-substrate systems at contact load during indentation [L. 17]
Rys. 1. Deformacja układów powłoka–podłoże przy obciążeniach działających w styku skoncentrowanym podszas indentacji **[L. 17]**

a diamond indenter with a rounding radius R = 20 μm was pressed with a normal force from 0 to 1N or 3 N, depending on the thickness of the coating. Simulations were carried out with constant successive steps of load 0.1 N. It was assumed that models with an infinitely thick coating and an infinitely thick substrate will be treated as models having the properties of homogeneous materials adopted for the coating and the substrate, respectively. It was assumed that the models are axially-symmetrical. The mesh of models was created by Plane182 quadrangle elements with 4 nodes located in the corners. The ability to move along the axis of symmetry along the X-Y plane was restricted. At the contact point of the indenter with the coating, the mesh was additionally compacted and the friction coefficient μ = 0.1 was assumed. This value of the friction coefficient corresponded to experimental results of scratch test at the same load range as given above. In simulations, the Bilinear Isotopic Hardening model, taking into account plastic deformations but without strengthening during plastic flow, for the substrate was adopted. However, in the case of the coating, it was assumed that material is perfectly elastic. Using the same assumptions in FEM, calculations were performed for models with residual stress **[L. 1]**. The results were considered when two values (2 and 5 GPa residual stress) were introduced for both compressive and tensile stresses. The material properties of coating and substrate, used in FEM analysis, are given in **Table 1**. The value of E = 1041 GPa and ϑ = 0.07 was adopted for the indenter.

Table 1. Material properties used in FEM models [L. 1]
Tabela 1. Parametry materiałowe powłoki i podłoża użyte do modelowania **[L. 1]**

	Young's modulus E [GPa]	Yield strength R_e [MPa]	Poisson ratio ϑ
Substrate	210	800	0.3
Coating	420	-	0.25

RESULTS AND ANALYSIS

Excessive deformation of the substrate in coated systems could lead to catastrophic forms of coating wear. To avoid typical forms of coating destructions, such as fracture, delamination, the permissible loads should be determined **[L. 18, 19]**. **Figure 2** shows the results of the radial stress distribution, which are the most important because they lead to the formation of typical cracks formation around the ball-coating contact, i.e. to circumferential cracks in the shape of circles around the imprint. Stress analysis was performed at 0.2 N and 1 N loads for systems with 1 to 5 μm thick coatings. Two models reflecting homogeneous material were also added, i.e. one with the properties of the substrate itself, the other with the properties of the coating. The graph indicates that, as the system stiffness increases, the contact area is getting smaller. That is, the intersection of the curves with the x-axis in the coating-substrate systems approaches the contact axis as the coating thickness increases **(Fig. 2a)**. This means that, for

a) b)

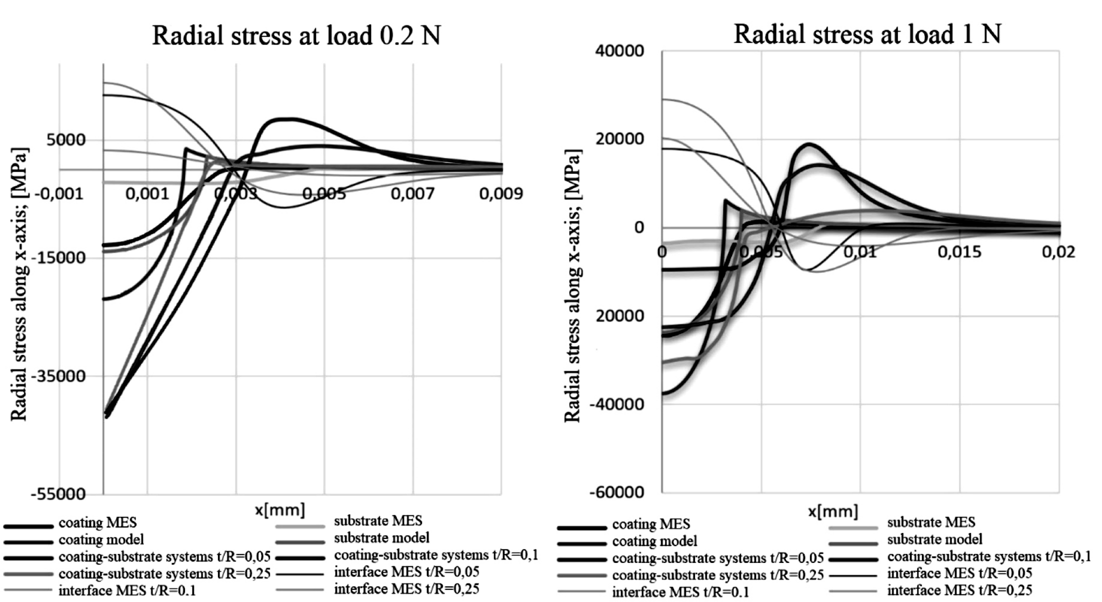

Fig. 2. Distribution of radial stress on the surface of the coating and at the interface for systems with 1, 2, and 5 μm coatings at loads: a) 0.2 N, b) 1 N
Rys. 2. Rozkład naprężeń promieniowych na powierzchni powłoki i na granicy połączenia powłoki z podłożem dla układów z powłoką 1,2 i 5 μm a) dla siły 0,2 N, b) dla siły 1 N

rigid coatings, these contact stresses can be very high, because it deforms very little even at a maximum load of 1N **(Fig. 2b)**. However, the most interesting are tensile stresses outside the contact zone, because they lead to the cracking of thin coatings. It was noticed that, as the thickness of the coating decreases, the contact diameter increases, but stress outside the contact zone increases. However, such analyses cannot be limited to stresses that are only on the surface of the coating. Mainly in the case of thicker coatings, the interface of the coating and the substrate is important. In this area, radial stresses can reach high tensile values. On the surface, the highest stresses are just beyond the contact zone, while, at the interface, these maxima are in the contact axis at both the minimum and maximum loads. The highest stresses at the interface for thin coatings (1 and 2 µm thick, under 0.2 N load) are 15 and 12 GPa, respectively **(Fig. 2a)**. However, in the case of the thickest coating (5 µm), it can be seen that, at 0.2 N load, the tensile stress is much smaller, only 4 GPa **(Fig. 2a)**. Increasing the load to 1 N, it can be seen that the compressive stresses on the surface (in the axis of symmetry) corresponds to high tensile stresses at the interface on the other side of coating, which indicates a state similar to pure bending **(Fig. 2b)**. The value of tensile stress (19 and 21 GPa at 1 N load) for a system with a 5 µm coating is similar to that of a thin 1µm coating. The same maximum values, but as a function of a normal force range up to 1 N and 3 N, are shown in **Fig. 3**. It was observed that, for the 5 µm coating and for an infinitely thick coating, these maxima are very similar, i.e. the substrate has almost no effect on deformations in this load range. However, for 1 and 2 µm coatings, these stresses increase very quickly on the surface and at interface, achieving very high values 18 GPa on surface and 29 GPa at interface for 1 µm thick coatings. Of course, there are no materials

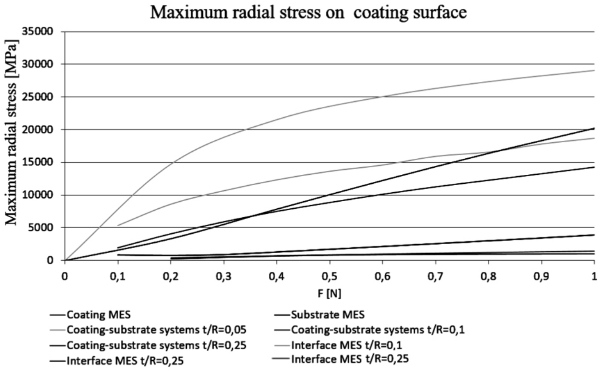

Fig. 3. Maximum radial stress on the coating surface as a function normal force F [N] for systems with 1, 2, and 5 µm coatings

Rys. 3. Maksymalne naprężenia promieniowe na powierzchni powłoki w funkcji siły F[N] dla układów z powłoką 1,2 i 5 µm

that can transfer such stress values obtained as a result of modelling without destroying it. This is confirmed by the results of experimental studies, which are not presented in this paper, where there was always a net of many cracks visible on the surface of the coating a range of loads up to 3 N.

An additional problem in analysis, which is very rarely considered in the literature, is the occurrence of residual stress, which can reach values up to several GPa and which are inevitable in coating depositions by PVD and CVD methods. Compressive stresses are desirable, but in concentrated contact, at higher external loads, they change to tensile causing cracking of brittle coatings. The values of the maximum radial stress at loads of 0.2 N and 1 N at the interface for 1 and 5 µm coating with the introduced residual stresses are shown in **Fig. 4**. The maximum tensile stresses at

a) b)

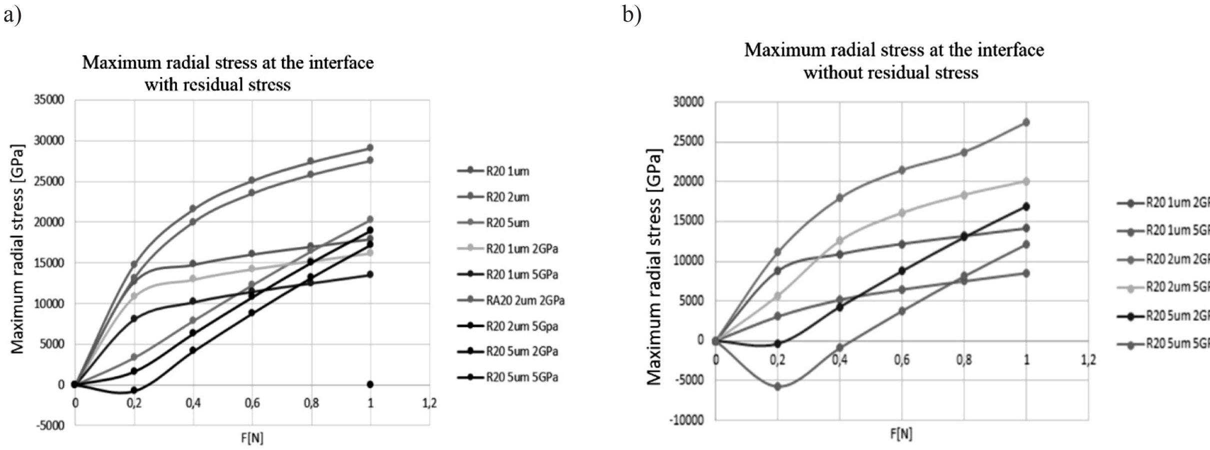

Fig. 4. Maximum radial stress at the interface as a function of force F [N]: a) without residual stress and with residual stress 2 and 5 GPa, b) analogously after subtraction of residual stress

Rys. 4. Maksymalne naprężenia promieniowe na granicy połączenia powłoki z podłożem w funkcji siły F[N]: a) bez naprężeń własnych i z wprowadzonymi naprężeniami własnymi 2 i 5 GPa, b) analogicznie po odjęciu naprężeń własnych interface for the 5µm coating system are reduced by introduced compressive residual stresses from 21 GPa to 16 GPa. A similar phenomenon was observed in the case of other coatings. However, as the load increases, the value of the maximum radial stress increases only in the case of the thickest coating **(Fig. 4a)**. Subtracting from the total maximum radial the residual stress, the value of maximum stress is on a very similar level **(Fig. 4b)**.

Figure 5 shows the maximum stress as a function of h/t (maximum penetration depth of indenter is to coating thickness) for systems with 1 and 5 µm coatings. Thanks to this combination, it is easier to compare contact mechanics, because it breaks free from coating thickness and analysing only coatings bending in relation to its thickness. For both coatings, with rising penetration depth, the maximum radial stress at the interface also increases **(Fig. 5)**. The smaller the value of introduced compressive residual stresses, the greater is the value of the maximum radial stresses at the same penetration depth at the interface.

The average contact pressure p_m in the contact zone resulting from external loads of the system can be referred to stresses at every place in the coating, obtaining the values of the stress concentration coefficient. The values of this coefficient σ_{max}/p_m for coatings with a 1 and 5µm thickness are shown in **Fig. 6**. At the interface, an continuous increase in stress concentration is visible as the deformation increases, and the σ_{max}/p_m ratio increases from 0.1 to 2.5 for a relative penetration depth of h_{max}/t = 1.7 of the 1µm coating. For a 5 µm thick coating, the concentration coefficient in the substrate is two times smaller, and their maximum value reaches 0.9, but at lower penetration depth h_{max}/t = 0,17. Substrate plastic deformations lead to an increase of coating deformation and an increase of tensile stress at the interface, **Fig. 6b**. After subtraction **(Figs. 6c–d)**, it turns out that, for a thin 1µm coating, the relative radial stress at the interface is constant above the relative depth of 0.5 **(Fig. 6c)**. However, the differences are visible for thicker 5 µm coatings. But, with the increase of the value of residual stresses up to 5 GPa, this difference increases to σmax/pm = 0.7 **(Fig. 6d)**. This difference is probably the result of a smaller zone of plastic deformation of the substrate and therefore a smaller bending of the coating.

The impact of increasing external loads not only causes elastic deformations of the coating and substrate, but the formation of plastic deformations in the substrate was also observed. Images of the plastic deformations of the substrate for systems with 1, 2, and 5 µm coatings are shown in **Figs. 7a–c**. It can be clearly seen that, for a thin 1µm coating, the range of these plastic deformations is large. Plastic deformations arise in the substrate at a certain depth. The depth of maximum plastic deformations moves away from the interface with increasing load **(Fig. 8a)**. The thicker the coating, the smaller are the plastic deformations, but they are very dangerous because the yielding begins just below the coating **(Figs. 8b, c)**. The coating could lose contact and the ability to transfer loads to the substrate. In this case, the load increase may result in coating delamination **(Fig. 8c)**.

a) b)

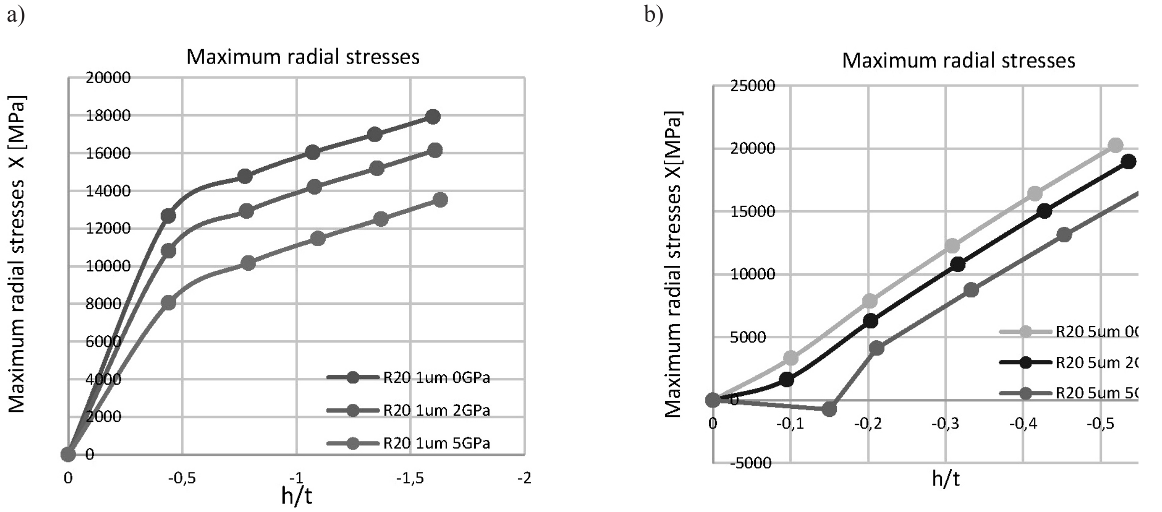

Fig. 5. Maximum radial stresses at the interface between the coating and the substrate as a function of h / t
Rys. 5. Maksymalne naprężenia promieniowe na granicy połączenia powłoki z podłożem w funkcji h/t

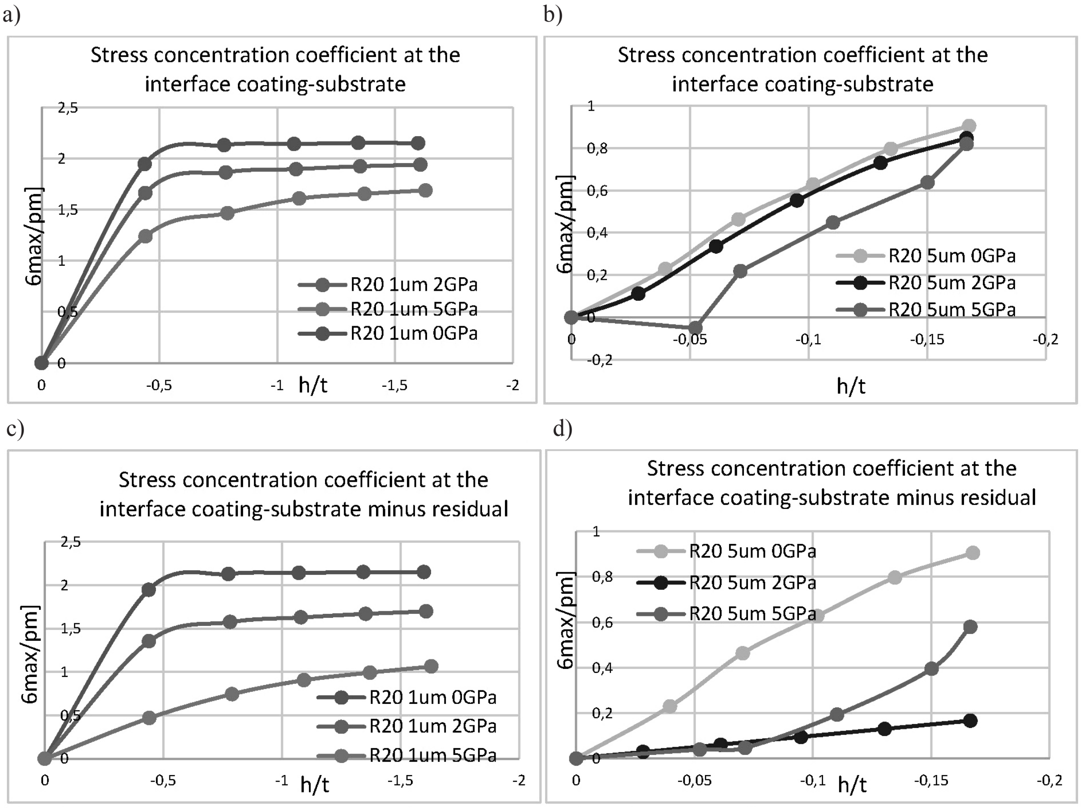

Fig. 6. Stress concentration coefficient as a function of relative penetration depth with residual stresses at 1 N load for coatings: a) 1 µm, b) 5 µm, and without residual stress for coatings, c) 1 µm, d) 5 µm,

Rys. 6. Współczynnik koncentracji w funkcji wględnej głębokości penetracji z wprowadzonymi naprężeniami własnymi dla powłok o grubości a) 1 µm, b) 5 µm, c) 1 µm minus residual, d) 5 µm minus residual przy obciążeniu 1 N

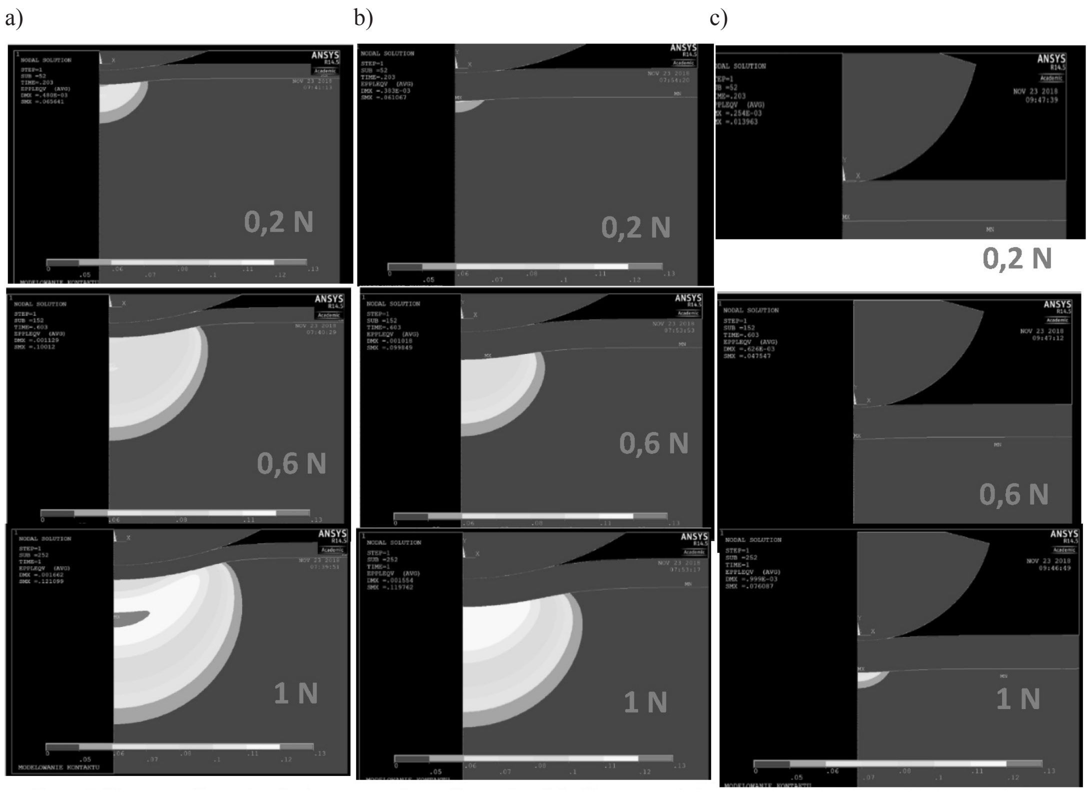

Fig. 7. Images of plastic deformation of the substrate for systems with a coating thickness: a) 1 µm, b) 2 µm, and c) 5 µm

Rys. 7. Obrazy odkształceń plastycznych podłoża dla układów z powłoką o grubości a) 1 µm, b) 2 µm i c) 5 µm

4. CONCLUSIONS

Modelling using finite element method (FEM) of the indentation test allowed us to assess the effect of coating thickness on stress distribution and deformation at the interface between coating and substrate. Results showed a significant relationship between the maximum radial stress in the substrate and the relative thickness of the coating. The maximum radial stress in the substrate in relation to the relative coating thickness in systems with a thin 1 µm coating is two times higher than in systems with the thickest 5 µm coating. The increase in load at which initial plastic deformation of the substrate occurs is visible when the thickness of the applied coating changes. In the case of a system with a 5 µm coating thickness, the yielding of the substrate appears at 0.32N normal force. It is clear that thicker coatings protect the formation of plastic deformations in the substrate at low loads. However, it should be remembered that, often at the coating-substrate interface, coating cracks and delaminations could happen for very thick coatings.

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