Vereschaka, AA, Grigoriev, SN, Sitnikov, NN and Batako, ADL

 Delamination and longitudinal cracking in multi-layered composite nanostructured coatings and their influence on cutting tool life

http://researchonline.ljmu.ac.uk/id/eprint/7975/

Article

Delamination and longitudinal cracking in multi-layered composite nano-structured coatings and their influence on cutting tool life

A.A. Vereschaka[1], S.N. Grigoriev[1], N.N. Sitnikov[2,3] and Andre Batako[4]

[1]Moscow State Technological University STANKIN, Vadkovsky per. 1, Moscow, 127994, Russia

[2]Federal State Unitary Enterprise "Keldysh Research Center", Onezhskaya St. 8, Moscow 125438, Russia

[3]National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe shosse 31, Moscow 115409, Russia

[4]Liverpool John Moores University (LJMU), Byrom Street, Liverpool, L3 3AF, UK

Abstract. This paper presents the results of a study of the mechanisms of delamination and the formation of longitudinal cracks in the structure of multi-layered nano-structured coatings to predict the mechanisms for further improvement of tool life and the reliability of metal-cutting tools. Various mechanisms of formation of longitudinal cracks and delaminations in coatings on rake and flank tool surfaces, which vary based on the compositions and architectures of the coatings, are addressed. In addition, the influence of internal defects, including embedded microdrops and pores, on the formation of cracks and delaminations and the failure of coatings is discussed. The importance of ensuring a balance of the basic properties of coatings to achieve high wear resistance and maximum tool life of coated metal cutting tools is shown. The properties of coatings and the natures of their failures, as investigated during scratch testing and dry turning of steel C45, are provided.

Highlights

- Differences in the mechanism of formation of delaminations and longitudinal cracks depending on the elemental composition and architecture of multi-layered nano-structured coatings.
- Specifics for formation of cracks and delaminations on rake and flank surfaces of the cutting tool.
- A balanced combination of hardness and ductility as an important condition for good performance of coatings.
- Influence of coating defects on cracking and failure.

Keywords: wear-resistant coatings; wear; crack; fracture; tool life; PVD coatings; delamination; nanoscale structures

Nomenclature

NMCC - nano-scale multi-layered composite coatings
FCVAD - filtered cathodic vacuum arc deposition
FEM - finite element method
VCCT - virtual crack closure technique
SERR – strain energy release rate

σ_{ld} - concentration of local tensile stresses in the head of a number of edge dislocations

τ – edge stresses

2d –length of slip band or distance between slip bands

x –distance of the band to the head of dislocation cluster

τ_i –stress of resistance to movement of dislocations (friction stress)

σ_{theor} –theoretical strength of crystalline body

a_0 –equilibrium distance between atoms

E –modulus of elasticity

γ – plastic shear deformation

b – Burgers vector

B_d - delamination length (mm)

N - number of cycles

C - Paris coefficient for delamination growth

n_p - Paris exponent for delamination growth

G- strain energy release rate (N/mm)

G_{max}- strain energy release rate at maximum fatigue load (N/mm)

F_{Av} - avulsion force

F_P - thrust force

F_C - cutting force

F_Z - resultant force

1. Introduction

1.1. Background

Further increases in efficiency of machining and cutting speeds as well as tightening of reliability requirements associated with greater levels of automation of production result in the need to create new tool materials with enhanced performance characteristics.

One way to improve the performance characteristics of tool materials is to enhance their surface properties by applying modified coatings [1]. In turn, the properties of modified coatings continue to be improved, and their architecture and elemental composition become more complicated. In particular, multi-layered composite coatings, nano-structured and gradient coatings, and coatings with multi-component elemental composition have been used extensively in recent years [2-8].

The use of a multi-layered architecture of coatings and the use of nano-structured technology can significantly improve the performance characteristics of a new generation of coatings. However, along with the use of such coatings comes new problems that did not occur with monolithic coatings of the first generation. In particular, problems arose concerning interlayer delamination and formation of specific longitudinal cracks in the structure of coating.

A large number of studies examining problems of cracking have been conducted. The general assumption is that the formation of microcracks is associated with the displacement of dislocations [9-12]. A number of mechanisms for the formation of dislocation microcracks are well known [9,10,12]. In principle, those mechanisms provide for blocking of the progress of dislocation by some obstacle (for example, a grain boundary, a boundary of nano-layers, or inclusion). If in some slip plane, dislocations stop before a sufficiently powerful obstacle, then a

cluster of dislocations is formed, and it causes a high concentration of stresses at the obstacle. This concentration of stresses results in formation of a dislocation microcrack.

It should be noted that the problems of crack formation and delamination in the structures of multi-layered coatings have not been studied as thoroughly as have other aspects of operation and wear of such coatings. Section 1.2 highlights some of the research that has been conducted regarding crack formation and delamination of coatings.

1.2. Literature review

V.P. Tabakov et al. [13,14] considered mechanisms of cracking with respect to single-layer macro-scale coatings on the basis of systems composed of TiN, TiCN, (Ti,Zr)N, and (Ti,Zr)CN. They discovered that coatings of a complex composition of (Ti,Zr)N and (Ti,Zr)CN are characterized by better resistance to intensive cracking. V.P. Tabakov et al. also considered multi-layered coatings with macro-scale structure: in particular, on the basis of systems composed of TiCN-(Ti,Zr)N-TiN, TiN-(Ti,Zr)N-TiN, TiCN-(Ti,Al)N-TiN, and TiCN-(Ti,Mo)N-TiN [15]. These studies proved that the introduction of zirconium nitride in the coating composition significantly reduces the tendency to cracking.

The problems of cracking and brittle fracture of coatings consisting of Ti-TiN-(Ti,Cr,Al)N, Zr-(Zr,Cr)N-CrN, and Ti-TiN-(Ti,Cr,Al)N; and Ti-(Al,Cr)N-(Ti,Al)N, Ti-(Al,Cr)N-(Ti,Cr,Al)N, and Zr-(Al,Cr)N-(Zr,Cr,Al)N also were addressed in papers [16-22]. A detailed review of existing papers in the field of crack formation in multi-layered coatings, with classification of types of cracks and analysis of the mechanisms of their formation, is given in [23].

The topic of mathematical modeling of cracking in multi-layered coatings with the use of an axis-symmetrical finite element method (FEM) model was considered by G. Skordaris et al. [24]. Xiang-FaWu et al. [25,26] modeled cracking in single-layer coatings within the framework of linear elastic fracture mechanics (LEFM). R. M'Saoubi et al. [27] investigated the nature of wear, including brittle fracture and cracking of physical vapor deposition (PVD)-coated (TiN, (Ti,Si)N, (Ti,Al)N, and (Al,Cr)N) polycrystalline cubic boron nitride. S. Koseki et al. [28] examined the cutting performance of TiN-coated cutting tools. Defects (e.g., droplets, voids) in the coating were found to be the starting point of damage. The breakdown region is enlarged as the work material is caught in the damaged portion of the coating.

S. Kumar et al. [29] considered the probable mechanisms of development and inhibition of cracks in microstructures: particularly at crack bridging by ductile ligaments, crack deflection by second-phase particles, microcrack formation, and stress-induced phase transformations. The same paper also includes an overview of methods for modeling the development of cracks using FEM and incorporating cohesive elements at the continuum level, as well as discrete dislocation methodology at the mesoscopic level, and coupled atomistic/continuum methods that transition atomic level information to the microscopic level.

A large number of studies have been devoted to the investigation of causes and conditions for the formation of delaminations in multi-layered composite macrostructures. To predict the occurrence of delaminations, the methods of layer wise-interface elements [30], classical finite element analysis (FEA) [31, 32], and the virtual crack closure technique (VCCT) [33] are widely used.

2. Materials and Methods

2.1. Deposition method

For deposition of nano-scale multi-layered composite coatings (NMCC), a vacuum-arc VIT-2 unit [2], which was designed for the synthesis of coatings on substrates of various tool materials, was used. The unit was equipped with an arc evaporator with filtration of vapor-ion flow. In this

study, the process, termed filtered cathodic vacuum arc deposition (FCVAD) [16-22], was used for deposition of coatings on the tools to significantly reduce the formation of the droplet phase during formation of the coating. The use of the FCVAD process does not cause structural changes in carbide and provides the following:

• High adhesive strength of the coating in relation to the carbide substrate
• Control of the level of the "healing" of energy impact on surface defects in carbide in the form of microcracks and micropores and formation of favorable residual compressive stresses in the surface layers of the carbide material
• Formation of the nano-scale structure of the deposited coating layers (grain size, sublayer thickness) with high density due to the energy supplied to the deposited condensate and transformation of the kinetic energy of the bombarding ions into thermal energy in local surface volumes of carbide material at an extremely high rate of approximately 10^{14} Ks^{-1}

When choosing the composition of NMCC layers, in forming the coating of the three-layered architecture [2,16], the Hume-Rothery rule was used. This rule states that the difference in atomic dimensions in contacting compounds should not exceed 20% [34].The parameters used at each stage of the deposition process of NMCC are shown in Table 1.

Table 1. Parameters of stages of the technological process of deposition of NMCC.

Process	p_N (Pa)	U (V)	I_{Al} (A)	I_{ZrNb} (A)	I_{Ti}(A)	I_{Cr},(A)
Pumping and heating of vacuum chamber	0.06	+20	120	80	65	75
Heating and cleaning of products with gaseous plasma	2.0	100DC/ 900 AC f = 10 kHz, 2:1	80	-	-	-
Deposition of coating	0.36	-800 DC	160	75	55	70
Cooling of products	0.06	-	-	-	-	-

Note: I_{Ti}=current of titanium cathode, I_{Al}=current of aluminum cathode, I_{ZrNb}=current of zirconium-niobium cathode, I_{Cr}-current of chromium cathode, p_N=gas pressure in chamber, U=voltage on substrate.

An uncoated carbide tool and a carbide tool with "reference" coating TiN, deposited via standard vacuum-arc technology of arc-PVD, were used as objects for comparative studies of tool life.

2.2. Microstructural studies

For microstructural studies of samples of carbide with coatings, a raster electron microscope FEI Quanta 600 FEG was used. The studies of chemical composition were conducted using the same raster electron microscope. To perform X-ray microanalysis, characteristic X-ray emissions resulting from electron bombardment of a sample were examined.

The hardness (HV) of coatings was determined by measuring the indentation at low loads according to the method of Oliver and Pharr [35], which was conducted on a micro-indentometer micro-hardness tester (CSM Instruments) at a fixed load of 300 mN. The penetration depth of the indenter was monitored so that it did not exceed 10 – 20% of the coating thickness to limit the influence of the substrate.

The adhesion characteristics were studied on a Nanovea scratch-tester, which represents a diamond cone with apex angle of 120° and radius of top curvature of 100 µm. The tests were conducted with the load linearly increasing from 0.05 N to 40 N. Crack length was 5 mm. Each

sample was subjected to three trials. The obtained curves were used to determine two parameters: the first critical load, L_{C1}, at which the first cracks appeared in the coating, and the second critical load, L_{C2}, which caused the total failure of the coating.

2.3. Study of cutting properties

A study of the cutting properties of the tool made of carbide with developed NMCC was conducted using a lathe CU 500 MRD for longitudinal turning of steel C45 (HB 200). In the experiment, the cutters featured mechanical fastening of inserts made of carbide (WC+15%TiC+6% Co) with square shapes (SNUN ISO 1832:2012) and with the following figures for the geometric parameters of the cutting part: $\gamma = -8°$; $\alpha = 6°$; $K = 45°$; $\lambda = 0$; and $R = 0.8$ mm. The study was performed for the following cutting modes: f = 0.2 mm/rev; $a_p = 1.0$ mm; and $v_c = 250$ mmin^{-1}.

Flank wear-land values (VB_c) were measured with a toolmaker's microscope MBS-10 as the arithmetic mean of four to five tests. A value of $VB_c = 0.4$ mm was taken as failure criterion. The study included statistical processing of tests of wear of cutting tools, sample mean value of wear, and sample mean square deviation of tool wear, which are random variables with different values in repeated experiments. Of note, during the experiments, outlying results were excluded. To exclude outlying results of the experiments, the Irwin's criterion was used. To do that, the value of the Irwin's criterion K_λ was defined, if the outlying result was the maximum value VB_{max}:

$$K_\lambda = (VB_c - VB_{max})/K_\sigma$$

and if the doubts were provoked by the wear value with minimum value VB_{min}:

$$K_\lambda = (VB_c - VB_{min})/K_\sigma$$

The calculated value K_λ was compared to the critical value $K_{\lambda A}$, defined theoretically for a given level of significance level A and selection criterion n. If $K_\lambda < K_{\lambda A}$, then deviation of questionable value VB_c was considered as valid.
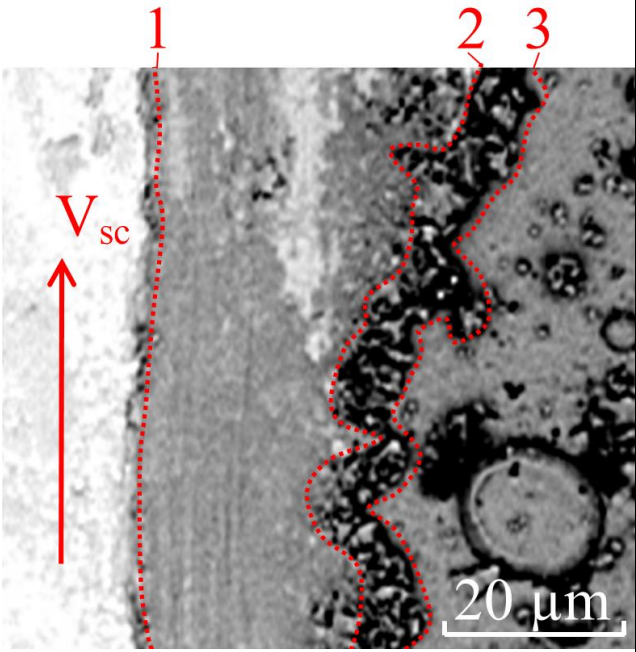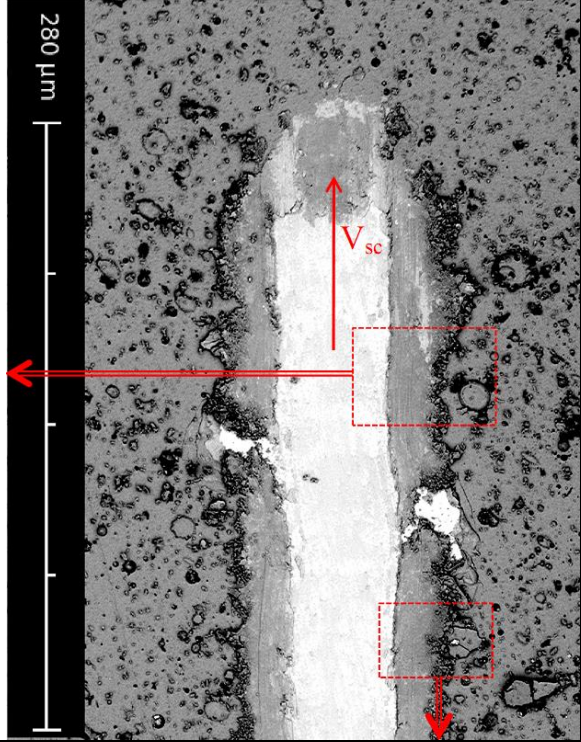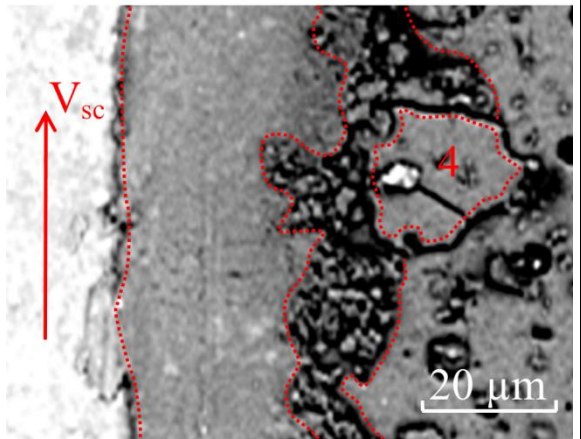
3. Results and discussion

3.1. Adhesion characteristics

The classical test that enables determination of the strength of the adhesive bond of a coating with a substrate by the scratch-test method also can be used for qualitative evaluation of the strength of the adhesive bond between individual coating layers and cohesive bond between nano-sublayers. The tests were conducted on a Nanovea scratch-tester. The indenter was a diamond cone with an apex angle of 120° and radius of top curvature of 100 µm. The tests were performed with a load linearly increasing from 0.05 N to the final load (40 N). Crack length was 5 mm. Each sample was subjected to 3 trials. The obtained curves were used to determine two parameters: the first critical load L_{C1}, at which first cracks appeared in NMCC, and the second critical load L_{C2}, which caused the total failure of NMCC.

Typical types of failure are presented in Fig. 1 (standard coating TiN), Fig. 2. (NMCC Zr-ZrN–(Nb,Zr,Ti,Al)N), and Fig. 3 (NMCC Ti-TiN-(Ti,Al)N). All investigated coatings showed a sufficiently high level of adhesion bonds with substrate. Numerous research efforts and the experience of the authors of this paper show that a scratch-test does not have a unique correlation with the tool life of a coated tool [1]; the test allows only "rejecting" coatings with insufficient strength of adhesion bonds. However, this test enables a study of the nature of the coating failure, particularly from the point of view of delaminations that occur in its structure. Let us consider the nature of the failure of the single-layer monolithic TiN coating (Fig. 1). A fairly smooth scribing groove is clear, with a clearly visible area of brittle fracture of the outer area of the coating. On the edges of the groove, cracks and splintered areas of the coating are visible. Patterns of failure of NMCC Zr-ZrN–(Nb,Zr,Ti,Al)N (Fig. 2) and (NMCC Ti-TiN-(Ti,Al)N)

(Fig. 3) are characterized by a number of significant differences. The failures of those coatings occur under the mechanism of "wedging spallation". Meanwhile, NMCC Zr-ZrN-(Nb,Zr,Ti,Al)N shows extensive interlayer delaminations, whereas in NMCC Ti-TiN-(Ti,Al)N, similar delaminations are less pronounced, and delaminations between nano-sublayers also occur. Generally, this picture correlates with the nature of the failure of those coatings observed during cutting tests.

A boundary of a scribing "groove" in monolayer monolithic coating TiN.

A general view of an end of a scribing groove in monolayer monolithic coating TiN.

Figure 1. The nature of failure of coating TiN along a longitudinal crack, caused by a diamond indenter at critical (breaking) load. V_{sc}- scribing direction. 1 – "substrate-coating" boundary, 2 – boundary of the brittle fracture zone of the coating, 3 – boundary of the scribing groove, 4 – splintered section of the coating.

A boundary of a scribing "groove" in monolayer monolithic coating TiN. Separation of a fragment of coating.
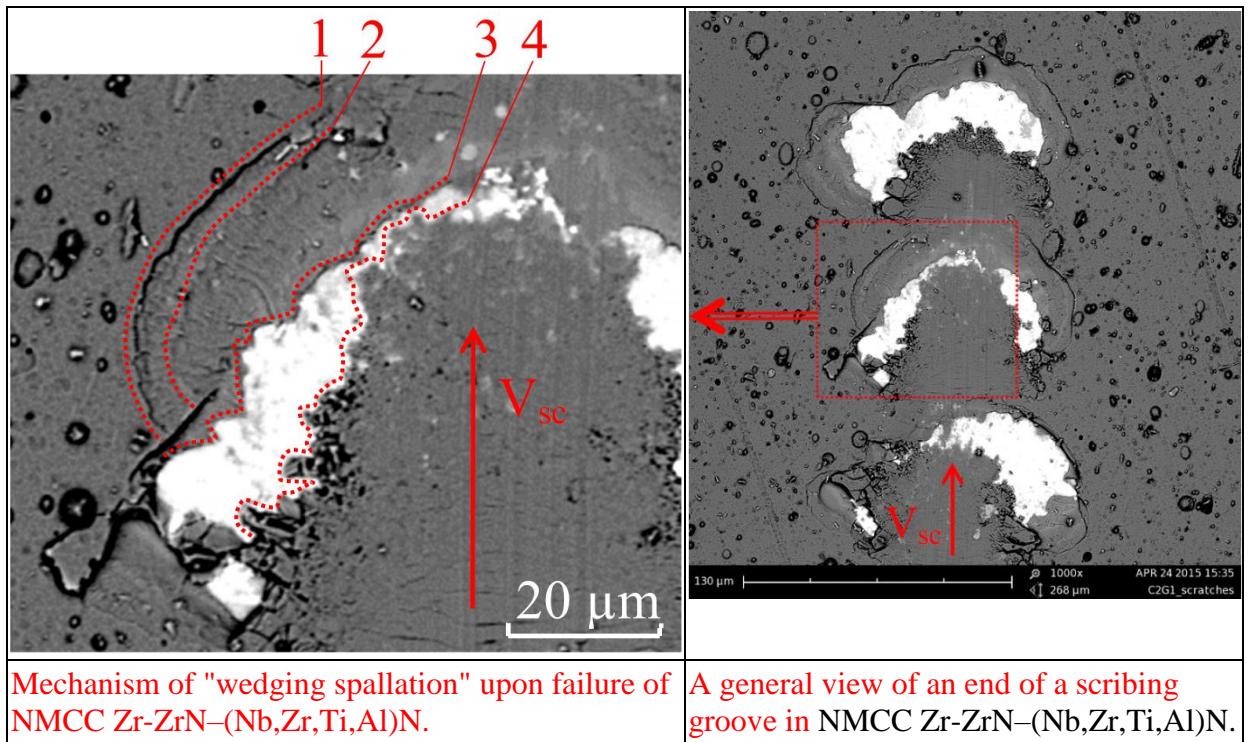
Mechanism of "wedging spallation" upon failure of NMCC Zr-ZrN–(Nb,Zr,Ti,Al)N.

A general view of an end of a scribing groove in NMCC Zr-ZrN–(Nb,Zr,Ti,Al)N.

Figure 2. The nature of failure of NMCC Zr-ZrN–(Nb,Zr,Ti,Al)N (coating thickness 5 µm) along a longitudinal crack, caused by a diamond indenter at critical (breaking) load. V_{sc}- scribing direction. 1 – the boundary of the wedging spallation zone, 2 – the delamination boundary between the intermediate and wear-resistant layer, 3 – the boundary of "adhesion coating layer-substrate" delamination, 4 – the boundary of the coating zone, pressed by the tip of the scratch tester.

Figure 3. The nature of failure of NMCC Ti-TiN-(Ti,Al)N (coating thickness 5 µm) along a longitudinal crack, caused by a diamond indenter at critical (breaking) load. V_{sc}- scribing direction.
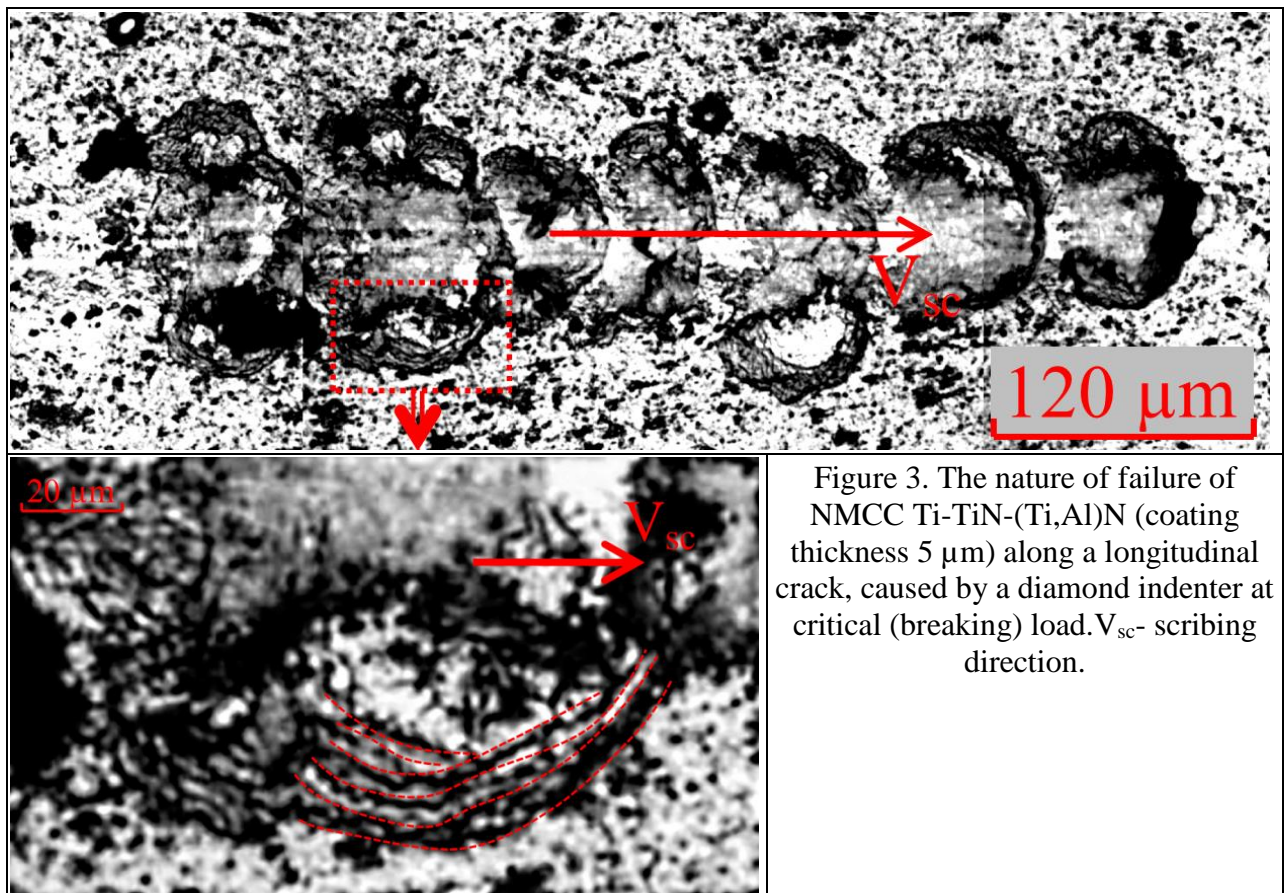
The study of the scribing process for nano-structured coatings of large thickness (exceeding 10 µm) is of particular interest. In this case, it is possible to observe both coating failure caused by violation of adhesion bonds between layers and cohesive bonds between nano-sublayers and failure of a coating as a whole, when failure is not accompanied by delamination. Signs of failure of coating Ti-TiN-(Ti,Al)N (with coating thickness 13 µm) at scribing is shown in Fig. 4 and 5.
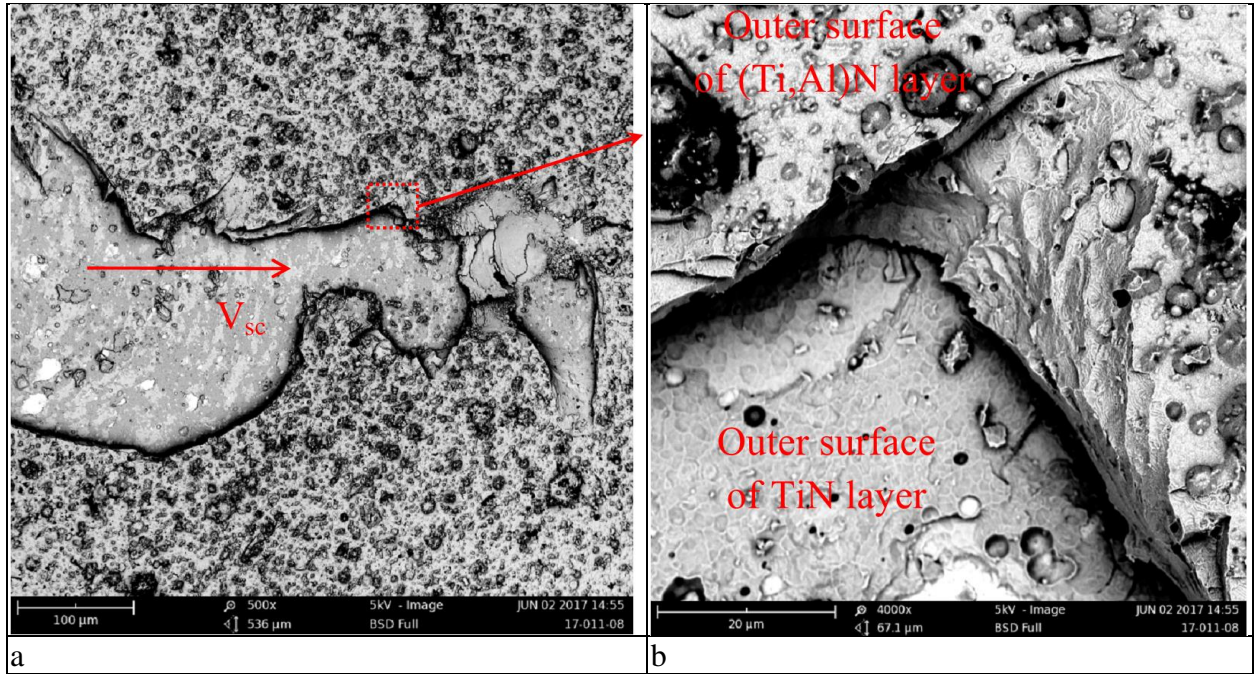

Figure 4. The nature of failure of NMCC Ti-TiN-(Ti,Al)N (coating thickness 13 µm) along a longitudinal crack, caused by a diamond indenter at critical (breaking) load.

In particular, Fig. 4 (b) shows both violation of the interlayer interface between layers TiN and (Ti,Al)N and persistence of strong adhesion bonds between nano-sublayers of layer (Ti,Al)N. At zoom-in, it is possible to notice in Fig. 5 that in some cases, at critical loads, there is also failure of cohesive bonds between nano-sublayers, and that fact results in formation of a kind of "terraces", i.e., flat microsites with surface structure of a nano-sublayer. It is also possible to see signs of a tear-out of microdroplets embedded in the coating structure. Fig. 5 (b) shows the "terrace-like" structure of failure zone of a nano-structured coating. A general structure of the coating under the study and the nature of cracking in it during the cutting tests are shown below, in Fig. 21 and 22.
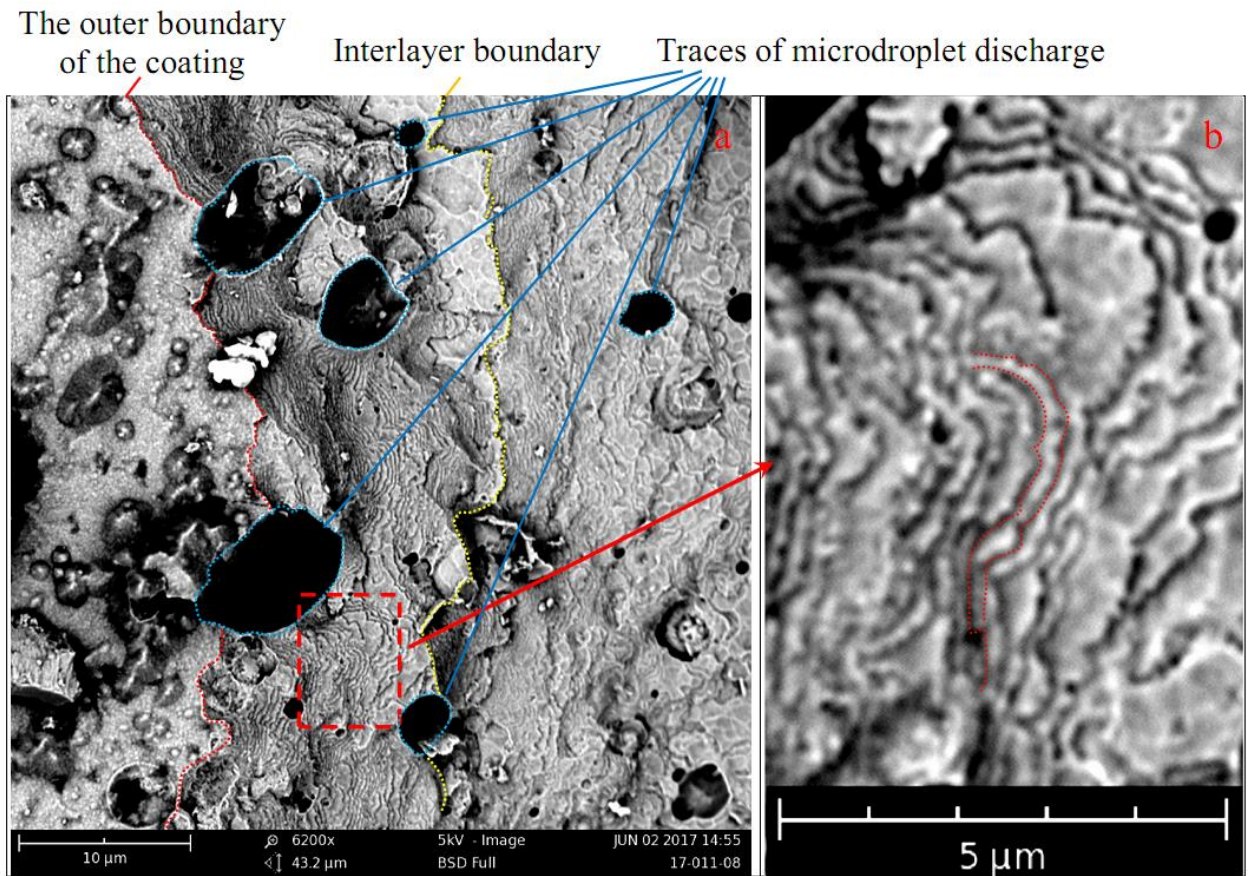
Figure 5. The nature of failure of NMCC Ti-TiN-(Ti,Al)N (coating thickness 13 µm) along a longitudinal crack, caused by a diamond indenter at critical (breaking) load.

3.2. Determination of basic properties of NMCC under cutting tests

This study was focused on the NMCC containing nitrides of Ti, Al, Cr, Zr, and Nb in its composition. For the detailed studies of various properties, NMCC were selected based on the following conditions:
- If earlier studies show significant increase in cutting properties and reliability of the tool [10-16]
- If the thermodynamic criterion $\Delta_r G$ (Gibbs free energy change per mole of reaction) favored the formation of the NMCC

To accomplish the research tasks, NMCC of various compositions were selected to meet the above conditions and were deposited using the FCVAD technology. The thicknesses of the coatings used in the studies were 2.4–13.0 μm. A wide range of thicknesses were selected on the basis of previous studies (in particular, [16-22]), indicating the improvement in cutting performance with increase in coating thickness. The basic properties of the NMCC under study are presented in Table 2.
Table 2. The basic properties of NMCC and periods of tool life of the carbide tools under study with the NMCC under study.

#	Composition of NMCC	Tool life T_c (min) VB=0,4 mm	Sublayer thickness (nm)	Total thickness (µm)	Adhesion, L_{C2}, N	Hardness, HV GPa
1	Uncoated	8	-	-	-	18
2	TiN	18	-	2.8	31	30
3	Zr-ZrN-(Nb,Zr,Ti,Al)N	31	45–60	3.3	>40	34
4	Zr-ZrN-(Zr,Cr,Al)N	37	15–45	2.4	39	36

5	Ti-TiN-(Ti,Al)N (5 μm)	30	65–90	5.0	>40	38
6	Ti-TiN-(Ti,Al)N (13 μm)	26	50-75	13.0	>40	38
7	(Zr,Nb)N-(Zr,Al,Nb)N	34	80-110	4.0	>40	36

The NMCC Ti-TiN-(Ti,Al)N shows better resistance for approximately 19 minutes of operation due to its high surface hardness; however, subsequently, the tool with such a coating begins to experience intensive wear. This fact can be related to the start of intense cracking and wear of this coating. As a result, the tool with NMCC Zr-ZrN-(Zr,Cr,Al)N showed better resistance, and it was characterized by a balanced combination of sufficiently high hardness and resistance to brittle fracture. Let us consider in detail the mechanism of cracking and failure of coatings, paying special attention to such aspects of those processes as longitudinal cracks and delaminations (interlayer delaminations and delaminations between nano-sublayers) form. Two basic mechanisms for the formation of longitudinal cracks and delaminations can be distinguished in a nano-structured multi-layered coating:

1. Because of the tearing force related to the adhesion interaction between the outer boundary of the coating and the material being machined (Fig. 6), which has a prevailing fatigue characteristic and results in the formation of fatigue cracks due to the alternating processes of formation and failure of adhesion bridges in the system of "coating-material being machined." The considered mechanism is more typical for coatings on the rake face of the tool.
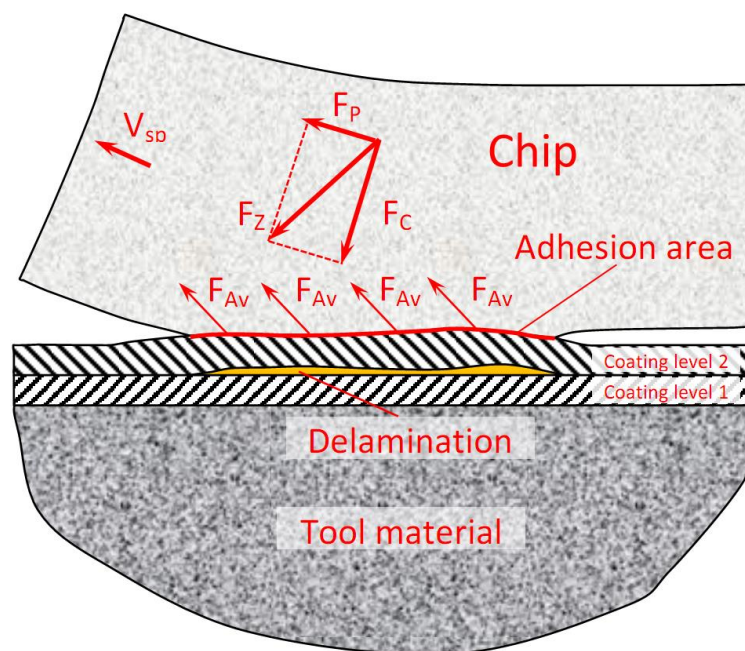

Figure 6. The mechanism of formation of longitudinal cracks and delaminations in a nano-structured multi-layered coating during cutting due to the tearing force associated with adhesion interaction between the outer boundary of the coating and the material being machined.

The action of the mechanism shown in Figure 6 can result not only in the formation of longitudinal cracks and delaminations, but also in the destruction of the surface layers of the coating, and, consequently, in the deterioration of the tool life of the metal-cutting tool (Fig. 7).
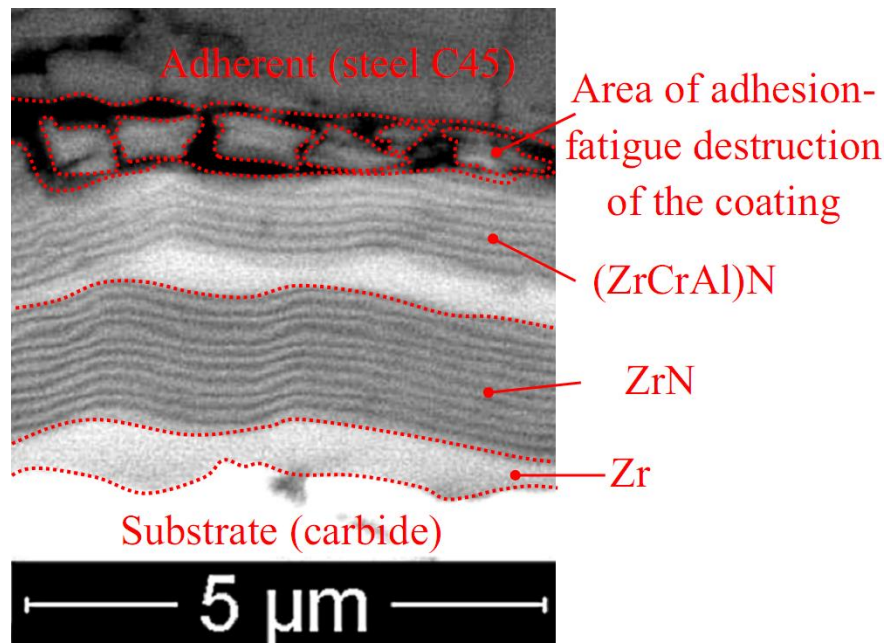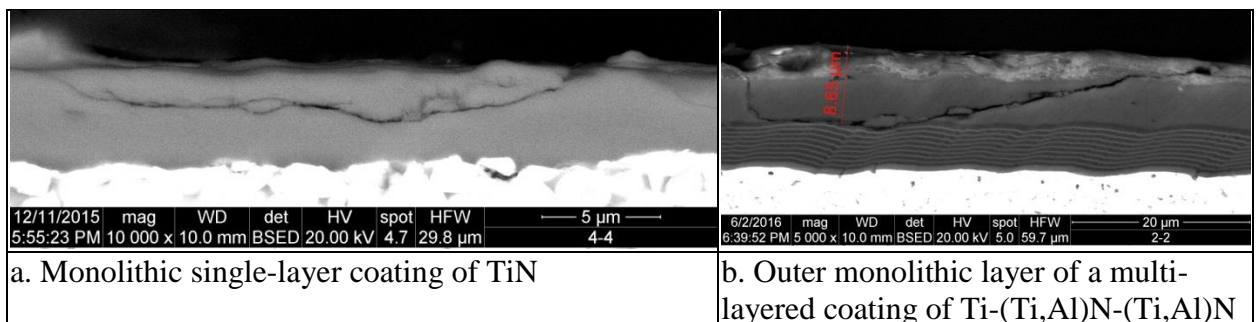
Figure 7. An example of the failure of the upper layer of NMCC Zr-ZrN-(Zr,Cr,Al)N because of the tearing force related to the adhesion interaction between the outer boundary of the coating and the material being machined (steel C45).

Meanwhile, the strength of adhesion bonds between the coating layers and the cohesive bonds between nano-sublayers of the same layer is of great importance. If those bonds are sufficiently strong, longitudinal cracks will form; that is, the coating will collapse as a whole. In this case, the mechanism of formation and character of longitudinal cracks resembles the formation of a longitudinal crack in a monolithic single-layer coating (see Fig. 8.). Otherwise, with less strong adhesion bonds, interlayer and intralayer (between nano-sublayers) delaminations are formed. Note that the formation of longitudinal cracks can be combined with delamination, as can be seen in Fig. 8(d). Also consider that the strength of cohesive bonds between different nano-sublayers can differ substantially because of changes in conditions during the deposition of the coating and the occurrence of plasma-chemical reactions (in particular, temperature on product surface, gas pressure, etc. may change). At present, no techniques are available to accurately control the gas pressure in a volume that is directly adjacent to the surface of the substrate. Neither are methods available to control the temperature on the surface of the substrate. All available methods and devices for monitoring pressure (vacuum gauges, etc.) and temperature (pyrometers, thermocouples) make it possible to obtain only more or less accurate information about some average value of the appropriate parameter.

| a. Monolithic single-layer coating of TiN | b. Outer monolithic layer of a multi-layered coating of Ti-(Ti,Al)N-(Ti,Al)N |

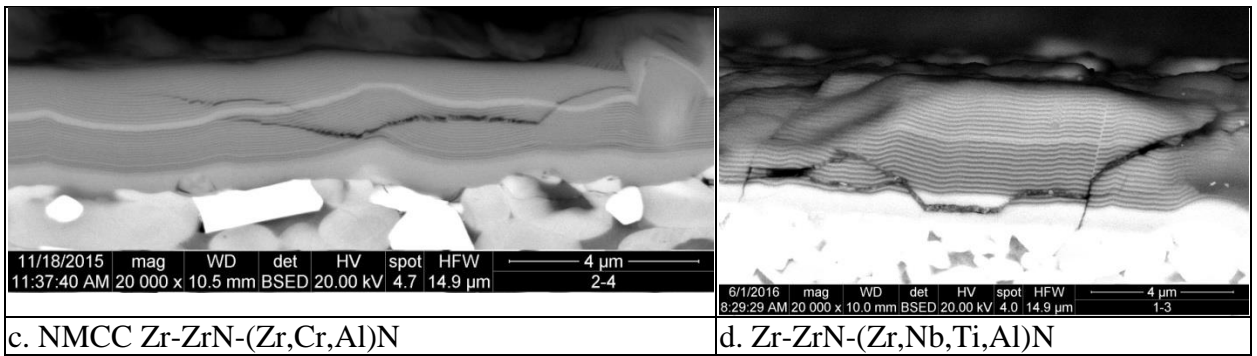| c. NMCC Zr-ZrN-(Zr,Cr,Al)N | d. Zr-ZrN-(Zr,Nb,Ti,Al)N |

Figure 8. An example of the formation of longitudinal cracks.

An important distinctive feature of the development of longitudinal cracks in nano-structured coatings is the formation of bridges in the process of cracking due to the alternation of less plastic sublayers with more plastic ones in the coating structure. Such bridges inhibit the development of a crack by exerting a positive influence on coating crack resistance, and consequently, on the tool life of a cutting tool (Fig. 9). This mechanism of inhibition of cracking is fairly close to the mechanism of action of bridges from a particle of a more-plastic phase embedded in the brittle phase described, in particular, by S. Kumar et al. [29]. It should be noted that the studies of the propagation of longitudinal cracks in monolithic coatings revealed no such bridges. The strength of the bridges depends on the composition of the coating layers. In particular, in layers of (Zr,Cr,Al)N (Fig. 9(a)), the bridges show significantly higher strength and ductility than in (Zr,Nb,Ti,Al)N (Fig. 9(b)), where the bridges show a tendency to failure.

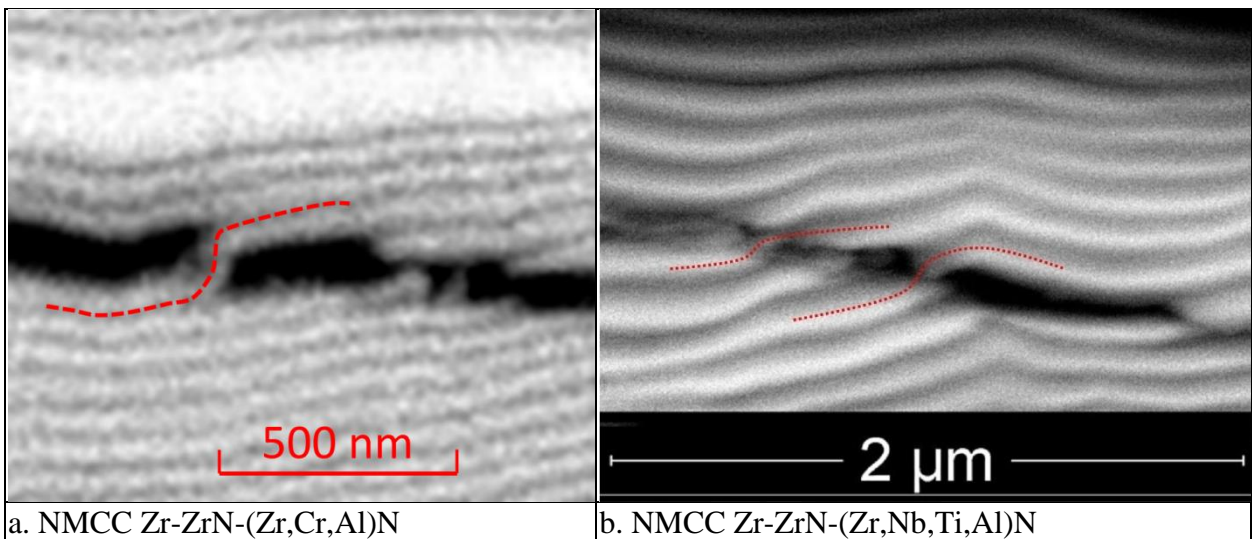| a. NMCC Zr-ZrN-(Zr,Cr,Al)N | b. NMCC Zr-ZrN-(Zr,Nb,Ti,Al)N |

Figure 9. Deceleration of a longitudinal crack due the formation of bridges of more-plastic nano-layers.

No such bridges are observed in NMCC Ti-TiN-(Ti,Al)N, and that may be connected with the high hardness and brittleness of the layer (Ti,Al)N. The failure of NMCC Ti-TiN-(Ti,Al)N often occurs in accordance with a pronounced "brittle fracture" scenario with the formation of a network of longitudinal and transverse cracks (Fig. 10).
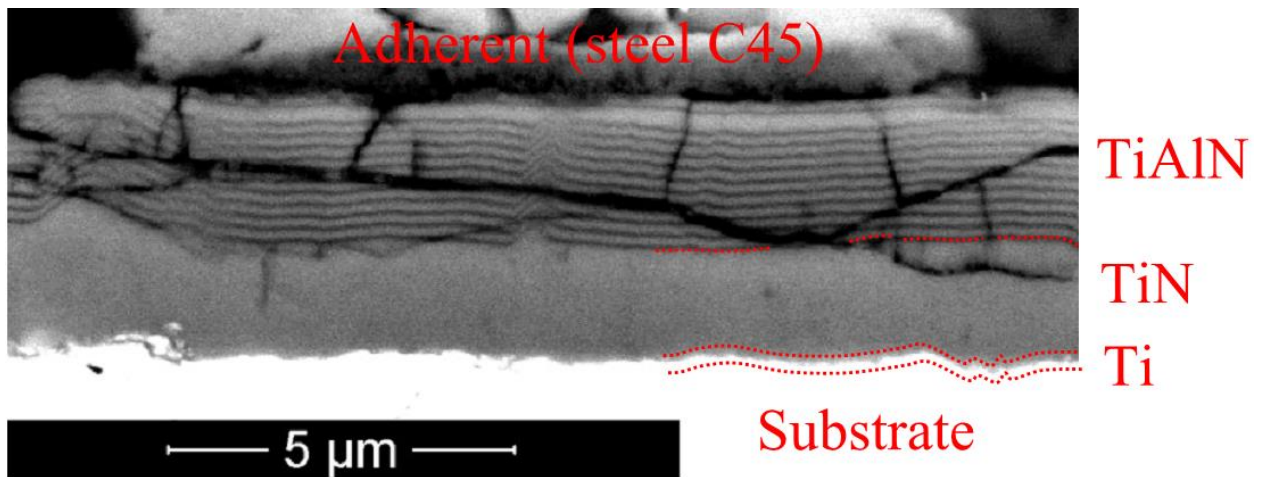
Figure 10. Failure of NMCC Ti-TiN-(Ti,Al)N with the formation of a network of longitudinal and transverse cracks.

In the case of insufficiently strong adhesion bond between the coating layers or cohesive bonds between its nano-sublayers, delaminations of the classical form are formed between the layers of the coating or between its nano-sublayers. In particular, Fig. 11 and Fig. 12 show obvious delamination between the intermediate TiN layer and the wear-resistant (Ti,Al)N layer. In the structure of the coating presented in Fig. 12, transverse cracks and delaminations also occur between nano-sublayers of the wear-resistant layer. In addition, it is possible to note a relatively positive role of delamination (1) as a factor of inhibition of transverse cracks (3). The transverse cracks (3) are decelerated at the boundary of the intermediate and wear-resistant layers, and they are not spreading in the intermediate TiN layer (Fig. 12).
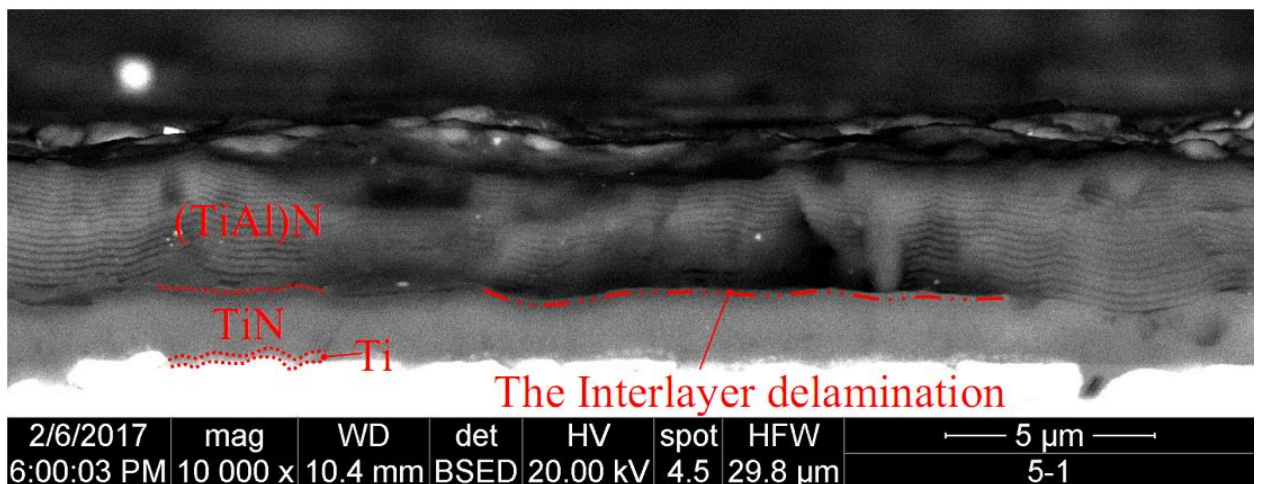

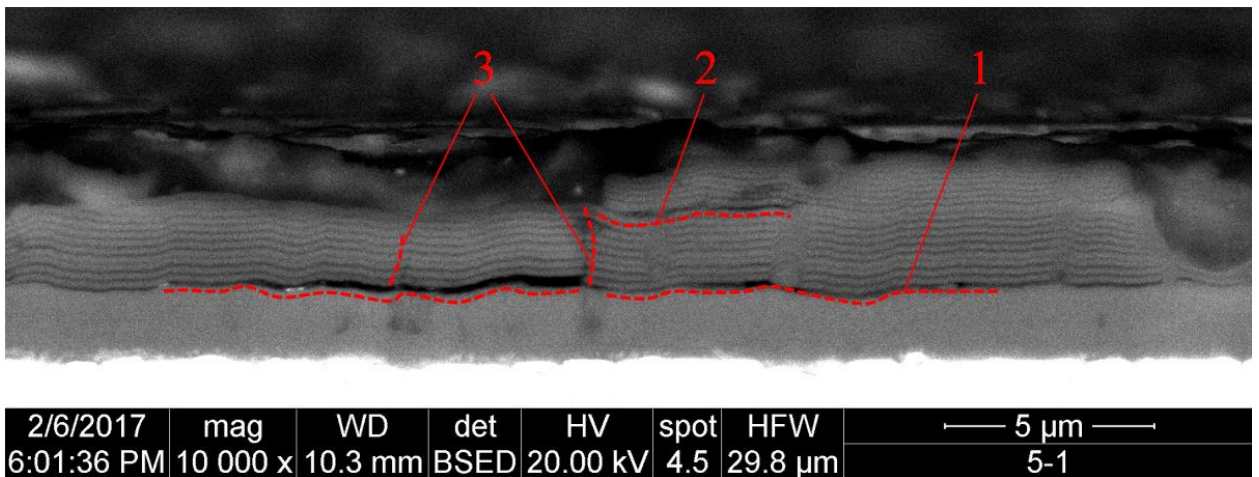Figure 11. Interlayer delamination in the structure of NMCC Ti-TiN-(Ti,Al)N.

Figure 12. Interlayer delamination (1), delamination between nano-sublayers (2), and transverse cracks (3) in the structure of NMCC Ti-TiN-(Ti,Al)N.

The patterns of formation of longitudinal cracks and delaminations often appear to be complex. In particular, Fig. 13 shows the mechanisms of cracking and delamination in NMCC Zr-ZrN-(Zr,Cr,Al)N. The area of this picture that is marked as AREA I contains a crack of a complex kind, combining delamination between the substrate and the adhesion layer Zr, passing into a transverse crack that cuts the adhesive layer, and turning into a series of delaminations between nano-sublayers of the intermediate coating layer. The initial factor stimulating the formation of this crack is microroughness of the substrate, formed by high carbide grain. In contrast, the area indicated as AREA II contains an example of extended delamination, reaching a width of 200-300 nm. The formation of this delamination resulted in chipping of microcomponents of the coating (1) and formation of bridges of more-plastic nano-layers (2). The crack development boundary is indicated by (3).
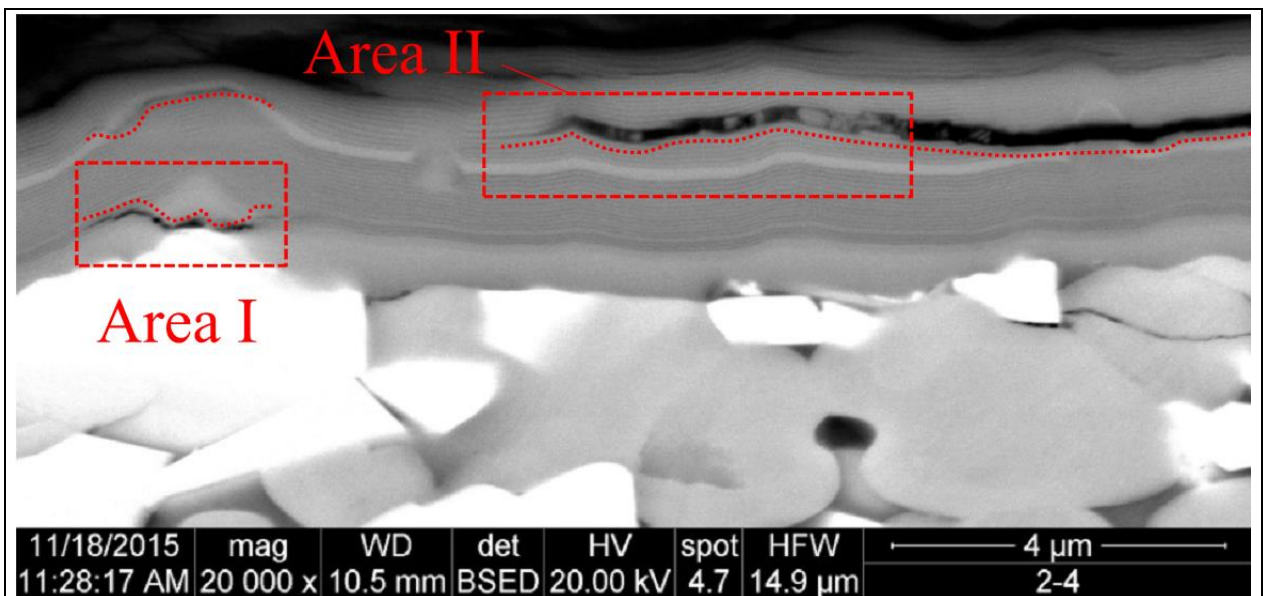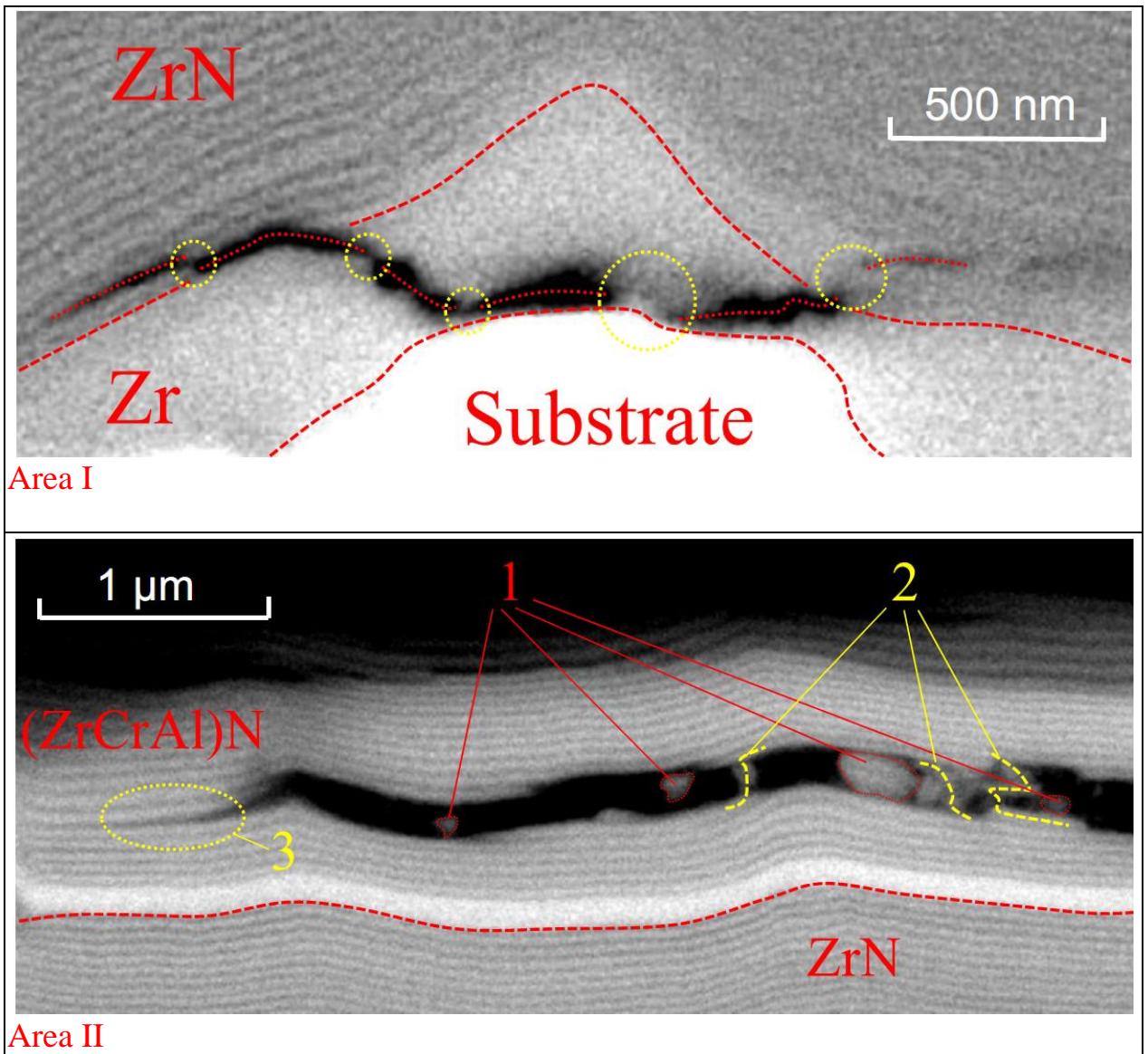
Figure 13. An example of formation of longitudinal cracks and delaminations in NMCC Zr-ZrN-(Zr,Cr,Al)N.

The conducted studies show that harder coatings with thicker nano-sublayers (in particular, NMCC (Zr,Nb)N-(Zr,Al,Nb)N with thickness of nano-sublayers of up to 110 nm) show higher tendency to delamination that coatings of the same hardness, but with thinner nano-sublayers. Fig. 14 shows an example of "pure" delamination, without formation of transverse and longitudinal cracks. Delamination goes strictly through the interlayer interface. Meanwhile, it is possible to notice a broken bridge of bond between two nano-sublayers (Fig.14 (b)).
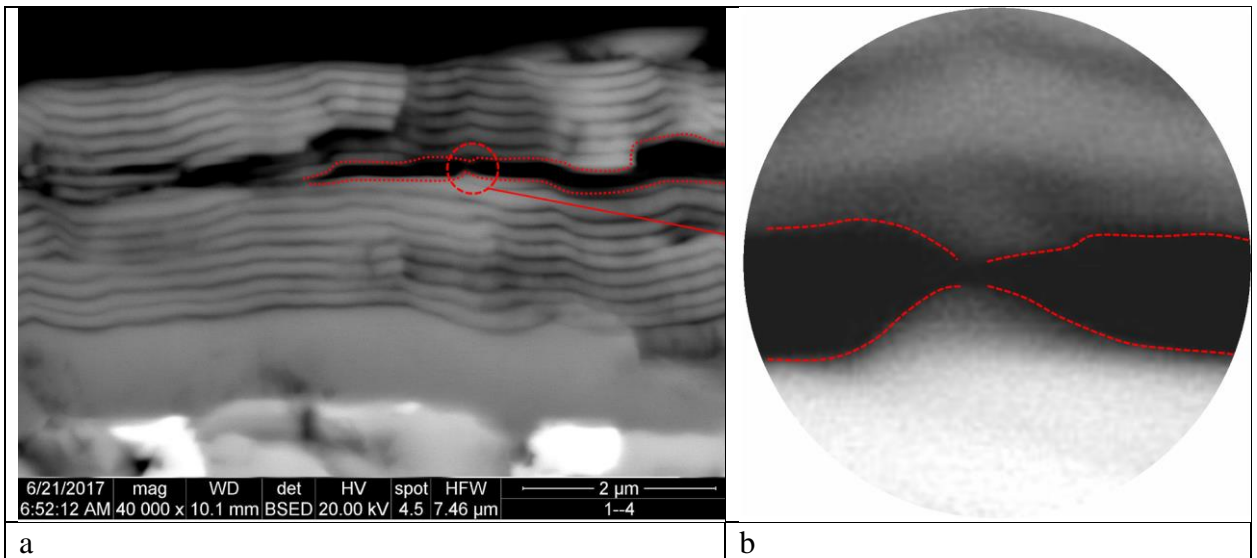
a | b

Figure 14. An example of formation of longitudinal cracks and delaminations in NMCC (Zr,Nb)N-(Zr,Al,Nb)N.

Various defects in coatings (in particular, embedded microdrops and pores) can play an important role in the formation of longitudinal cracks and delamination. Figure 15 shows how a crack reaches a macro droplet and forms branches. Meanwhile, one of the branches of the crack passes through a macro droplet, while the second crack branch traverses it along the contour. This photomicrograph reveals a separation of the material being machined from the coating; this separation indicates a low adhesive bond between the materials. Meanwhile, no separation of the coating from the tool material occurs due to a strong adhesive bond between them.
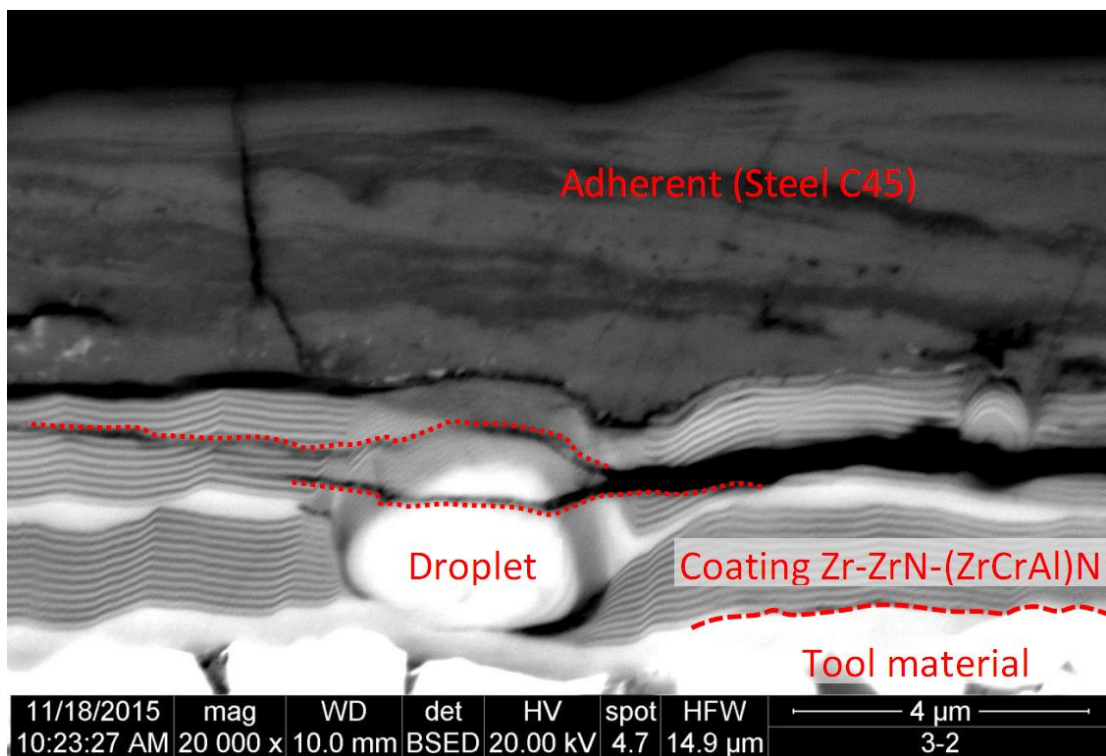

Figure 15. An example of development of a longitudinal crack in NMCC Zr-ZrN-(Zr,Cr,Al)N.

Another example of the effect of a micro droplet embedded in the structure of the coating on the formation of delaminations is shown in Fig. 16. Here, a crack is formed directly above a micro

droplet, and several parallel delaminations exist in the area adjacent to a micro droplet. These occurrences may be related to internal stresses arising during the coating deposition.
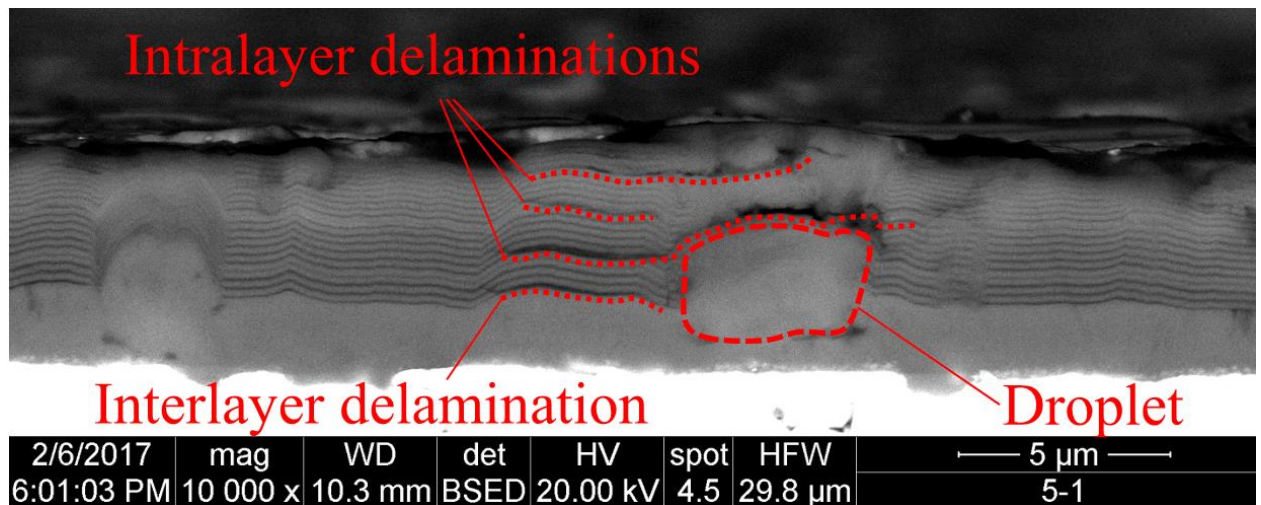

Figure 16. An example of development of a longitudinal crack in NMCC Ti-TiN-(Ti,Al)N.

Defects of the coating in the form of embedded pores are much less frequent and, as a rule, are related to burnout of organic micropollution on the surface of the substrate during the coating deposition. Figure 17 shows the sponge structure formed around a micropore, which in turn creates distortion in the coating structure. These distortions result in numerous delaminations in the structure of the (Ti,Al)N layer and a longitudinal crack in the structure of the TiN layer.
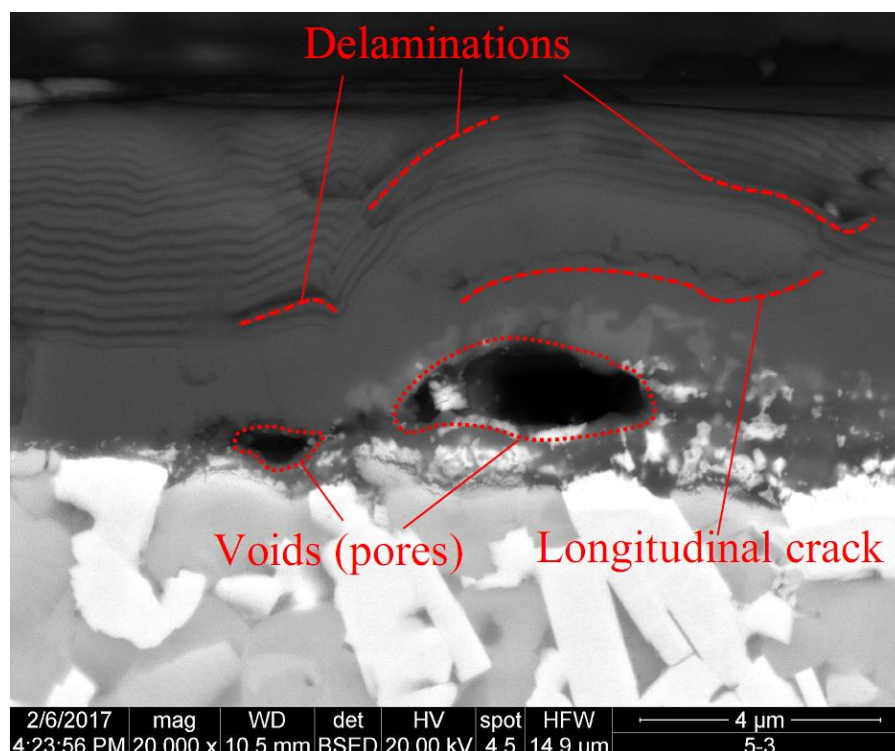

Figure 17. An effect of an internal pore on the development of longitudinal crack and delaminations in NMCC Ti-TiN-(Ti,Al)N.

Another mechanism of the formation of longitudinal cracks and delaminations takes place because of the tearing force related to plastic microdeformations in the surface layer of the tool substrate

(Fig. 18). In the process of plastic deformation of the tool substrate, the layers of the coating also are subjected to deformation, and the lower layers, which are in adhesive bond with the substrate, are deformed to a greater extent than the surface layers. This results in a tearing force between the layers of the coating. This mechanism is more typical for a coating on the flank face of a tool.
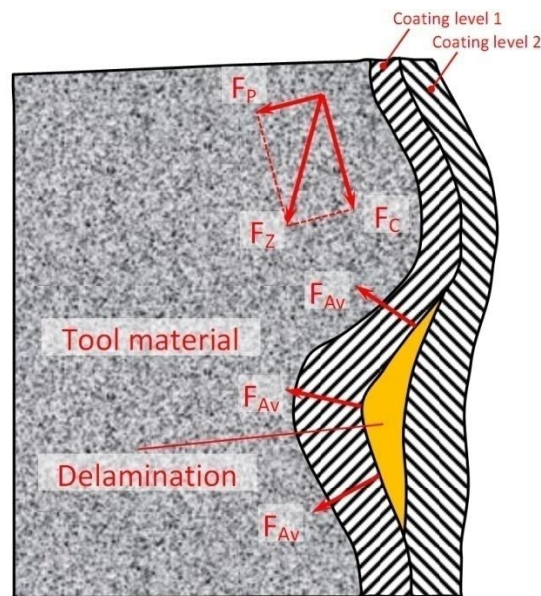

Figure 18. Mechanism of formation of transverse cracks and delaminations in a nano-structured multi-layered coating during the cutting process because of the tearing force related to plastic microdeformations in the surface layer of the tool substrate.

Figure 19 shows examples of the formation of transverse cracks and delaminations in the structure of multi-layered nano-structured coatings on the flank face of the tool. It is clear that in NMCC Zr-ZrN-(Zr,Cr,Al)N (Fig. 19 (a)), the direction of crack propagation is generally the same as the direction of nano-sublayers of the coating. The spread of a crack cutting the nano-sublayers of the coating is combined with delaminations of the nano-sublayers. In contrast, NMCC Ti-TiN-(Ti,Al)N (Fig. 19 (b)) shows no "longitudinal crack-transverse crack" transitions and practically no delaminations. The crack cuts the coating "as a whole," slightly relating to the direction of the nano-sublayers.
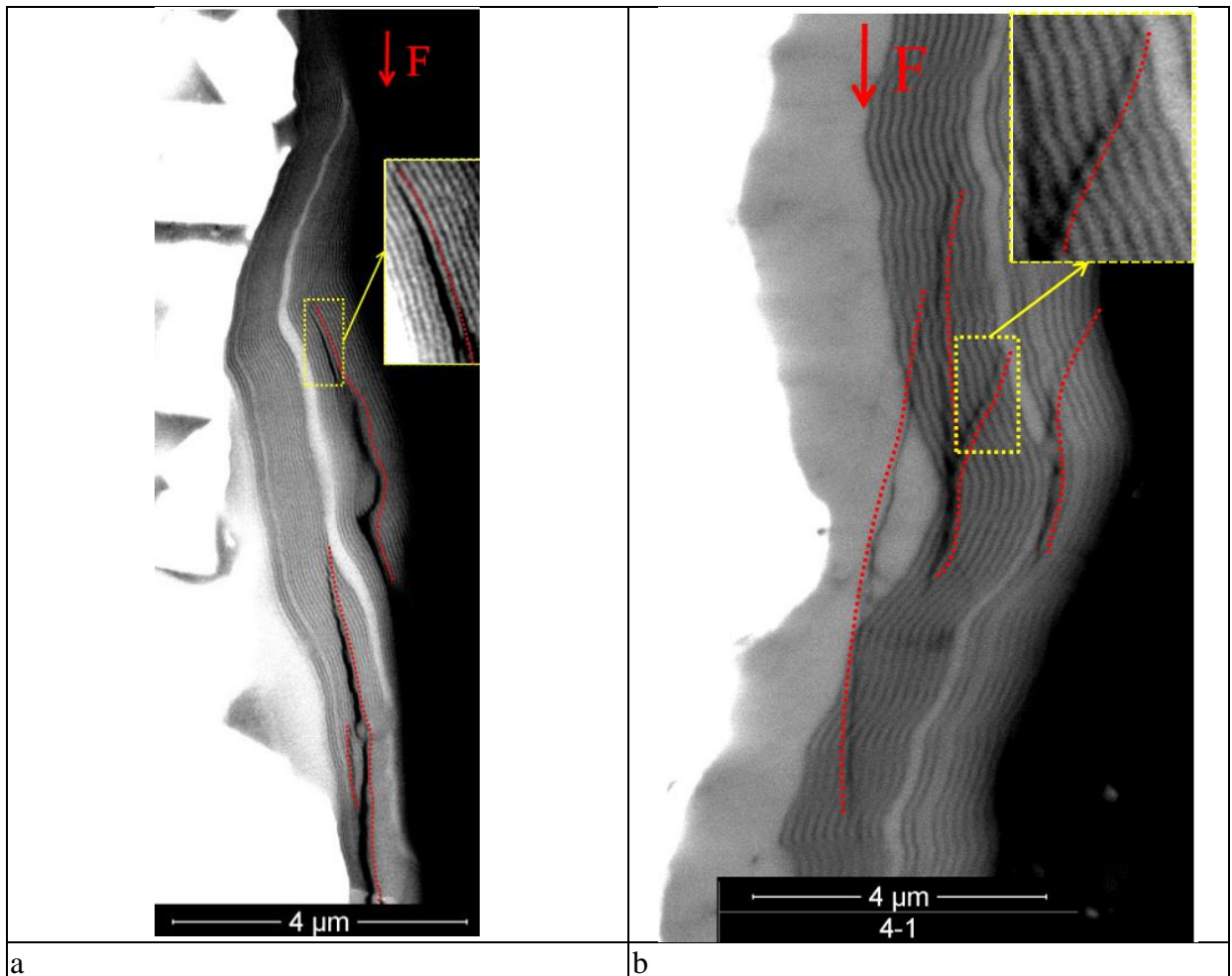
Figure 19. An example of development of longitudinal cracks in NMCC Zr-ZrN-(Zr,Cr,Al)N (a) and Ti-TiN-(Ti,Al)N (b) because of the formation of plastic deformations on the flank surface of a tool.

Let us individually consider delaminations formed in NMCC of heavy thickness (usually exceeding 10 µm) because of heavy internal compressive stresses. Such delaminations can be formed with equal probability in the coating both on the rake and flank face of a tool. An example of formation of delaminations in "thick" NMCC is presented in Fig. 20. It is possible to observe four clear delaminations located at approximately equal distance (about 20 nano-sublayers) from each other. Meanwhile, the delamination closest to the substrate (area A on Fig. 20) passes exclusively along the boundary between the sublayers. At the same time, delaminations B, C, and D are rather longitudinal cracks because they also are characterized by breaks in the structures of nano-sublayers.
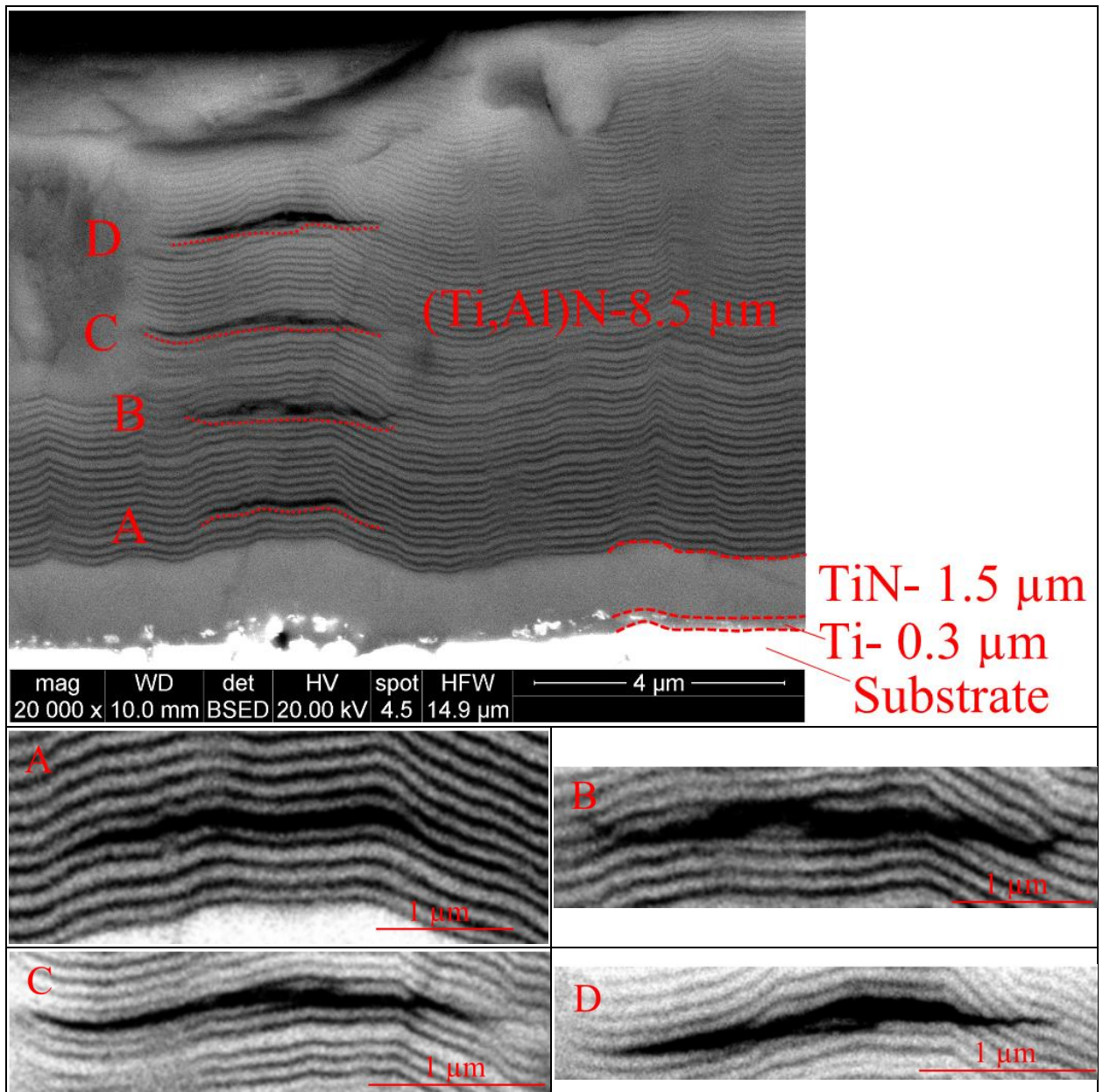
Figure 20. An example of the formation of delaminations in NMCC Ti-TiN-(Ti,Al)N (total thickness of the coating is 13 µm).

Various internal defects in "thick" NMCC (in particular, microdroplets embedded in the structure of the coating) become particularly important and result in local fracture of the coating because of the formation of multiple delaminations that weaken the coating structure and ultimately result in the formation of a transverse crack (Fig. 21). As a result of the distortion of the coating structure associated with the curvature of the nano-sublayers because of rounding of an embedded microdroplet, internal stresses arise, which in turn result in the formation of corresponding delaminations and longitudinal cracks. Because (Ti,Al)N is a very hard, yet brittle compound, the chipping of fragments of nano-sublayers and formation of a transverse crack occur in the coating structure weakened by delaminations.
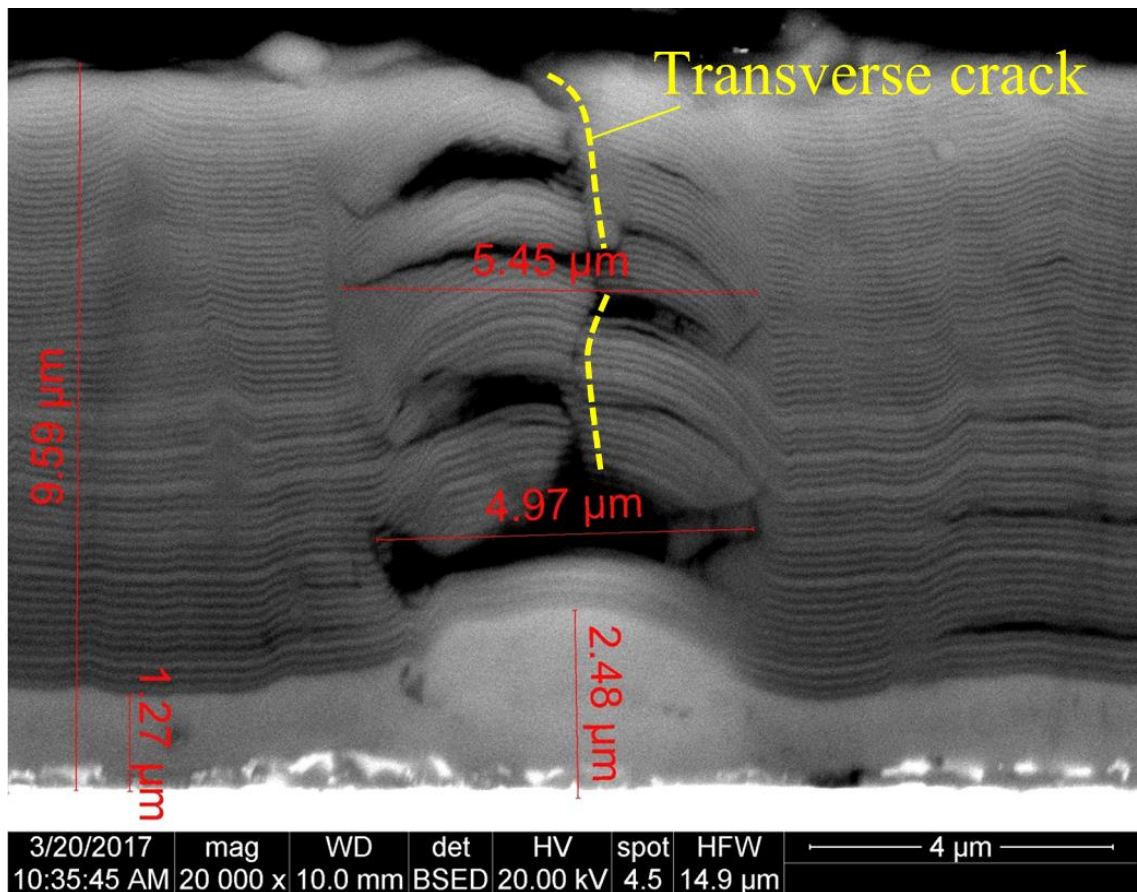
Figure 21. Formation of a transverse crack in the structure of NMCC Ti-TiN-(Ti,Al)N as a result of weakening of the structure of NMCC by multiple delaminations formed under the influence of internal stresses.

4. Conclusions

This study of the nature of the formation of longitudinal cracks and delaminations in multi-layered nano-structured coatings reveals the following:

1. Two important mechanisms result in formation of transverse cracks and delaminations:

- Tearing force associated with adhesion interaction between the outer boundary of the coating and the material being machined (typical for the rake face of the tool)

- Tearing force associated with plastic microdeformations in the surface layer of the tool substrate (more typical for the flank face of a tool)

2. The nature of the formation of longitudinal cracks and delaminations varies significantly for different coating compositions. In coatings with more plastic nano-layers, bridges can be formed, which inhibit the development of cracks. This can be clearly observed in NMCC Zr-ZrN-(Zr,Cr,Al)N, and to a lesser extent in NMCC Zr-ZrN-(Zr,Nb,Ti,Al)N, while in coatings with more hard and brittle nano-layers (for example, (Ti,Al)N), such bridges are not formed and coatings are destructed under the mechanism of brittle failure.

3. Such coating defects as embedded microdrops and micropores can stimulate the development of longitudinal cracks and delaminations.

4. The following factors reduce the probability of formation of longitudinal cracks (delamination):

- Reduction of adhesion interaction between the outer boundary of the coating and the material being machined

- Increase of adhesion bonds between coating layers and cohesive bonds between the nano-sublayers

- Decrease in the level of plastic microdeformations of the tool substrate; in particular, through heat strengthening and/or diffusion saturation with alloying elements

5. NMCC of relatively large thickness (larger than 8 µm) may experience delamination during the deposition as a result of significant internal stresses. The presence of such delamination can contribute to brittle fracture of coatings, particularly NMCC based on a hard and brittle compound (Ti, Al) N.

References
[1] A.S. Vereschaka. *Working capacity of the cutting tool with wear resistant coatings.* Mashinostroenie. Moscow, 1993 (in Russian).

[2] A.A. Vereshchaka, A.S. Vereshchaka, O. Mgaloblishvili, M.N. Morgan, and A.D. Batako Nano-scale multilayered-composite coatings for the cutting tools. International Journal of Advanced Manufacturing Technology, Vol. 72, Iss. 1 (2014), pp. 303-317.

[3]   G.S. Fox-Rabinovich, A.I. Kovalev, M.H. Aguirre, B.D. Beake, K. Yamamoto, S.C. Veldhuis, J.L. Endrino, D.L. Wainstein, A.Y. Rashkovskiy, Design and performance of AlTiN and TiAlCrN PVD coatings for machining of hard to cut materials, Surf. Coatings Technol. 204 (2009) 489–496. doi:10.1016/j.surfcoat.2009.08.021.

[4]   K. Yamamoto, T. Sato, K. Takahara, K. Hanaguri, Properties of (Ti,Cr,Al)N coatings with high Al content deposited by new plasma enhanced arc-cathode, Surf. Coatings Technol. 174–175 (2003) 620–626. doi:10.1016/S0257-8972(03)00580-2.

[5] G.S. Fox-Rabinovich, K. Yamamoto, A.I. Kovalev, S.C. Veldhuis, L. Ning, L.S. Shuster, A. Elfizy, Wear behavior of adaptive nano-multilayered TiAlCrN/NbN coatings under dry high performance machining conditions, Surf. Coat. Technol. 202 (2008) 2015–2022. doi:10.1016/j.surfcoat.2007.08.067

[6] M.G. Faga, G. Gautier, R. Calzavarini, M. Perucca, E. Aimo Boot, F. Cartasegna, L. Settineri, AlSiTiN nanocomposite coatings developed via Arc Cathodic PVD: Evaluation of wear resistance via tribological analysis and high speed machining operations. Wear. 263 (2007) 1306–1314.

[7] K.-D. Bouzakis, N. Michailidis, N. Vidakis, K. Efstathiou. Failure mechanisms of physically vapour deposited coated hardmetal cutting inserts in turning, Wear 248 (2001) 29-37

[8] S. PalDey, S.C. Deevi, Single layer and multilayer wear resistant coatings of (Ti, Al)N: A review, Mater. Sci. Eng. A 3 (42) (2003) 58.

[9] Y.G. Matvienko. The models and criteria of fracture mechanics. FIZMATLIT. Moscow. 2006 (in Russian).

[10] K.B. Broberg. Cracks and Fracture. San Diego: Academic Press, 1999.

[11] T.A. Zehnder. Lecture Notes on Fracture Mechanics, Cornel University, Ithaca, New York, 2007.

[12] T.L. Anderson , Fracture mechanics: Fundamentals and applications. New York, CRC Press LLC, 1995.

[13] V.P. Tabakov. The Influence of Machining Condition Forming Multilayer Coatings for Cutting Tools. Key Engineering Materials. 496 (2012) 80-85.

[14] V.P. Tabakov and A.S. Vereschaka. Development of technological means for formation of multilayer composite coatings, providing increased wear resistance of carbide tools, for different machining condition. Key Engineering Materials. 581 (2014) 55-61.

[15] V.P. Tabakov, M. YU. Smirnov, and A.V. Tsirkin. Productivity of end mills with multilayer wear-resistant coatings. Ulyanovsk: UlSTU 2005 (in Russian).

[16] A.A.Vereschaka, A.S. Vereschaka, J.I. Bublikov, A.Y. Aksenenko, and Sitnikov N.N. Study of properties of nanostructured multilayer composite coatings of Ti-TiN-(TiCrAl)N and Zr-ZrN-(ZrNbCrAl)N. Journal of Nano Research. 40 (2016) 90-98.

[17] A.A. Vereschaka, A.S. Vereschaka, A.D.Batako, O.Kh.Hojaev, and .Y. Mokritskii. Development and research of nanostructured multilayer composite coatings for tungsten-free carbides with extended area of technological applications. International Journal of Advanced Manufacturing Technology. 87:(2016) 3449–3457.

[18] A.O. Volkhonskii, A.A.Vereshchaka, I.V. Blinkov, A.S. Vereshchaka and
A.D. Batako. Filtered cathodic vacuum Arc deposition of nano-layered composite coatings for machining hard-to-cut materials. International Journal of Advanced Manufacturing Technology. 84 (2016) 1647–1660.

[19] Alexey A.Vereschaka, Sergey N.Grigoriev, Anatoly S.Vereschaka, Alexey Yu.Popov, and Batako A.D. Nano-scale multilayered composite coatings for cutting tools operating under heavy cutting conditions. Procedia CIRP. 14, 2014, 239–244.

[20] A.A. Vereschaka, M.A. Volosova, A.D. Batako, A.S. Vereshchaka, and
B. Y. Mokritskii. Development of wear-resistant coatings compounds for high-speed steel tool using a combined cathodic vacuum arc deposition. International Journal of Advanced Manufacturing Technology.84, (2016) 1471 –1482.

[21] Sergey N. Grigoriev and Alexey A. Vereshchaka. Methodology of formation of multi-layered coatings for carbide cutting tools. Mechanics& Industry. 17, 706 (2016) DOI: 10.1051/meca/2016065.

[22]Alexey A. Vereschaka, Anatoly S. Vereschaka, Andre D.L. Batako, Boris J. Mokritskii, Anatoliy Y. Aksenenko, and Nikolay N. Sitnikov. Improvement of structure and quality of nano-

scale multi-layered composite coatings, deposited by filtered cathodic vacuum arc deposition method. Nanomaterials and Nanotechnology. 7 (2016),1-13.

[23] A.A. Vereschaka and S.N. Grigoriev. Study of cracking mechanisms in multi-layered composite nano-structured coatings. Wear. 378-379 (2017) 43–57.

[24] G. Skordaris, K.-D. Bouzakis, and P. Charalampous. A dynamic FEM simulation of the nano-impact test on mono- or multi- layered PVD coatings considering their graded strength properties determined by experimental–analytical procedures. Surface & Coatings Technology 265 (2015) 53–61.

[25] Xiang-FaWu, Yuris A. Dzenis, and Kyle W. Strabala. Free-edge stresses and progressive cracking in surface coatings of circular torsion bars. International Journal of Solids and Structures 45 (2008) 2251–2264.

[26] Xiang-FaWu, Robert A. Jenson, and Youhao Zhao. Stress-function variational approach to the interfacial stresses and progressive cracking in surface coatings. Mechanics of Materials 69 (2014) 195–203.

[27] R. M'Saoubi, M. P. Johansson, and J. M. Andersson. Wear mechanisms of PVD-coated PCBN cutting tools. Wear 302 (2013) 1219–1229.

[28] S. Koseki, K. Inoueb, and H. Usuki. Damage of physical vapor deposition coatings of cutting tools during alloy 718 turning. Precision Engineering 44 (2016) 41–54.

[29] S. Kumar and W. A. Curtin. Crack interaction with microstructure. Materials Today.10 (9) (2007) 34-44.

[30] H. Hosseini-Toudeshky, S. Hosseini, and B. Mohammadi. Delamination buckling growth in laminated composites using layer wise-interface element. Composite Structures 92 (2010) 1846–1856.

[31] J.A. Pascoe, C.D. Rans, R.C. Alderliesten, and R. Benedictus. Fatigue Disbonding of Bonded Repairs – An Application of the Strain Energy Approach. 27th ICAF Symposium – Jerusalem, 5 – 7 June 2013.

[32] J.A. Pascoe, C.D. Rans, and R.Benedictus. Characterizing fatigue delamination growth behavior using specimens with multiple delaminations: The effect of unequal delamination lengths. Engineering Fracture Mechanics 109 (2013) 150–160.

[33] E. Rybicki and M. Kanninen. A finite element calculation of stress intensity factors by a modified crack closure integral. EngngFractMech 1977; 9(4):931–8.

[34] W. Hume-Rothery, *Atomic Theory for Students of Metallurgy*, The Institute of Metals, London, 1969 (fifth reprint).

[35] W.C. Oliver and G. M. J. Pharr, An improved technique for determining hardness and elastic modulus using load and displacement sensing indentation. Journal of Materials Research, 7 (1992) 1564-1583.