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Influence of substrate roughness on structure and mechanical property of TiAlN coating fabricated by cathodic arc evaporation

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Abstract

The aim of the present research was to investigate the influence of different substrate roughness on structure and mechanical properties of Titanium Aluminium Nitride (TiAlN) coatings. Tungsten carbide rectangular block was used as substrate. Different surface roughness was achieved by using grinding discs with different grain sizes and diamond polishing powder, and TiAlN coatings were deposited on these substrates under the same preparation technique and parameters. Morphologies of substrates and coatings, crystal structure, thickness and mechanical properties of coatings were investigated using optical microscope, AFM, XRD, CSM scratch tester and tribometer. It was shown that surface morphology of cathodic arc TiAlN coating was mainly affected by the morphology of the substrate surface and the coating growth process. The influence of substrate roughness on crystal structure and thickness of the coatings could be ignored. With the decreasing of the substrate roughness, the adhesion force between coating and substrate increased. Three stresses model was applied to interpret this result. The wear resistance of the coating was also improved with decreasing the substrate roughness.

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1. Introduction

The use of surface coatings is well established in many sectors of engineering. TiAlN coating is one of the most representational commercial coatings. It has been found a range of applications, particularly in the tool industry, based on its desirable properties including high micro-hardness, relatively low residual stress, low friction, good thermal stability, superior oxidation resistance, high hot hardness, low thermal conductivity and so on [1-4]. Ternary TiAlN coatings have been chosen as the subject of preparation and property investigations for many years.

With the development of coating preparation technology, a substrate surface pretreatment, e.g. sand blasting, grinding and polishing or honing, is required for improving the performance of the coatings [5, 6]. Different pretreatment processing results in different substrates surface roughness, and its evaluation is very important for many fundamental problems such as friction, adhesion property, contact deformation, heat and electric current conduction, tightness of contact joints and positional accuracy [7]. However, the influence of different substrate surface roughness on structure and mechanical properties of TiAlN coatings has not been systematically studied. In

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the present study the morphologies of the tungsten carbide substrates were varied by using grinding discs with different grain sizes and diamond polishing powder. TiAlN coatings were deposited on these substrates by cathodic arc evaporation technology. The aim of this work is to investigate the influence of different substrate roughness on structure and mechanical properties of TiAlN coatings.

2. Experimental Details

2.1. Sample preparation

Tungsten carbide rectangular block was used as substrate, fixed size was 12.7mm ×12.7mm×4.76mm. Substrates were burnished by a mechanical polisher combined with diamond grinding disc. Different surface roughness was achieved by using grinding discs of different grain sizes (600 and 1200 mesh) and diamond polishing powder through different wet grinding processing procedure. Table.1 shows the pretreatment of the substrates in details. Subsequently, all the substrates were ultrasonically cleaned for 10 min, each successively in acetone and absolute ethyl alcohol. TiAlN coatings were deposited by a cathodic arc unit (Oerlikon Balzers, Switzerland) from $Ti_{33}Al_{67}$ alloy target. All the coatings were deposited under the same deposition parameters which are listed in Table.2.

Table 1 Pretreatment of the substrates

Samples	Processing procedure
1	untreated
2	600 mesh 10 min
3	600 mesh 10 min + 1200 mesh 10 min
4	600 mesh 10 min + 1200 mesh 10 min + polishing cloth 15 min

Table 2 Operation parameters for deposition of TiAlN coatings

Parameter	Value
Base pressure	8×10^{-4} Pa
N_2 gas pressure	1.0 Pa
Substrate biasing	-50 V
Target current density	0.8 Acm^2
Substrate temperature	500 ℃

2.2. Characterization of structure and morphology

The phase composition was investigated using Panalytical X'pert PRO X-ray diffraction (Philips, Netherland). The diffraction experiments were performed at grazing angle scanning using Cu Kα radiation, 2 theta angles ranged from 10 degree to 90 degree. The coating thicknesses were determined by a Dektak3 profilometer (VEECO, U.S.). The thicknesses of the coatings are around 3.5 ± 0.05 μm. The roughness of the substrate (Ras) and coating (Rac) was measured by a Nano Scratch Tester combined with atomic force microscope (AFM) analysis software produced by CSM instruments SA, Switzerland. Optical microscope (OM, Nikon, Japan) and AFM (SIS, Germany) were applied to investigate the morphology of the substrates and coatings.

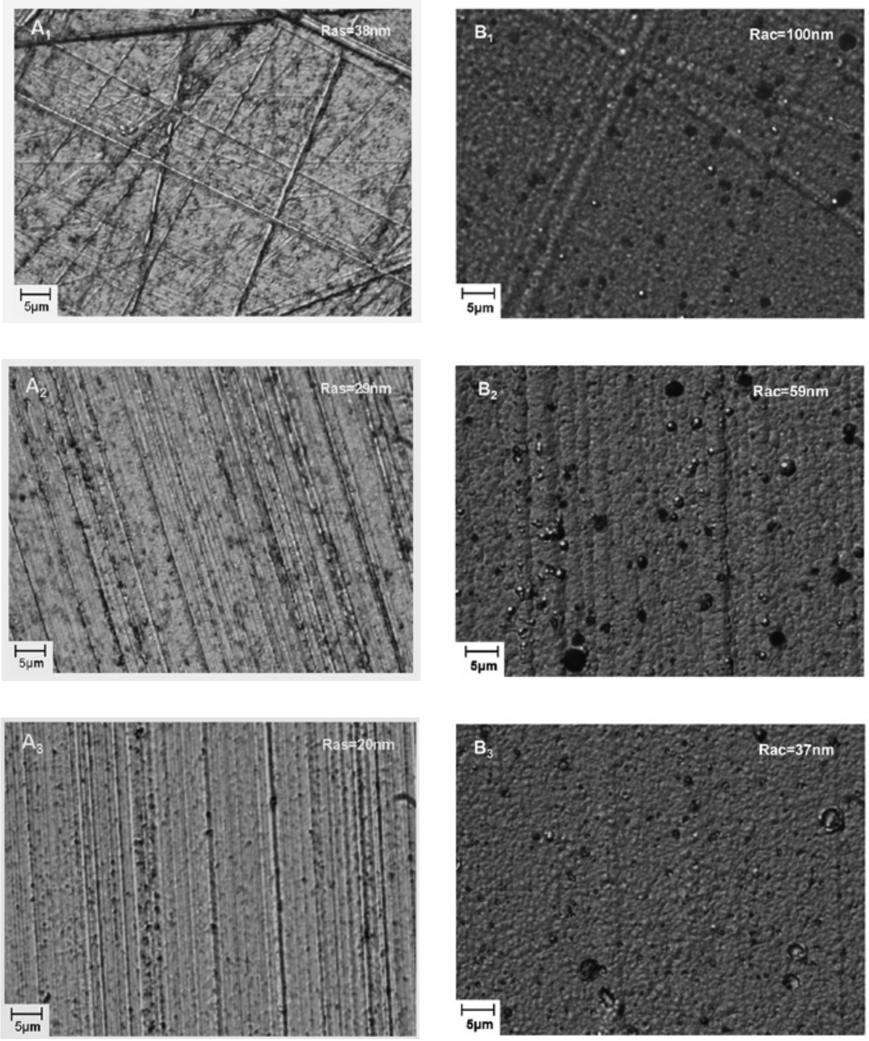
2.3. Characterization of mechanical properties

Scratch testing was performed to determine the film adhesion using a CSM Revetest scratch tester (CSM instruments SA, Switzerland) fitted with a Rockwell C diamond (120° cone with a 200 μm radius hemispherical tip). The load was increased linearly from 0 to 100 N at a loading rate of 200 N/min, the diamond was drawn across the film surface at a table speed of 6 mm/min and the length of scratch tester's track was 3 mm. In this sort of scratch test, care has to be taken in setting the critical load Lc, defined as the load where film complete flaking starts, which was determined by optical examination of the trace [8-10]. The critical load given in this work was the mean value of three scratching tests. Sliding tests were carried out using a tribometer (pin-on-disc, CSM Instruments SA) allowing measuring friction coefficient continuously during the sliding test at elevated temperatures up to 1000 ℃ in controlled condition. In this study the testing was performed at room temperature using an Al_2O_3 (diameter of 6 mm) ball as a counterpart. All measurements were done under the load of 1 N, linear speed of 0.05 ms^{-1} and relative humidity of air (50±5) %. The radius of a wear test track was 2.5 mm. The number of cycles was 3000 for sliding with Al_2O_3 ball. The ball was changed after each test. The tracks were measured using Nano Scratch Tester and optical microscopy.

3. Results and discussion

3.1. Morphology

OM morphologies of the samples before and after depositing coatings are shown in Fig.1. Different roughness substrates are obtained through different pretreatments. It is shown that the substrate roughness significantly affects the coating surface morphology. There are still some fringes on the coatings which were deposited on unpolished substrates. In addition, microparticles as large as 1 to 3 μm are observed on each coated sample surface. The production of microparticles and their subsequent incorporation in ceramic coatings have also been documented by Johnson and Randhawa [11]. They indicated that during the deposition process, the arc spots have a tendency to dwell in particular locations on the surface of the target material, producing localized pools of molten metal from which microdroplets are ejected. Some of the microdroplets impinge on the surface and become incorporated in the growing coatings. These microparticles affected the measurement of coating roughness.



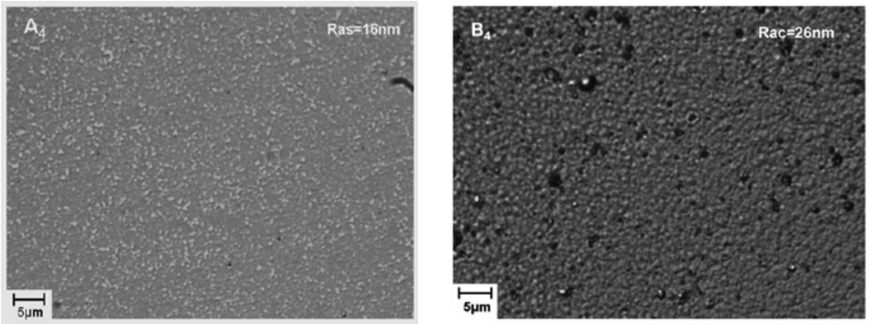


Fig.1 The OM morphologies of the substrates (A) and TiAlN coatings (B)

The AFM images of the TiAlN coating surfaces deposited on various roughness substrates are shown in Fig.2. Variations of surface roughness, before and after coating depositing, are shown in Fig.3. After depositing, the surface roughness of all the coatings increased. With the decreasing of the substrate roughness, the surface of the obtained coatings became smoother and smoother. On the other hand, the disparity of surface roughness between substrate and coating ranged from 62 nm to 10 nm. It can be explained that coating surface roughness results from the sharps of initial nucleus, from preferential nucleation at substrate inhomogeneities, from substrate roughness, and from preferential growth [12]. The fluctuation of substrate surface results in surface energy fluctuation. It is easier to form nucleus at peak points, where energy is higher than valleys. Nucleation, which uses up many atoms around, results in forming low-concentration area in mass transfer process, and then a concentration gradient is present. Therefore, atoms diffuse and transfer to peak points on which coating grows preferentially. Compared with peak points, it is harder to form nucleus and receive diffusing atoms at valleys, so coating grows slowly here. Finally, overlapping-island morphology is formed. Inhomogeneous substrate surface and different growing processing increase the height deviations between peaks and valleys of coating. The measured roughness is the average of the absolute values of these height deviations [7]. If coating is deposited on a very smooth substrate, it can overcome the influence of inhomogeneity of substrate and initial nucleation. Thus, the coating surface is very smooth, similarly.

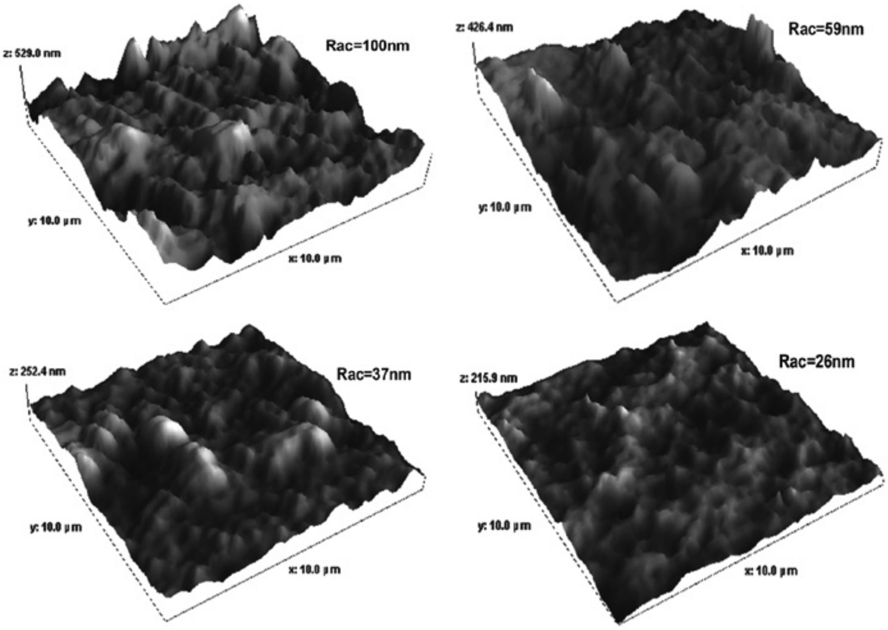
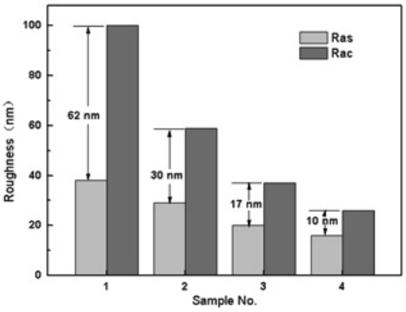


Fig.2 The AFM images of the surface of TiAlN coatings deposited on various roughness substrates

From the surface morphology investigation it can be deduced that the surface morphology of cathodic arc TiAlN coating is mainly affected by two parameters, i.e. the morphology of the substrate surface and the morphology induced by the coating growth process. On the other hand， the substrate roughness is reproduced on coating surface, which has been exaggeratedly formed.



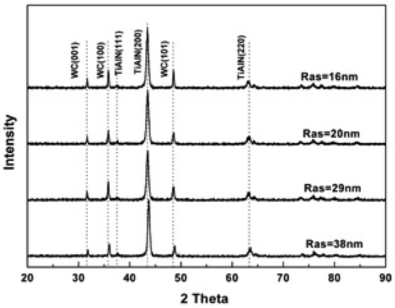
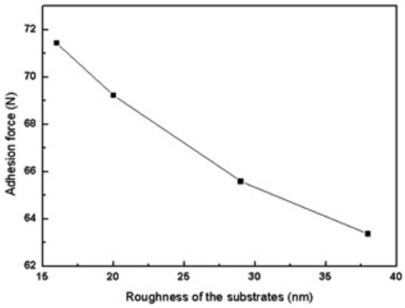


Fig.3 Variations of surface roughness of the samples before and after depositing coatings

Fig.4 The XRD patterns of TiAlN coatings with different substrate roughness

3.2. X-ray structural analysis

The diffraction peaks of TiAlN with B1-NaCl structure and WC (substrate) with hexagonal crystal structure are both exhibited in Fig.4. The intensity of second peak for TiAlN coating is considerably higher due to the (200) preferred orientation. The lattice parameter in the B1-NaCl structure decreases from 4.242 for pure TiN to 4.156 for TiAlN. Such lattice parameter's changes were observed by M. Zhou et al [13]. Substitution of Ti atoms with Al atoms in the B1-NaCl structure of TiN results in TiAlN phase. As a result of this substitution, the TiN lattice parameter decreases since the atomic size of Al is smaller than Ti. Results of XRD characterization reveals that phase of coatings does not show dependence on the substrate roughness as well as the diffraction angles for TiAlN (200) does not vary with substrate roughness.



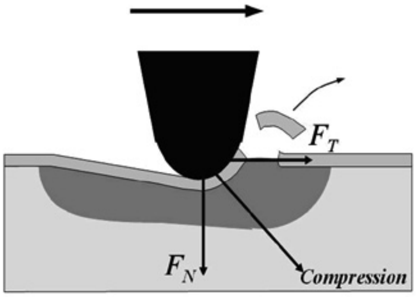


Fig.5 The critical loads of the coatings deposited on different roughness substrates

Fig.6 Principle of the scratching test method used in the present study

3.3. Scratching testing

Fig.5 shows the critical loads of the coatings deposited on the substrates with different roughness. The coating adhesion increases with the decreasing of the substrate roughness. The difference of two decades of nanometers on substrate roughness results in variation of adhesion force, which is up to 10%, as shown in Fig.5. It can be interpreted that the stresses generated are modeled as a combination of an indentation stress field, an internal stress present in coating and a tangential frictional stress during the scratching test [14]. The necessary requirement for coating failure is a sufficient compression [15]. In this work, all the coatings were deposited under the same condition. XRD analysis and thickness test indicate that substrate roughness is not a significant factor to affect the internal stress of TiAlN coatings. Therefore, the effect of internal stress on different samples in the scratch testing is almost the same. So the compression can be considered as the combined effect of indentation stress and tangential frictional stress in this study, as shown in Fig.6. Furthermore, it makes the difference of critical load among the samples. Frictional force is the product of indentation force and friction coefficient. So the indentation stress and the friction coefficient decide the compression, i.e. for the indentation is equal, the friction coefficient is higher, the compression is greater. Fig.7. shows the friction coefficient of coatings with different roughness during the scratching test. As shown in Fig.7, the roughness of coating is smaller, the friction coefficient is lower. The smoother coating bears a smaller frictional force during the scratching test. Under the combined effect of indentation stress and tangential frictional stress, the sufficient compression which makes the coating delamination needs a larger indentation stress for the smoother coating. And the critical load that measures the adhesion force is defined with the indentation stress. So the coating roughness is smaller, the critical load is higher. It can be deduced that the adhesion force between coating and substrate is affected by the morphology of the substrate surface, and we conclude that the best adhesion will be achieved at atomic level roughness of substrate.

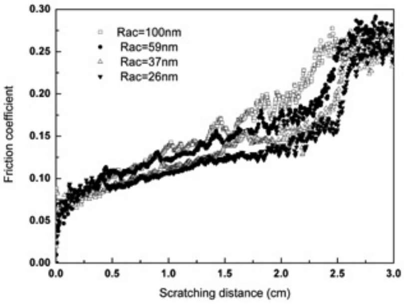


Fig.7 The friction coefficient of coatings with different roughness

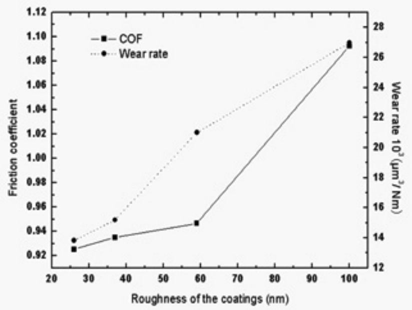


Fig.8 The variation of stabilized friction coefficient and coating wear rate with coating roughness for TiAlN coatings

3.4. Friction and wear testing

The variation of stabilized friction coefficient (COF) and coating wear rate with coating roughness for TiAlN coatings is shown in Fig.8. The ball wear rate was not measurable, since the wear scars were too small and smooth to observe.

It presents that the coating exhibits slightly higher level of friction coefficient (stabilized) at rougher surface, while the friction curves of the samples are all stabilized at a high level which is more than 0.9, shown in Fig.9. It can be seen that there is not quite significant difference on steady-state friction coefficient level for different coating roughness, but the sliding time when steady-state conditions are reached is longer for rougher coating surfaces. The similar result was obtained in Ref. [16].

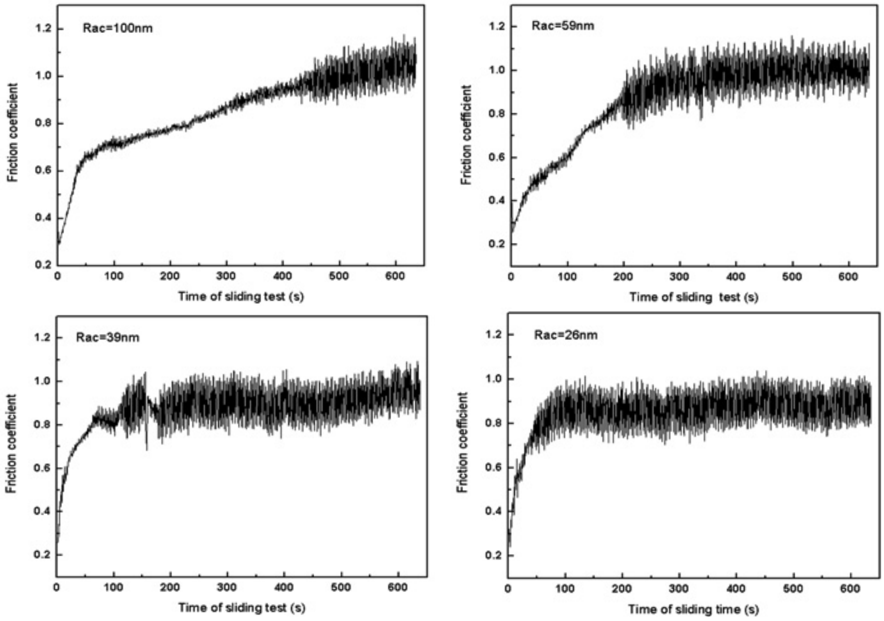


Fig.9 The friction curves for TiAlN coatings of different roughness

Wear rate was calculated by the following formula:

$$\text{wear rate} = \frac{\text{wear volume}}{\text{load} \times \text{sliding distance}}$$

where sliding distance was measured in m. The coatings were not worn out, since the depths of the coating tracks were less than 0.7 μm, much less than the coating thickness of 3 μm. Fig. 8 shows that the coating wear rate increases with increase in roughness of coating surface. In general, the wear rate depends on the initial roughness of the coating surface to some extent. Rougher surfaces show higher wear than smoother ones. It can be understood that contact occurs at the surfaces' summits during wear testing, while a rough surface has a smaller real contact area, therefore, a relatively greater surface pressure is loaded. Thus, low surface roughness of coating is believed to be responsible for relatively good wear resistance. For substrate roughness strongly affects deposited coating roughness, the pretreatment of substrate before deposition is considered as an important step for production of wear resistance coating, such as grinding and polishing, which effectively decrease substrate's roughness, then coating's. This is also in good agreement with the influence of substrate roughness on adhesion between coating and substrate, as previous part.

It should be mentioned that the influence of coating surface roughness is limited to the range of "top layer" of the coating. Thus, there can be a conjecture that the coating wear rate of different surface roughness will tend to the same value with the increase of sliding time, assuming the substrate's influence is neglected, which needs further study.

4. Conclusions

The structure and mechanical properties of TiAlN coatings deposited on substrates of different surface roughness have been systematically studied. The major results are as follows：

- The substrate roughness is reproduced in exaggerated form on the coating surface. The surface morphology of cathodic arc TiAlN coating is mainly affected by the morphology of the substrate surface and coating growth process.
- The crystal structures of TiAlN coatings do not show dependence on the substrate roughness.
- The adhesion force of coating-substrate system is affected by the morphology of substrate surface. The difference of two decades of nanometers on substrate roughness results in variation of adhesion force, which is up to 10%. Three stresses model is applied to interpret this result. It can be deduced the best adhesion will be achieved at atomic level roughness of substrate.

The steady-state friction coefficients for different coating roughness are all approximately 1.0, but the rougher coating surface needs longer time to reach the steady state. The wear test shows that the coating with smoother surface has better wear resistance.

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