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The Mechanical and Tribology Properties of Sputtered Titanium Aluminum Nitride Coating on the Tungsten Carbide Insert Tool in the Dry Turning of Tool Steel

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Abstract

The effect of the sputtering parameters on the mechanical tribology properties of Titanium Aluminum Nitride coating on the tungsten cabide insert tool in the dry turning of tool steel has been investigated. The coating was deposited using a Direct Current magnetron sputtering system with various substrate biases (-79 to -221 V) and nitrogen flow rates (30 to 72 sccm). The dry turning test was carried out on a Computer Numeric Code machine using an optimum cutting parameter setting. The results show that the lowest flank wear (~0.4 mm) was achieved using a Titanium Aluminum Nitride-coated tool that was deposited at a high substrate bias (-200 V) and a high nitrogen flow rate (70 sccm). The lowest flank wear was attributed to high coating hardness.

Abstrak

Sifat Mekanik dan Tribologi Lapisan Titanium Aluminium Nitrida pada Perkakas Tungsten Karbida dalam Pemotongan Kering Baja. Telah dilakukan penelitian mengenai pengaruh parameter sputering terhadap sifat mekanik dan tribologi lapisan Titanium Aluminum Nitrida pada perkakas potong tungsten karbida dalam proses pemotongan *turning* kering baja perkakas. Deposisi lapisan tipis dilakukan menggunakan sistem sputtering magnetron dengan variasi tegangan substrate (-79 s/d -221 Volt) dan laju alir gas nitrogen (30 s/d 72 sccm). Pemotongan *turning* kering dilakukan menggunakan mesin bubut otomatis CNC dengan parameter pemotongan optimum. Hasil percobaan menunjukan bahwa aus sisi terendah (~0.4 mm) perkakas ditunjukan oleh lapisan Titanium Aluminum Nitrida yang dideposisikan pada tegangan substrat (-200 V) dan laju alir gas nitrogen (70 sccm) tinggi. Rendahnya aus sisi perkakas diakibatkan oleh tingginya nilai kekerasan lapisan.

Keywords: dry turning, flank wear, hardness, sputtered TiAlN coating, tool steel

1. Introduction

The mechanical properties of Titanium Aluminum Nitride (TiAlN) coating on the tungsten carbide insert tool, such as hardness and adhesion strength, is required to improve its performance, such as its wear resistance in the machining process. During the reactive magnetron sputtering process, the coating properties, such as composition, structure, and morphology, can be controlled by varying the process parameters, and then the tool performance thus the tool performance can be compared based on the process parameters. The sputtered coating composition may depend on the target composition (the metallic to metallic ratio of the alloy target). A stoichiometric of the TiAl target (50:50 at.%) may produce a different sputtered TiAlN coating composition due to the varying sputtering parameters [1]. The sputtered coating crystal was a columnar structure, which consists of pores between the grain boundaries due to low ion bombardment energy during coating deposition [2]. The structure transformation of the TiAlN coating crystal occured because of the varying substrate biases and the nitrogen gas pressure [3].

The increase of the TiAlN coating hardness was achieved by increasing the negative substrate bias and resulted in the improvement of wear resistance [4]. The hardness of the TiAlN coating also increased with the increasing nitrogen flow rate, but it had low wear resistance [5]. An early finding was reported that better wear resistance was shown by the TiAlN-coated insert deposited at a high nitrogen flow rate above the critical nitrogen flow rate [6].

The improvement of the wear resistance of the sputtered TiAlN-coated insert tools may have been due to the improvement of the coating properties. Thus, the optimization of the sputtering parameters, such as the substrate bias and the nitrogen flow rate, in depositing the TiAlN coating on the insert tool is related to the improvement of the tool performance. The objective of this investigation was to determine the influence of the substrate bias and the nitrogen flow rate on the hardness and the tool wear of the sputtered TiAlN-coated insert tool in the dry cutting of tool steel. The sputtering parameters were optimized using Response Surface Methodology (RSM).

2. Experiment

The TiAl alloy (50:50) target was used to deposit the coating on the tungsten carbide insert tool (SPGN 120308). The dimension of the target (length x width x thickness) was (60 x 10 x 3) cm^3. The uncoated insert was ultrasonically cleaned in ethanol for 30 minutes at room temperature. Prior to deposition, the insert was etched by Ar ion bombardment with a flow rate of 180 sccm and a substrate bias of -300 V for 30 minutes. To improve the coating adhesion, the TiAl interlayer was deposited using a 123 sccm argon flow rate and a substrate bias of -100 V for 10 minutes. The deposition of the TiAlN coating on the tungsten carbide insert tool was conducted in an Ar-N_2 mixture with a constant Ar flow rate of 123 sccm, a target current of 5 A, and a substrate temperature of 350 °C for 90 minutes. The deposition was carried out at various substrate biases (-79 to -200 V) and nitrogen flow rates (30 to 72 sccm). A pump at a constant speed of 2050 L/s was utilized to achieve an ultimate chamber pressure of 5 x 10^{-5} mbar. After the deposition was completed, the chamber was cooled down for 50 minutes before the chamber was vented.

The TiAlN coating hardness was measured using a Shimadzu Dynamic Ultra-Microhardness tester at applied loads of 5 grams. In the present study, the hardness samples were characterized using a triangular pyramid diamond indenter with a 115° tip angle (standard). The holding time of the indentation process was 10 s. The tool performance test was conducted using a Computer Numerical Code (CNC) for the dry turning of the tool (D2) steel. The cutting parameter setting used was adopted from a previous study [7]. The flank wear of the TiAlN-coated insert tools was measured using an optical microscope. The RSM analysis used to identify the relationship between the sputtering parameters and the hardness and the flank wear of the sputtered TiAlN-coated insert tool was performed using the Central Composite Design. The ranges of the substrate bias and the nitrogen flow rate analyzed were from -100 V to 200 V and 60 sccm to 70 sccm, respectively. The experiment runs consisted of 13 tests in which 4 tests were run for the factorial points, 4 tests were run for the axial points, and 5 tests were run for the center points.

3. Results and Discussion

13 samples of TiAlN coating on the tungsten carbide inserts deposited at various substrate biases and nitrogen flow rates and its composition, hardness, and flank wear are shown in Table 1. The thickness of the TiAlN coatings deposited on the tungsten carbide insert tool varied between 0.6 to 2 μm. Figure 1(a) shows the cross-section area of TiAlN coatings deposited at the substrate bias of -100 V and the nitrogen flow rate of 60 sccm with a coating thickness of about 2 μm. The EDX analysis (Figure 1(b)) showed that the elemental compositions of the coating were 32.18 at.% Ti, 27.38 at.% Al, and 40.44 at.% N.

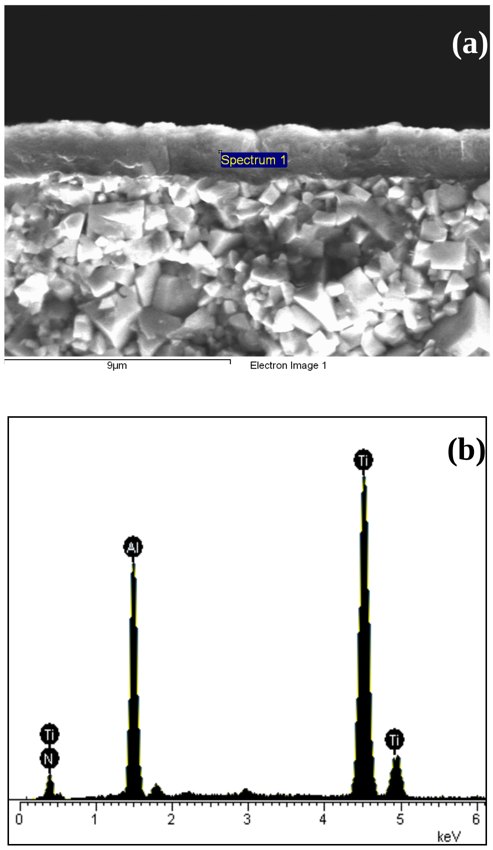
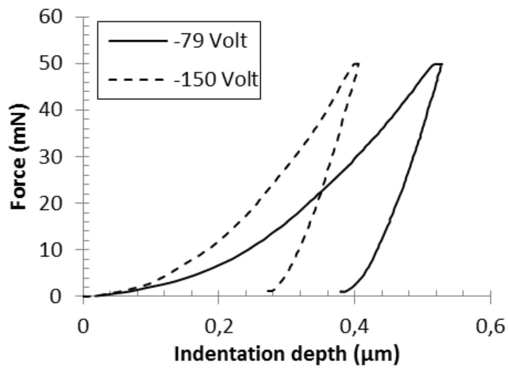


Figure 1. (a) SEM Image of a TiAlN Coating Fracture with a Thickness of ~ 2 μm and (b) its EDX Composition Deposited at the Substrate Bias of -100 V and the Nitrogen Flow Rate of 60 sccm

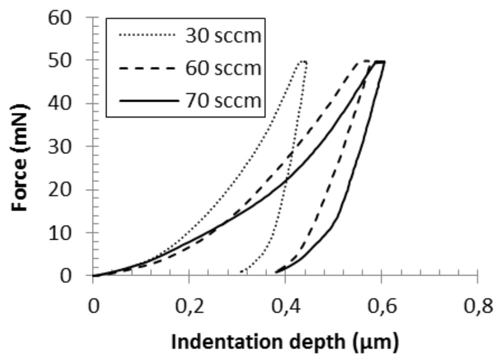
Table 1. TiAlN Coating Composition at Various Substrate Biases and Nitrogen Flow Rates

Run	V_b (-V)	N_2 flow rate (sccm)	Ti at.%	Al at.%	N at.%	Hardness (GPa)	VC (mm)
1	150	65	27.22	28.49	44.30	16.28	0.375
2	150	58	20.08	30.68	49.24	20.56	0.544
3	200	70	25.64	24.59	49.77	18.07	0.405
4	150	65	19.96	23.85	56.20	18.48	0.466
5	100	60	32.18	27.38	40.44	9.67	0.496
6	150	65	18.70	27.48	53.82	16.35	0.506
7	150	65	23.18	32.43	44.39	19.04	0.529
8	221	65	31.89	32.63	35.47	24.04	0.413
9	150	72	14.52	42.08	43.40	17.56	0.425
10	79	65	18.80	32.35	48.86	10.90	0.437
11	200	60	17.04	38.62	44.34	20.17	0.419
12	100	70	23.23	27.66	49.11	8.15	0.419
13	150	65	20.89	34.30	44.81	24.05	0.422

The coating hardness can be evaluated by loading/ unloading the curve measured by a dynamics micro-hardness tester, as shown in Figure 2. The hardness measured is defined by $H = L_{max}/[26.34\ (d_{cor})^2]$ where d_{cor} is the penetration depth in the plastic deformation area and is given in unit of kg/mm^2 or Giga Pascal (GPa) where 1000 kg/mm^2 = 9.807 GPa [8]. The area under the curve represented the elastic deformation energy, while the area between the curves represented the plastic deformation energy. The lower the indentation depth or the smaller the area between the curves, the harder the coating was.



(a)



(b)

Figure 2. Force vs Indentation Depth of TiAlN Coating at (a) Various Substrate Biases and Nitrogen Flow Rates of 65 sccm; (b) Various Nitrogen Flow Rates and Substrate Biases of -100 V

The average hardness values of the three measurements at various substrate biases and nitrogen flow rates are presented in Figures 3(a) and 3(b), respectively. It is shown that the hardness tend to increase as the substrate bias is increased, while it decrease as the nitrogen flow rate is increased.

The RSM experimental result of the coating hardness measurement as a function of the substrate bias and the nitrogen flow rate is presented in Table 1. From the sequential model sum of squares analysis and the lack of fit test, the linear model is suggested to represent the relationship between the TiAlN coating hardness and the sputtering parameters of the substrate bias and the nitrogen flow rate.

The analysis of variance (ANOVA) for the response surface linear model is summarized in Table 2. The model shows a significant value, which is indicated by the p-value of 0.0045. This means that the terms in the model have a significant effect on the response (TiAlN coating hardness). Based on the p-value, the main factor of the substrate bias significantly influences the TiAlN coating hardness. The ANOVA analysis showed that the substrate bias term was significant (p-value < 0.05) in influencing TiAlN coating hardness, while the nitrogen flow rate was not a significant factor.

Based on the regression analysis, the TiAlN coating hardness as a function of the substrate bias and the nitrogen flow rate can be predicted using Equation (1).

$$y = 17.17975 + 4.864274\ x_1 - 0.98839\ x_2 \qquad (1)$$

where: y = hardness (GPa)
x_1 = substrate bias (-V)
x_2 = nitrogen flow rate (sccm)

Equation (1) can be plotted as a three-dimensional (3D) graph of TiAlN coating hardness with respect to the substrate bias and nitrogen flow rate, as shown in Figure 4. It is shown that the highest coating hardness was achieved by high negative substrate bias and nitrogen flow rate.

The flank wear is mainly due to the abrasion between the tool and the workpiece during the dry cutting process. The fabricated TiAlN coating on the WC insert was tested using fixed optimum cutting parameters and shows that the flank wear VC is the dominant mode of the tool wear (Figure 5).

The experimental results show that the flank wear was influenced by the coating properties that were deposited at various substrate biases and nitrogen flow rates. The effect of the substrate bias on the flank wear is presented in Figure 6(a). It shows that, generally, the flank wear tended to decrease with an increasing negative substrate bias of up to about -200 V. The effect of the nitrogen flow rate on the flank wear is presented in Figure 6(b). It shows that, generally, the flank wear of -100 V, -150 V, and -200 V decreases with an increasing nitrogen flow rate of up to about 70 sccm.

The effect of the substrate bias and the nitrogen flow rate on the flank wear of the TiAlN coating was analyzed using RSM. The flank wear measurement data is taken from the experimental data in Table 1. From the sequential model sum of the squares of the flank wear and the lack of fit test, the linear model is suggested to predict the effect of the substrate bias and the nitrogen flow rate to the flank wear.

The Analysis on Variance (ANOVA) for the response surface linear model of the flank wear is presented in Table 3. Although the model is not significant, the lack of the fit test value is not significant. This means that the model can still be used to predict the relationship between the process parameters and the tool performance. Compared with the negative substrate bias, the nitrogen flow rate (p-value is 0.0841) is the influential parameter for the flank wear.

The linear model of the flank wear as functions of the substrate bias and the nitrogen flow rate can be written in Equation (2).

$$y = 0.451 - 0.016\ x_1 - 0.033\ x_2 \qquad (2)$$

where: y = flank wear (mm)
x_1 = substrate bias (-V)
x_2 = nitrogen flow rate (sccm)

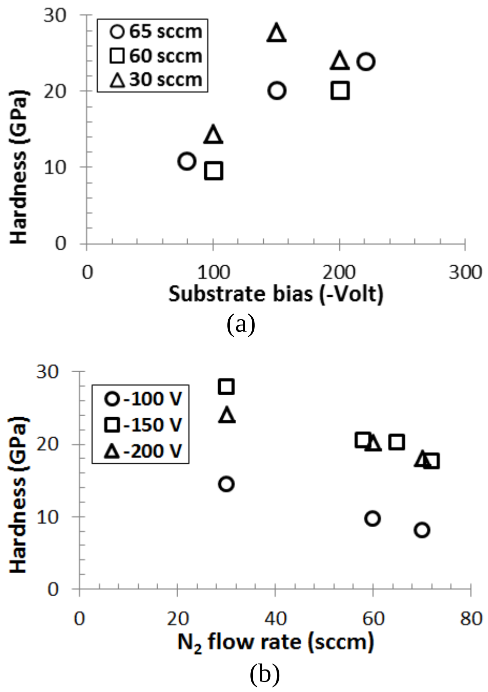


Figure 3. The TiAlN Coating Hardness at (a) Various Substrate Biases and (b) Nitrogen Flow Rates

Table 2. The ANOVA for the Response Surface Linear Model of the TiAlN Coating Hardness

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	197,8025	2	98,9013	9,7167	0.0045
A-Substrate bias	190,0653	1	190,0653	18,6732	0.0015
B-Nitrogen flow rate	7,7372	1	7,7372	0,7601	0.4037
Residual	101,7850	10	10,1785		
Lack of Fit	61,6819	6	10,2803	1,0254	0.5144
Pure Error	40,1031	4	10,0258		
Cor Total	299,5876	12			

Based on the suggested linear model, it is shown that the lowest flank wear (highest desirability) is achieved by a higher substrate bias and a higher nitrogen flow rate combination. Equation (2) can be illustrated by a 3D graph, as shown in Figure 7.

Generally, the TiAlN coating hardness increases with an increasing negative substrate bias. Similar results were reported by other researchers. The hardness of the TiAlN coating increased with an increasing substrate bias due to the increase in the coating density [6,9]. The increase of the coating density is attributed to reducing the coating crystal size and the finer microstructure. The decreased crystal size is due to the interruption of columnar structure growth by a re-nucleation process. The re-nucleation process is induced by high ion bombardment energy and enhanced by the increase of a negative substrate bias [10].

The high TiAlN coating hardness may also be attributed to the Al atom substitution at the Ti atom position in the TiN structure. Since the Al atom size is smaller than the Ti atom, the lattice parameter of the TiN structure decreases when the Al atom position replaces the Ti atom position [11]. Therefore, the TiAlN coating hardness increases with an increase of Al content. The hardness of the TiAlN coating should increase with an increasing negative substrate bias due to the increasing Al content; however, there is an optimum Al content that can enhance the TiAlN hardness [12]. The hardness increases with an increasing Al concentration and reaches a maximum value at an Al concentration of 50 mol% [13]. A further increase in the Al content causes the hardness to decrease rapidly due to the appearance of the B4 structure (hexagonal structure). The hexagonal structure (or Wurtzite structure) exhibits a lower hardness than the B1 structure (cubic structure) [14].

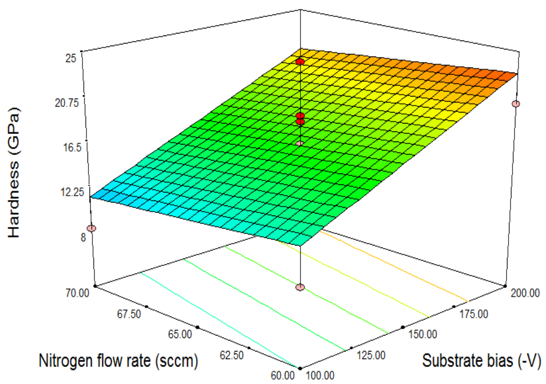


Figure 4. Three-dimensional Graph of the TiAlN Coating Hardness as a Function of the Substrate Bias and the Nitrogen Flow Rate

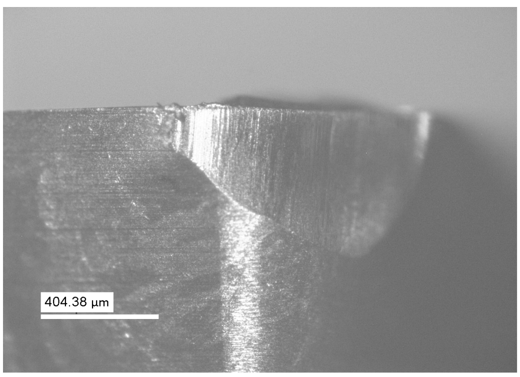


Figure 5. The Flank Wear VC Mode of the TiAlN-coated WC Insert Deposited at -150 V and 65 sccm in the Dry Turning of D2 Steel

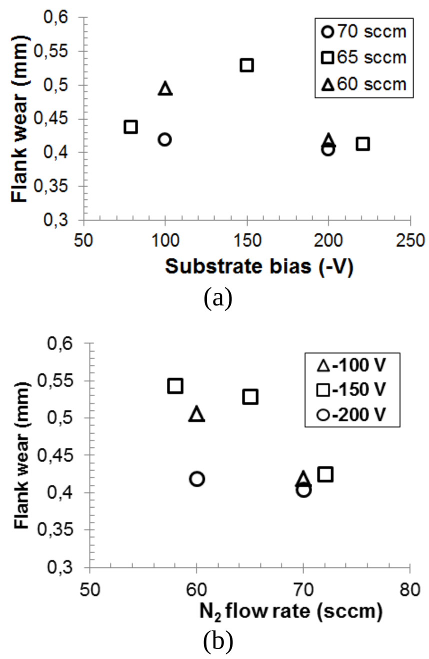


Figure 6. The TiAlN Coating Flank Wear at Various Substrate Biases (a) and Nitrogen Flow Rates (b)

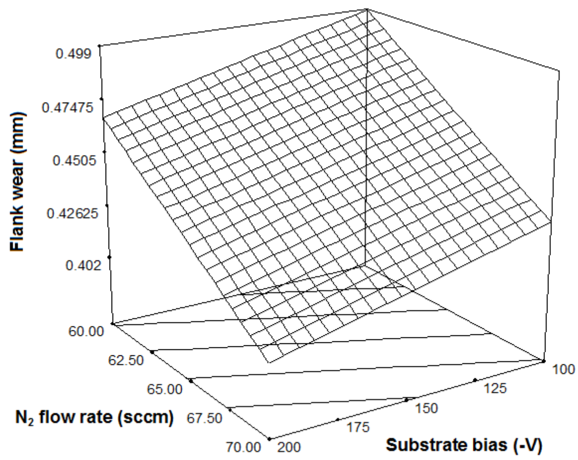


Figure 7. Three-dimensional Graph of the TiAlN Coating Flank Wear as a Function of the Substrate Bias and the Nitrogen Flow Rate

Table 3. The ANOVA for the Response Surface Linear Model ofthe TiAlN Coating Flank Wear

Source	Sum of squares	df	Mean squares	F value	p-value prob> F
Model	0.0103	2	0.0052	2.267	0.1542
A-V_b	0.0019	1	0.0019	0.8552	0.3769
B-N_2 flow rate	0.0084	1	0.0084	3.6788	0.0841
Residual	0.0228	10	0.0023		
Lack of Fit	0.0072	6	0.0012	0.3078	0.9038
Pure Error	0.0156	4	0.0039		
Cor Total	0.0331	12			

The present study results show that when the substrate bias is increased to up to -150 V, the Ti content increases and causes the increase in the coating hardness. The Ti content decreases with a further increasing substrate bias (except at a high nitrogen flow rate of 65 sccm), but the coating hardness tended to increase with a further increase in the negative substrate bias. The coating hardness may be attributed to the composition heterogeneity, the coating thickness, and the texture variation of the TiN-structure. From the experimental results, it appears that the coating hardness is not related to the coating composition.

The TiAlN coating hardness is also influenced by the nitrogen flow rate. The TiAlN coating hardness increased with an increasing nitrogen flow rate due to the presence of the AlN phase along with the TiN phase [5]; however, a further increase in the nitrogen flow rate increases the presence of the AlN phase, and it is not useful for the wear resistance application. The TiAlN coating hardness increased with an increasing nitrogen flow rate due to the increase of the nitrogen content [12]. The nitrogen content influenced the amorphous and crystalline phase formation and affected the coating hardness. The columnar morphology of the TiAlN became denser with an increasing nitrogen flow rate, which may increase the coating hardness [15]; however, the present study results show that, generally, the coating hardness decreased with the increase of the nitrogen flow rate. This is probably due to the new phase formation from the reaction between Al and N [11,16]. A small and disordered new phase could not be detected in the XRD measurement due to the weak diffraction intensity. The new phases potentially hinder the TiAlN crystal growth and can result in weak diffraction intensity. The new phases that may cause a reduction in TiAlN coating hardness are Ti_2AlN, $Ti_3Al_2N_2$ (hexagonal structure), or Ti_3AlN (perovskite structure).

There are other mechanisms involved in increasing the coating hardness, such as the refinement crystal size and the enhancement of the defect density, solution hardening, and/or second-phase precipitation [9,17]. It is shown that the substrate bias influenced the back-scattering process of the incoming ions. The Al content in the sputtered TiAlN coating decreases with an increasing negative substrate bias due to the back sputtering effect during the deposition because the Al atom is lighter than the Ti atom (the back-scattering process increased with an increasing negative substrate bias and caused a decrease of the Al content, which contributed to the hardness enhancement in terms of the defect hardening).

It has been shown that the TiAlN coating hardness strongly depends on its structure. The present study shows that the coating structure changes at various substrate biases [18]. In general, the increase of the coating hardness as the negative substrate bias increases is due to the reduction of the (111) peak. It was observed that the crystal plane (200) peak increases instead of reducing (111) the peak as the negative substrate bias increases [14]; however, the coating hardness did not depend on its structure in terms of the crystal plane orientation but did depend on its nanostructure [19]. The deformation mechanism of the nanocrystaline coating may be different from the normal bulk material. The nanocrystaline material may be deformed by the grain boundary rotation or the grain boundary sliding rather than by the dislocation slip via the slip system for the bulk material [20]. Therefore, the nanocrystaline coating hardness does not depend on the crystal plane orientation.

The RSM analysis result of the effect of the sputtering parameters on the TiAlN coating hardness shows a consistency compared with the conventional experiment-tal approach result in terms of the substrate bias effect on the coating hardness. It is shown that the substrate bias is a significant factor for the coating hardness.

An increase of a negative substrate bias increases the coating hardness. As mentioned previously, the coating hardness is related to the coating density and the coating crystal size. The decrease of the crystal size causes the increase of the density and eventually increases the coating hardness.

The wear rate of the TiAlN coatings decreases with an increasing negative substrate bias due to the increasing coating hardness and the residual stress [9]. This finding supports the present study results that the wear rate of the TiAlN-coated inserts decreases with an increasing negative substrate bias. Based on the analysis of the substrate bias effect on the coating hardness, it is found that the coating hardness increases with an increasing negative substrate bias.

It was found that the wear resistance of TiAlN improved when substrate bias was applied due to the columnar structure disappears [4]. The increase of the coating hardness with the increase of a negative substrate bias is usually followed by a decrease of adhesion strength due to the increase of residual stress. The optimum wear resistance of the TiAlN coating occurs at a higher substrate bias and nitrogen flow rate; however, after increasing the nitrogen flow rate further, the degraded wear resistance occurred [6]. The present study results show that the flank wear of the TiAlN-coated insert decreases with an increasing nitrogen flow rate. The decrease of the flank wear with the increasing nitrogen flow rate may be due to the presence of the AlN phase along with the TiN phase; however, increasing the AlN presence further is not useful for wear resistance application [5].

4. Conclusions

A negative substrate bias is a significant factor for the TiAlN coating properties, especially for coating hardness. Generally, the coating hardness increased with an increase in the substrate bias of up to -200 V due to the decreased coating crystal size. The cutting test result showed that the lowest flank wear (~0.4 mm) was achieved when the TiAlN coating was deposited at a high negative substrate bias of -200 V and a high nitrogen flow rate of 70 sccm.

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