

## Application of ANFIS in Predicting of TiAlN Coatings Hardness

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**Abstract:** In this paper, a new approach in predicting the hardness of Titanium Aluminum Nitride (TiAlN) coatings using Adaptive Neuro-Fuzzy Inference System (ANFIS) is implemented. TiAlN coated cutting tool is widely used in machining due to its excellent properties. The TiAlN coatings were formed using Physical Vapor Deposition (PVD) magnetron sputtering process. The substrate sputtering power, bias voltage and temperature were selected as the input parameters and the hardness as an output of the process. A statistical design of experiment called Response Surface Methodology (RSM) was used in collecting optimized data. The ANFIS model was trained using the limited experimental data. The triangular, trapezoidal, bell and Gaussian shapes of membership functions were used for inputs as well as output. The results of ANFIS model were validated with the testing data and compared with fuzzy and nonlinear RSM hardness models in terms of the root mean square error (RMSE) and model prediction accuracy. The result indicated that the ANFIS model using 3-3-3 triangular shapes membership function obtained better result compared to the fuzzy and nonlinear RSM hardness models. The result also indicated that the ANFIS model could predict the output response in high prediction accuracy even using limited training data.

**Key words:** ANFIS technique, hardness, TiAlN coatings, PVD magnetron sputtering

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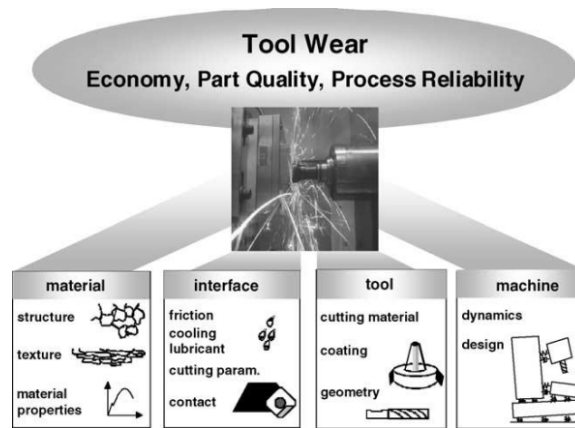
## INTRODUCTION

In high-speed machining process, the cutting tool is consistently dealing with high localized stress at the tool tip and high temperature which exceeds 800°C. In this process too, the cutting tool slides off the chip along the rake face and the newly cut workpiece surface (Kalpakjian and Schmid 2006). These conditions are causing tool wear, reducing the cutting tool performances and quality of parts and deteriorating the tool life. The tool wear problem also could be influenced by workpiece material, cutting interface, cutting tool performance and geometry and machine condition. In addition, tool wear condition has a direct effect on the economics of cutting operations, final product quality and process reliability (Yen *et al.* 2004). Fig. 1 shows the cause and effect of tool wear in machining process.

The wear problem could be addressed by improving the hardness of the cutting tool surface. This could be done by applying the thin film coating on the cutting tool. The main purpose of the thin film coating application is to improve the tool surface properties while maintaining its bulks properties. The performance of the coated tool has been proven in wear mechanism (Bhatt *et al.* 2010), hardness and adhesion (Jianxin *et al.* 2008) and tool life (Su *et al.* 2004). It is also has been ascertained that the coated tool is forty times better in tool wear performance compared to the uncoated tools (Tuffy *et al.* 2004). This finding promises prolonging of tool life and enables the implementation of minimum liquid lubrication to reduce cost of coolant that makes up 16 to 20% of manufacturing cost (Sreejith and Ngoi 2000). This finding too contributes in minimizing environmental impacts produced by discarding of cutting fluid (Byrne and Scholta 1993).

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**Fig. 1:** Four major functional elements influencing tool wear in machining process (Yen *et al.* 2004).

Physical Vapor Deposition (PVD) coating process plays essential roles in order to make the cutting tool perform better. It has been selected as a main coating process in hard coating purposes. However, two main challenging issues that need to be encountered in the coating process are cost and customization. The challenge to ensure reasonable cost in the process of coating and efficient process of treatment should be well-addressed as it directly affects the cutting tool market value (Bradbury and Huyanan 2000). Besides the equipment maintenance, other reasons that lead to high machining costs are the material usage and labor and the number of trial-and-error experiment. In PVD magnetron sputtering, process parameters like sputtering power, substrate bias voltage, substrate temperature (Md Nizam 2010), gas pressure (Sun *et al.* 2010) and turntable speed (Zhou *et al.* 2009) influence the coating performances. These conditions cause complexity in the coating process. In addition, the new application of coating needs trial and error experiments so that it could suit the parameters with the material used. Therefore, many researchers have developed models to address the coating process issues. Model development reduces resources wastage such as materials, equipment utilization, human resources and working time related to the trial and error experiments run.

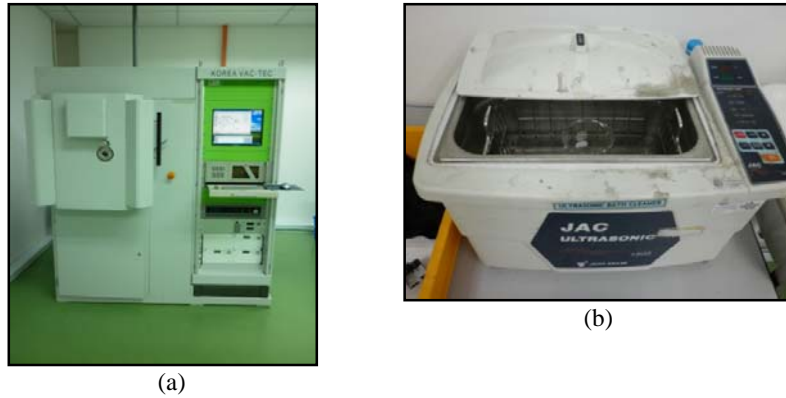
The coating process model is very useful to predict the coating performances while looking for the optimized value. However, limited number of experimental data due to experimental cost issue is a major constraint in modelling work. Various techniques such as design of experiment (Xiao and Zhu 2010), neural network (Cetinel *et al.* 2006), fuzzy logic (Manaila *et al.* 2002) and ANFIS (Buragohain and Mahanta 2008) have been applied. The design of experiment approaches like Taguchi, full factorial and Response Surface Methodology (RSM) are widely used to collect optimum and minimum experimental data (Karacan *et al.* 2007).

The Adaptive Neuro-Fuzzy Inference System (ANFIS) has been used in predicting the output response in many applications. The rules of the model is developed based on training data pairs and suggestion from the expert. The ANFIS has been proven to be well-suited for modelling nonlinear industrial processes such as end milling (Uros *et al.* 2009), wire-EDM (Ulas *et al.* 2009), welding (Zapata *et al.* 2010) and waterjet cleaning (Daoming and Jie 2006). In view of the nonlinear conditions of a the magnetron sputtering coating process, the ANFIS is employed for predicting the hardness value of TiAlN coatings. So far, there is no study has been carried out on application of ANFIS for predicting the hardness of TiAlN coatings. The main purpose of this study is to investigate the application of ANFIS model for predicting the hardness of TiAlN coatings with limited experimental data.

## MATERIALS AND METHODS

### *Experimental Run:*

The experiment was run in unbalanced PVD magnetron sputtering system made by VACTEC Korean model VTC PVD 1000 which has two vertically mounted TiAl alloys. This system also consists of substrate holder with adjustable planetary rotation. Fig. 2 (a) shows the PVD magnetron sputtering system. The titanium alloy was selected as the target material and the chemical compositions of the material was 50% of titanium and 50% of aluminum. The surface of tungsten carbide cutting tool insert was cleaned with alcohol bath in an ultrasonic cleaner for 20 minutes as shown in Fig. 2 (b). The substrates were loaded in the rotating substrate holder inside the coating chamber. The rotation speed was set at 5 rpm. Argon gas was used to produce electron and sputter the target material. The substrate was coated with the alloy in presence of nitrogen gas as the reactive gas.

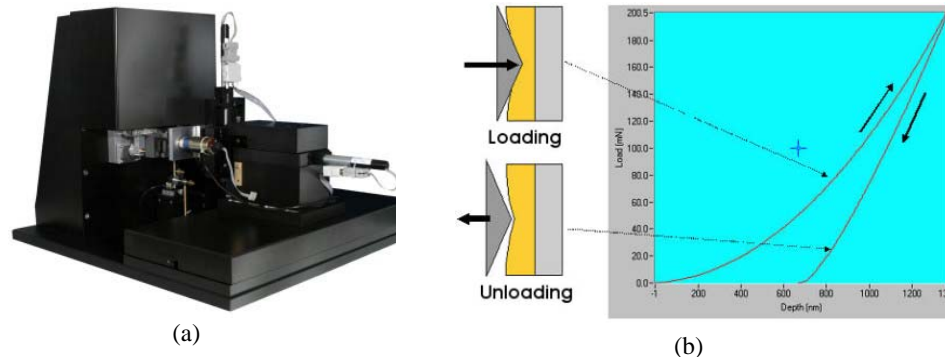


**Fig. 2:** (a) PVD unbalanced magnetron sputtering system model VTC PVD 1000, and (b) ultrasonic bath cleaner

**Table 1:** The experiment setting.

Process	Substrate ion cleaning	Interlayer coating deposition (TiAl)	TiAlN coating deposition
Argon pressure:	$5.5 \times 10^{-3}$ mbar	$4.0 \times 10^{-3}$ mbar	$4.0 \times 10^{-3}$ mbar
N <sub>2</sub> pressure:	-	-	$0.4 \times 10^{-3}$ mbar
Ion source power:	0.24 kV/ 0.4 A	0.24 kV/ 0.4 A	0.24 kV/ 0.4 A
Substrate bias:	-200V	-200V	-50-300V
Duration:	30 mins	5 mins (0.2 micron)	90 mins

The coating process consisted of three stages: 1). substrate ion cleaning, 2). interlayer coating deposition and 3). TiAlN deposition. The purpose of the substrate ion cleaning process is to remove impurity from the substrate surface for better adhesion. The interlayer coating deposition of TiAl was done to minimize the coefficient of thermal expansion gradient between the insert and TiAlN coatings. The detail process settings of the three stages are summarized in Table 1. The RSM centre cubic design (CCD) using Design Expert software version 7.03 was used to develop the experimental matrix. The influences of sputtering power, bias voltage and substrate temperature on the coating hardness were observed.



**Fig. 3:** (a) NanoTest nano-indentation system to measure the hardness of the coating. (b) The loading and unloading curve.

In this study, the hardness of TiAlN was measured using nano-indentation test. In nano-indentation system as shown in Fig. 3 (a), the hardness measuring process was done by indenting a specimen by a load from a very small set value to a maximum set value using a high precision instrument. Every load and displacement reading was recorded continuously. The mechanical properties of thin films coatings can be derived from the measure load-displacement loading/unloading curve through appropriate data analysis. A usual loading/unloading curve is shown in Fig. 3 (b). This curve is used to calculate the hardness and Young modulus as published by Oliver and Pharr (Oliver and Pharr 1992).

For this study, all of the samples were tested using Berkovitch indenter with maximum load set at 50mN. The dwell time at this load was set at 10 seconds. For each sample, six measurements were taken and the average value was calculated to be used as the harness value for the particular sample. Table 2 shows the input

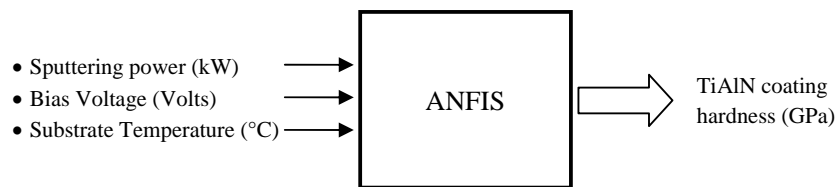
process parameter and experimental result of TiAlN coatings hardness. This data is used for training purpose. Table 3 shows another three experimental run with different combination of input value and the result was used for testing purpose. Fig. 4 shows the sputtering power, bias voltage and substrate temperature as the input variables to the model and the TiAlN coating hardness as the predicted output.

**Table 2:** Process variables and experimental result of hardness of TiAlN coatings for training purpose.

Run	Process variables			Result
	Sputter Power (kW)	Bias Voltage (Volts)	Substrate Temp. (°C)	Hardness (GPa)
1	6.00	50.00	400.00	3.54
2	4.81	100.67	518.92	5.27
3	4.81	249.33	281.08	13.17
4	6.00	175.00	400.00	10.96
5	6.00	175.00	200.00	8.06
6	4.81	100.67	281.08	4.33
7	7.19	249.33	281.08	4.04
8	6.00	175.00	400.00	16.12
9	6.00	175.00	400.00	7.77
10	4.81	249.33	518.92	3.53
11	7.19	100.67	281.08	9.76
12	6.00	175.00	600.00	7.48
13	7.19	249.33	518.92	15.26
14	6.00	175.00	400.00	8.91
15	8.00	175.00	400.00	22.64
16	6.00	300.00	400.00	14.14
17	7.19	100.67	518.92	8.88
18	4.00	175.00	400.00	15.69
19	6.00	175.00	400.00	11.27
20	6.00	175.00	400.00	12.34

**Table 3:** Data of TiAlN coating hardness for testing purpose

Run	Process variables			Result
	Sputter Power (kW)	Bias Voltage (Volts)	Substrate Temp. (°C)	Hardness (GPa)
1	5.00	100.00	280.00	5.2
2	6.50	150.00	350.00	10.3
3	7.00	145.00	450.00	14.2



**Fig. 4:** The inputs and output of the ANFIS model.

**ANFIS Modeling:**

Adaptive Neuro-Fuzzy Inference System (ANFIS) was presented by Jang in 1993 (Jang 1993). In this system, a hybrid learning procedure is used to construct an input-output mapping based on the human knowledge and training data pairs. The fuzzy inference system is employed in the framework of adaptive networks. ANFIS is normally contains a five-layer feed forward neural network excluding inputs to construct the inference system. Each layer consists of several nodes described by nodes function. The nodes in previous layer feed input to nodes in next layer.

ANFIS can be classified into two types based on the input space partition method which are grid and clustering partition. The grid partition (GP) construct the rules by enumerating all possible combination of membership functions (MFs). The Fig. 5 illustrates the structure of ANFIS-GP with three input and using two membership functions. This leads to an exponential explosion even when the number of inputs is moderately large. For example, the ANFIS with 3 inputs, each of which has 2 MFs, the GP creates  $2^3 = 8$  rules.

The five network layers are used in ANFIS to perform the following fuzzy inference steps: 1). fuzzification, 2). product, 3). normalization, 4). defuzzification, and 5). summation output.

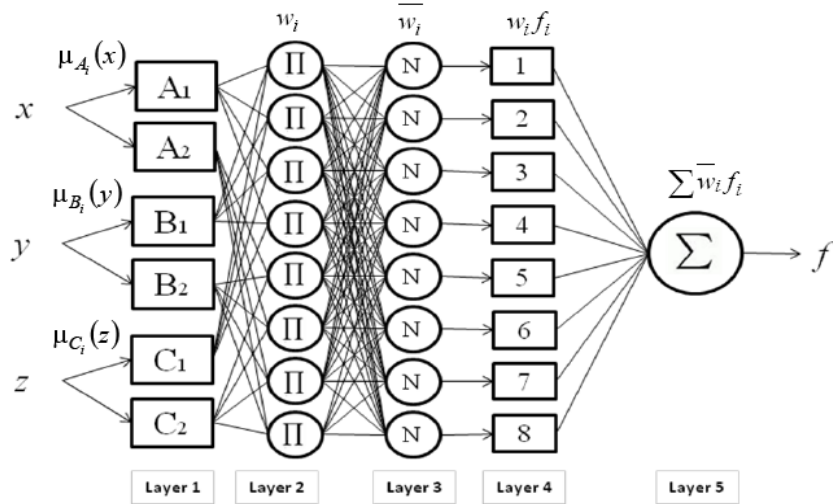


Fig. 5: The ANFIS structure with five layers and nodes.

**Layer 1: Transferring input data to the fuzzified values through membership functions.**

$\mu_{A_i}, \mu_{B_i}, \mu_{C_i}$  are membership functions.

Input data  $[x], [y]$  and  $[z], i = 1, 2$

$$[x] \Rightarrow [\mu_{A_i}(x)], [y] \Rightarrow [\mu_{B_i}(y)] \text{ and } [z] \Rightarrow [\mu_{C_i}(z)]$$

Consider, a bell-shaped membership function.

$$\mu_{A_i}(x) = \frac{I}{I + \left[ \left( \frac{x - c_i}{a_i} \right)^2 \right]^{b_i}} \tag{1}$$

where  $[a_i, b_i, c_i]$  is the premise parameter set.

**Layer 2: Multiplying the incoming signals and sending the product out.**

$$w_i = \mu_{A_i}(x) \times \mu_{B_i}(y) \times \mu_{C_i}(z), i = 1, 2 \tag{2}$$

Each node output represents the firing strength of a rule.

**Layer 3: Normalizing the firing strengths.**

$$\bar{w}_i = \frac{w_i}{\sum_i w_i}, i = 1, 2 \tag{3}$$

**Layer 4: Defuzzification**

$$\bar{w}_i \cdot f_i = \bar{w}_i \cdot (p_i \cdot x + q_i \cdot y + r_i \cdot z + s_i) \tag{4}$$

where  $(p_i, q_i, r_i, s_i)$  is the consequent parameter set, which is determined during the training process. If  $p_i, q_i, r_i$  are zero ( $f = \text{constant}$ ), the model is called zero-order-Sugeno model. Alternatively, first-order-Sugeno model.

**Layer 5: Summation of all incoming signals.**

$$\text{Overall output} = \sum_i \bar{w}_i \cdot f_i = \frac{\sum_i w_i \cdot f_i}{\sum_i w_i}, i = 1, 2 \tag{5}$$

The output of each rule is a linear combination of input variables plus a constant term and the final output is the weighted average of each rule's output.

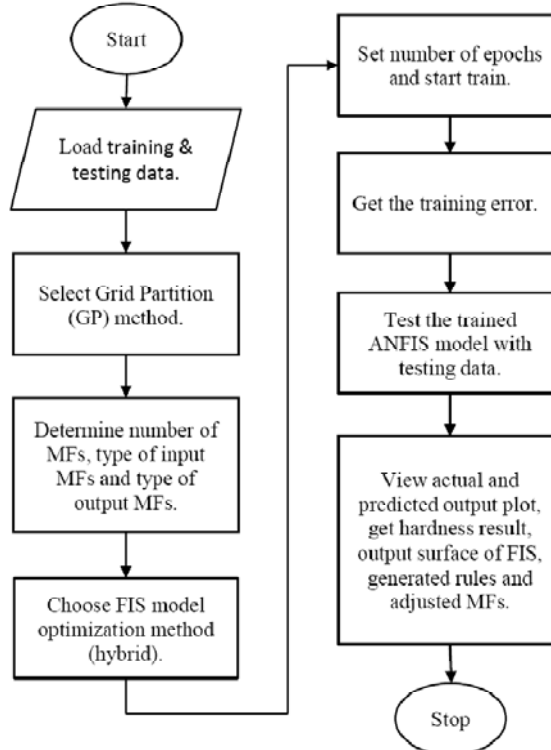
There are many type of parameters need to be set in ANFIS modelling. The parameters give a minor and major influence to the prediction output performance.

- i. the type of membership function (MFs) (triangular, Gaussian, bell shape, trapezoidal etc),
- ii. the type of consequent part (linear or constant),
- iii. the number of MFs (>1),
- iv. the number of training epoch,
- v. the number of training data,
- vi. the selection method (grid partition or subtractive clustering)
- vii. the optimization method (back-propagation, or hybrid of the least-squares and the back propagation gradient descent).

In this study, three variables were selected for inputs of the ANFIS model to predict an output response. The model were developed using different shape of input membership function (MFs) type which were triangular, Gaussian, bell shape and trapezoidal, with number of the MFs were two, three, four and five. In purpose of training the model, a hybrid of the least-squares method and the back propagation gradient descent method was used to emulate a given training data set. The linear and constant of output MFs type were employed to produce the hardness value. Fig. 6 shows the flowchart for predicting TiAlN coating hardness using ANFIS system. The model setting is shown in Table 3.

**Table 3:** Parameters setting for ANFIS model

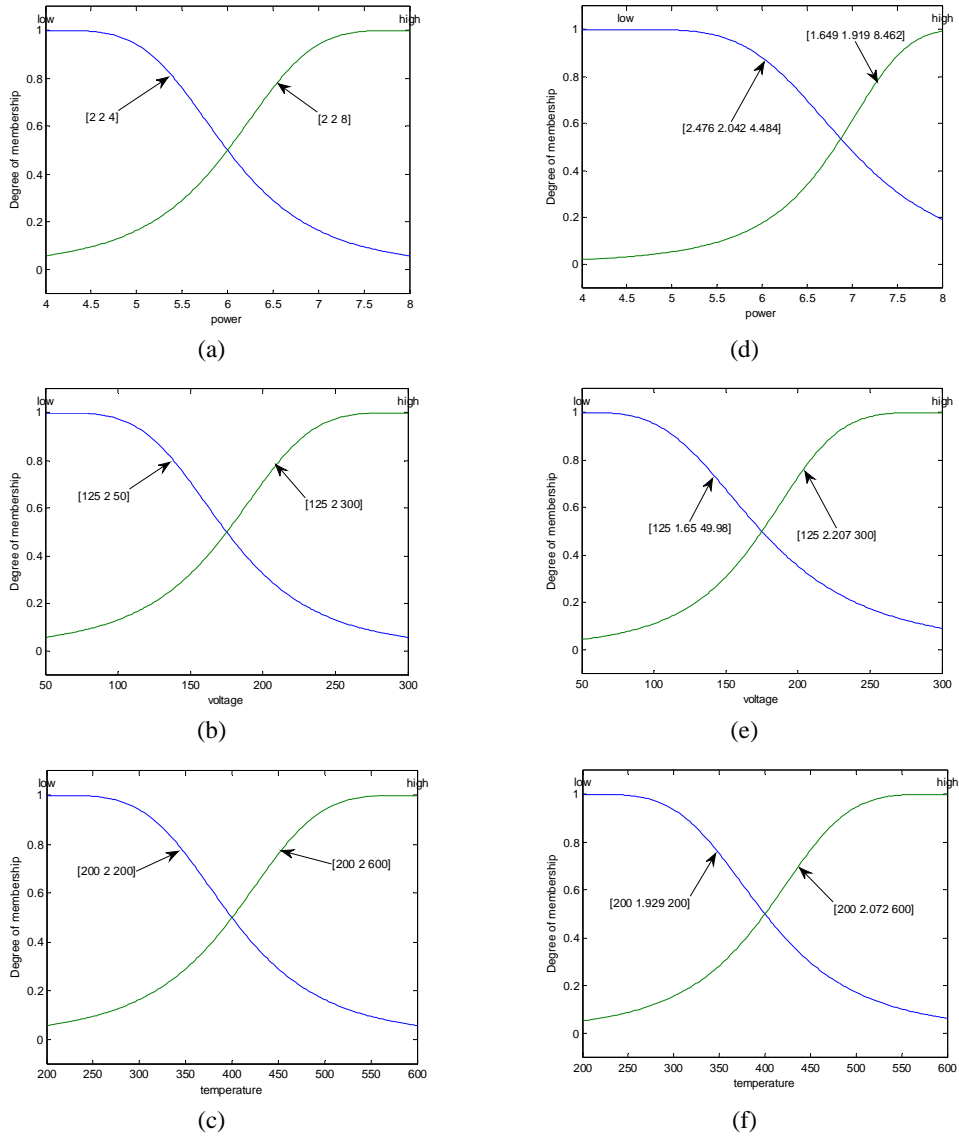
ANFIS Setting	Details
Input Variables	Power, Voltage, Temperature
Output Response	Hardness
Type of Input MFs	Triangular, Gaussian, Bell Shape, and Trapezoidal
No. of MFs	2,3, 4 and 5
Type of Output MFs	Linear and constant
Optimization Method	Hybrid of the least-squares and the back propagation gradient descent method.
Epochs	100



**Fig. 6:** Flowchart of hardness prediction of ANFIS system.

**RESULTS AND DISCUSSION**

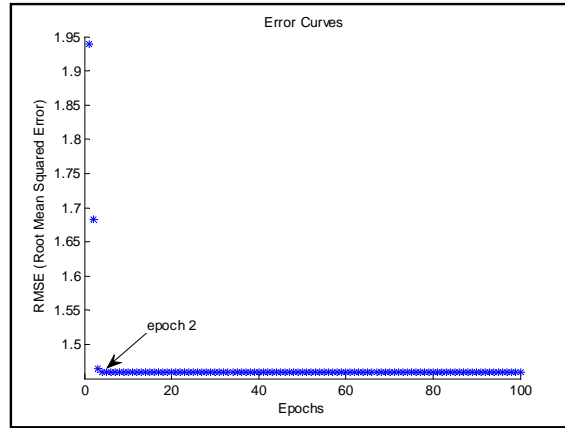
An example of ANFIS model details using two MFs with linear output is shown in Table 4. This info was indicated in MATLAB program during the training process. Three input with two MFs each created eight fuzzy rules. After the training process, the initial membership functions for input variables were derived by training. Fig. 7 (a)-(c) show the initial of MFs (constant output), while Fig. 7 (d)-(f) show the final MFs after training process. From the figures, major change can be seen on the shapes of the membership function in the POWER variable. Otherwise, the shapes of the membership function in the VOLTAGE and TEMPERATURE indicated only slight changes. Meanwhile, Fig. 8 shows that after the 2 epochs, the root means square error become steady. This happen because the model was trained using limited experimental data.



**Fig. 7: (a)-(f).** The MFs before (a-c) and after (d-f) training process.

**Table 4:** Details of ANFIS model.

ANFIS Info
Number of nodes: 34
Number of linear parameters: 32
Number of nonlinear parameters: 18
Total number of parameters: 50
Number of training data pairs: 20
Number of checking data pairs: 3
Number of fuzzy rules: 8



**Fig. 8:** Convergence of ANFIS training.

To verify the performance of the proposed ANFIS model, the following measures were used. The root mean squared error (*RMSE*) in (6) was used to quantify the difference between predicted and actual values. Meanwhile, the prediction accuracy (*A*) in (7) was computed to determine the accuracy of the prediction models.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n \left( v_a - v_p \right)^2} \tag{6}$$

$$A = \frac{1}{n} \sum_{i=1}^n \left( 1 - \frac{|v_a - v_p|}{v_a} \right) \times 100\% \tag{7}$$

where *n* is number of testing data, *v<sub>a</sub>* is experimental value and *v<sub>p</sub>* is predicted value. Three testing dataset from separated experiment were used to verify the proposed model.

**Table 5:** Result of the ANFIS model with linear output.

Input			Triangular				Gaussian			
Power	Voltage	Temp.	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
5	100	280	5.60	4.70	4.28	4.95	5.06	4.72	4.29	4.47
6.5	150	350	11.04	10.94	13.74	3.46	11.78	10.85	14.67	4.90
7	145	450	13.24	13.96	15.97	3.03	14.85	15.87	14.77	4.58
Input			Bell Shape				Trapezoidal			
Power	Voltage	Temp.	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
5	100	280	4.81	4.82	4.24	4.42	4.46	4.81	4.05	4.31
6.5	150	350	11.83	10.51	15.34	4.70	12.08	9.79	17.04	2.61
7	145	450	14.96	16.62	13.52	4.43	14.86	18.25	10.65	1.77

Meanwhile, Table 5 and 6 show the hardness values for the ANFIS models with different type of output (linear or constant), different shapes of input membership function (triangular, trapezoidal, Gaussian and bell) and different number of membership function (2, 3 and 5). From the tables, the value of hardness for all MFs with five shapes indicated far from the target values. The hardness result for model with two, three and four MFs showed around the target values. This pattern happen for both constant and linear output MFs.

**Table 6:** Result of the ANFIS model with constant output.

Input			Triangular				Gaussian			
Power	Voltage	Temp.	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
5	100	280	5.89	4.62	4.15	4.97	5.62	4.57	4.12	4.49
6.5	150	350	10.11	10.88	12.08	3.25	10.15	11.32	12.52	4.86
7	145	450	11.54	13.47	16.50	3.41	11.65	15.12	15.63	4.80
Input			Bell Shape				Trapezoidal			
Power	Voltage	Temp.	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
5	100	280	5.49	4.66	4.22	4.43	5.29	4.73	4.51	4.33
6.5	150	350	10.21	11.36	13.03	4.75	10.27	11.23	14.57	2.72
7	145	450	11.62	15.68	14.97	4.61	11.82	16.93	13.28	2.00



Table 7 and 8 show the RMSE and prediction accuracy of the ANFIS models for linear and constant output respectively. The tables indicate that the 2-2-2 and 3-3-3 structure gave high prediction accuracy with greater than 85%. In the table 7, the 3-3-3 triangular MFs obtains the highest prediction accuracy and the lowest RMSE with 94.15% and 0.4884 respectively. Meanwhile, the table 8 shows that the 2-2-2 trapezoidal MFs obtains the highest prediction accuracy with 93.75%. Otherwise, the lowest RMSE is indicated by the 3-3-3 triangular MFs with 0.6344.

**Table 7:** The RMSE and the prediction accuracy of the ANFIS model with linear output.

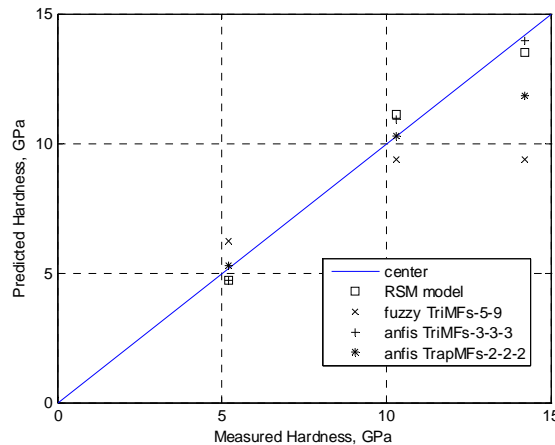
Performance Measures	Triangular				Gaussian			
	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
RMSE	0.7344	0.4884	2.2938	7.5642	0.9345	1.0510	2.5971	6.3809
A (%)	92.79	94.15	78.84	50.03	92.83	91.21	78.69	55.28
Performance Measures	Bell Shape				Trapezoidal			
	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
RMSE	1.0115	1.4201	2.9850	6.5143	1.1765	2.3700	4.4476	8.4515
A (%)	90.74	91.99	75.97	53.95	87.96	86.33	62.49	44.40

**Table 8:** The RMSE and the prediction accuracy of the ANFIS model with constant output.

Performance Measures	Triangular				Gaussian			
	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
RMSE	1.5922	0.6344	1.7865	7.4427	1.4934	0.8696	1.6483	6.2847
A (%)	88.75	92.67	82.08	50.37	90.83	90.53	82.54	55.75
Performance Measures	Bell Shape				Trapezoidal			
	2-2-2	3-3-3	4-4-4	5-5-5	2-2-2	3-3-3	4-4-4	5-5-5
RMSE	1.4995	1.0930	1.7337	6.4135	1.3764	1.6894	2.5553	8.3101
A (%)	91.79	89.65	83.10	54.61	93.75	87.54	79.57	41.23

Table 9 shows comparison of the best ANFIS model with fuzzy and RSM models in terms of RMSE and prediction accuracy. The fuzzy and the nonlinear RSM model were constructed based on same types and three input parameters. From the comparison, the 3-3-3 triangular linear ANFIS model indicates the highest prediction accuracy and the lowest RMSE compared to the others.

Fig. 9 shows the scatter diagram of the measured and predicted coating hardness (GPa) for the 3 testing value using RSM, fuzzy, ANFIS with triangular MFs 3-3-3 linear and ANFIS with trapezoidal MFs 2-2-2 constant models. It shows that the predicted values of ANFIS model between 4.7 to 14.2 GPa in a good agreement and follow the ideal center line very closely. In other words, the ANFIS model can be a good option in predicting hardness value of TiAlN coating for certain combination of input parameters.



**Fig. 9:** Scatter diagram of the measured and predicted coating hardness (GPa) for the testing data using RSM, fuzzy, ANFIS TriMFs 3-3-3 linear and ANFIS TrapMFs 2-2-2 constant models.

**Table 9:** Comparison of ANFIS model with single fuzzy and RSM model

Performance Measures	ANFIS Linear TriMFs 3-3-3	ANFIS Constant TrapMFs 2-2-2	Fuzzy TriMFs 5-9	RSM model (Md Nizam 2010)
RMSE	0.4884	1.3764	2.898	0.6782
A (%)	94.15	93.75	78.95	92.56

### Conclusion:

In this study, the ANFIS model was used in predicting the hardness of TiAlN coatings. The 20 experimental data were used for the model training purpose and 3 testing dataset were used for validation. The input parameters were the sputtering power, substrate bias voltage and substrate temperature. Meanwhile, the hardness of TiAlN coatings was selected as the output response. The triangular, trapezoidal, bell and Gaussian shapes were selected as input membership function with number of membership function were two, three, four and five. The linear and constant output were determine as the type of output membership function. After the training process, the *RMSE* became steady after 2 epochs. A major changes obviously could be seen on the shape of POWER membership function. However, only slightly changes happened to the shapes of the VOLTAGE and TEMPERATURE membership functions. The result showed that the 2-2-2 and 3-3-3 structures of ANFIS model gave a good prediction accuracy with greater than 85%. The ANFIS model also better than fuzzy and RSM model in terms of RMSE and prediction accuracy with the same input parameters and data. The result also indicated that the ANFIS model could predict the output response with high accuracy even using the limited experimental data for training purpose.

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