Computational Intelligence Approach for Predicting the Hardness Performances in Titanium Aluminium Nitride (TiA1N) Coating Process

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Abstract

This paper presents a computational approach on predicting of hardness performances for Titanium Aluminium Nitride (TiA1N) coating process. A new application in predicting the hardness performances of TiA1N coatings using a method called Support Vector Machine (SVM) and Artificial Neural Network (ANN) is implemented. TiAlN coatings are usually used in high-speed machining due to its excellent properties in surface hardness and wear resistance. Physical Vapor Deposition (PVD) magnetron sputtering process has been used to produce the TiA1N coatings. Based on the experimental dataset of previous work, the SVM and ANN model is used in predicting the hardness of TiA1N coatings. The influential factors of three coating process parameter namely substrate sputtering power, substrate bias voltage and substrate temperature were selected as input while the output parameter is the hardness. The results of proposed SVM and ANN models are compared to the experimental result and the hybrid RSM-Fuzzy model from previous work. The comparisons of SVM and ANN models against hybrid RSM-Fuzzy were based on predictive performances in order to obtain the most accurate model for prediction of hardness in TiA1N coating. In terms of predictive performance evaluation, four performances matrix were applied that are percentage error, mean square error (MSE), co-efficient determination (R^2) and model accuracy. The result has proved that the proposed SVM model shows the better result compared to the ANN and hybrid RSM-fuzzy model. The good performances of the results obtained by the SVM method shows that this method can be applied for prediction of hardness performances in TiA1N coating process with better predictive performances compared to ANN and hybrid RSM-Fuzzy.

Keywords: Support Vector Machine, Artificial Neural Network, RSM-Fuzzy, Hardness, TiA1N coatings, PVD Magnetron Sputtering.

1. INTRODUCTION

Nowadays coated material is widely used due to its excellent properties in surface roughness, hardness and tool wear. A particular study has indicated that coated tool wear performance is forty times better than the uncoated tools [1]. Generally, the performance of the coated tool is depending on the wear mechanism, hardness and adhesion, and tool life. Hardness is one of the characteristic of coated tool and it very important in order to reduce the tool wear [2].

The hardness performances can be improved by applying the thin film coating on the cutting tool. The main purpose of the thin film coating application is to improve the hardness performances. Meanwhile this application improves the tool surface properties while maintaining its bulks properties [2]. Physical Vapor Deposition (PVD) magnetron sputtering is the general coating process in applying thin film for hard coating purpose.

In PVD magnetron sputtering, the process parameters that influence the coating performance are sputtering power, substrate temperature, substrate bias voltage, turntable speed and gas temperature [3-6].To produce a good coating it is required the selection of values of coating process parameter. However, due to the best our knowledge, there are no methods that can be determining the parameters values accurately. By using the traditional approach, that is, through lab experiments, it involved lots of money and time because we need to conduct a few lab experiments until we obtained the best values. In other words, these conditions require trial and error process in order to determine the suitable parameters value for the material used, so that we could obtain the best coating performance. The trial and error process have resulted in the increase of coating process cost and more intricate process of customization in coating.

Therefore, with the help of computational approach that evolve nowadays, the coating process can be done in difference ways with the same objective. Using the computational approaches in estimating coating process performances, there is no traditional lab experiment need to be conducted and hence the coating process cost can be reduced. Thus, previous work conducted by Jaya et al. (2011), they proposed the hybridization RSM-Fuzzy method for prediction of hardness performance in TiA1N coating [7]. This model has achieved 88.49% accuracy compared to the experimental result. In addition, from literature survey, we found that another computational-based approach such as Support Vector Machine (SVM) and Artificial Neural Network (ANN) could be applied for the same purpose and might produce better accuracy.

To the best of our knowledge, no such work has been conducted to explore the ability of SVM and ANN in this particular matter. Thus, this study aims to explore these two methods to predict the value of parameters of hardness in TiA1N coating process. At the end of this study, the prediction results from SVM and ANN will be compared with the hybrid RSM-Fuzzy method. The comparison analysis will be based on predictive performances. In terms of predictive performance evaluation, four performances matrix will be applied were percentage error, mean square error (MSE), co-efficient determination (R^2) and model accuracy.

2. EXPERIMENTAL DESIGN

This section focuses on the experimental design that has been used in this study. The emphasis is on the prediction of hardness performances in Titanium Aluminium Nitride TiA1N coating process using two computational intelligence techniques, Support Vector Machine (SVM) and Artificial Neural Network (ANN). Based the literature, SVM and ANN were demonstrated its efficiency and reliability in prediction. Therefore, a proper experimental design must be carried out before the implementation of this study. It consists of five main phases which are problem definition, data definition and collection, model development, model validation and evaluation of predictive performance.

3. DATA DEFINITION

For this study, the result from the previous work [7] which are the value of hardness of TiA1N coating process were found using experimental approach is referred. The datasets used are the experimental result of TiA1N coating process. The datasets contains 20 instances as shown in TABLE 1. This instance has been used in this study as input/output data for the developed model using SVM and ANN.

TABLE 1: Referred Dataset Obtained from Previous Work by Jaya et al. (2011).

No of Dataset	Process Parameters			Output
	Sputter Power (kW)	Bias Voltage (Volts)	Substrate Temp. (^{0}C)	Hardness Value (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

In validating the performances of the models, three testing dataset were used. This three testing dataset were obtained from separated experimental [7]. This new three separated dataset is used instead of early 20 dataset to validating the performances of the RSM-Fuzzy model in order to avoid the model biasing the result. So, in validating the performances of SVM and ANN model, similar dataset were used. From TABLE 2, its shows the testing dataset were used to validate the predictive performances of prediction model.

TABLE 2: Testing Dataset for Evaluation of Predictive Performance.

No of Dataset	Input			Output
	Power (kW)	Voltage (Volt)	Temp (^{0}C)	Hardness (Gpa)
1	5.0	100	280	5.2
2	6.5	150	350	10.3
3	7.0	145	450	14.2

4. MODELLING PROCESS

4.1 Artificial Neural Network

Neural networks, as used in artificial intelligence, have traditionally been viewed as simplified models of neural processing in the human brain. It is accepted by the most scientists that the human brain is a type of computer. The origins of neural networks are based on efforts to model information processing in biological systems, which may rely largely on parallel processing as well as implicit instructions based on recognition of patterns of sensory input from external sources.

Human body consists of trillions of cells. A portion of them is the nerve cells called neurons. These neurons have different shapes and sizes [8]. A neuron collects signals from others through fine structures called dendrites. The neuron sends out spikes of electrical activity through a long, thin stand known as axon, which splits into thousands of branches. At the end of each branch, a structure called a synapse converts the activity from the axon into electrical effects that inhibit or excite activity in the connected neurons. When a neuron receives excitatory input that is sufficiently large compared with its inhibitory input, it sends a spike of electrical activity down its axon. Learning occurs by changing the effectiveness of the synapses so that the influence of one neuron on another changes.

4.2 Backpropagation

In this study, BP learning algorithm, which has a unique learning principle, generally called delta rule, is used, FIGURE 1 depicts a schematic illustration of BP networks. The three layer of the network architecture include the input layer, hidden layer and output layer. Layers include several processing units known as neurons. They are connected with each other by variable weights to be determined. In the network, the input layer receives information from external source and passes this information to the network for processing. The hidden layer receives from the input layer, and does all information processing. The output layer receives processed information from the network, and sends the results to an external receptor [9]. In the network, each neuron receives total input from all of the neurons in the proceeding layer as:

$$net_j = \sum_i W_{ji}^{(n)} X_i^{(n-1)} \tag{1}$$

Where net_j is the total or net input, $X_j^{(n)}$ is the output of the node *j* in the *n*th layer, and $W_{ji}^{(n)}$ represents the weights from node *i* in the (*n*−1)th layer to node *j* in the *n*th layer. A neuron in the network produces its input by processing the net input through an activation (transfer) function which is usually nonlinear. There are several types of activation functions used for BP. However, the sigmoidal activation function is most utilized. Three types of sigmoid functions are usually used, as follows [10]:

$$f(x) = \frac{1}{1+e^{-x}} \quad range\ (0,1) \tag{2}$$

$$f(x) = \frac{2}{1+e^{-x}} - 1 \quad range\ (-1,1) \tag{3}$$

$$f(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}} \quad range\ (-1,1) \tag{4}$$

the weights are dynamically updated using the BP algorithm. The difference between the target output and actual output (learning error) for a sample *p* is [7]

$$E_p = \frac{1}{2}\sum_{k=1}^{K}\left(d_{pk} - o_{pk}\right)^2 \tag{5}$$

where d_{pk} and o_{pk} are the desired and calculated output for *k*th output, respectively. *K* denotes the number of neuron in output of network. The average error for whole system is obtained by:

$$E_p = \frac{1}{2}\sum_{p-1}^{p}\sum_{k=1}^{K}\left(d_{pk} - o_{pk}\right)^2 \tag{6}$$

where *P* is the total number of instances. For the purpose of minimizing E_p, the weights of the inter-connections are adjusted during the training procedure until the expected error is achieved. To adjust the weights of the networks, the process starts at the output neuron and works backward to the hidden layer. The weights in BP based on the delta learning rule can be expressed as follows:

$$w_{ij}^{new} = w_{ij}^{old} + \Delta w_{ij} \tag{7}$$

$$\Delta w_{ij} = -\eta \frac{\partial E_p}{\partial w_{ij}} out_j \tag{8}$$

where out_j the *j*th neuron output. $\boldsymbol{\eta}$ is the learning rate parameter controlling stability and rate of convergence of the network, which is a constant between 0 and 1. Once the weights of all the links of the network are decided, the decision mechanism is then developed.

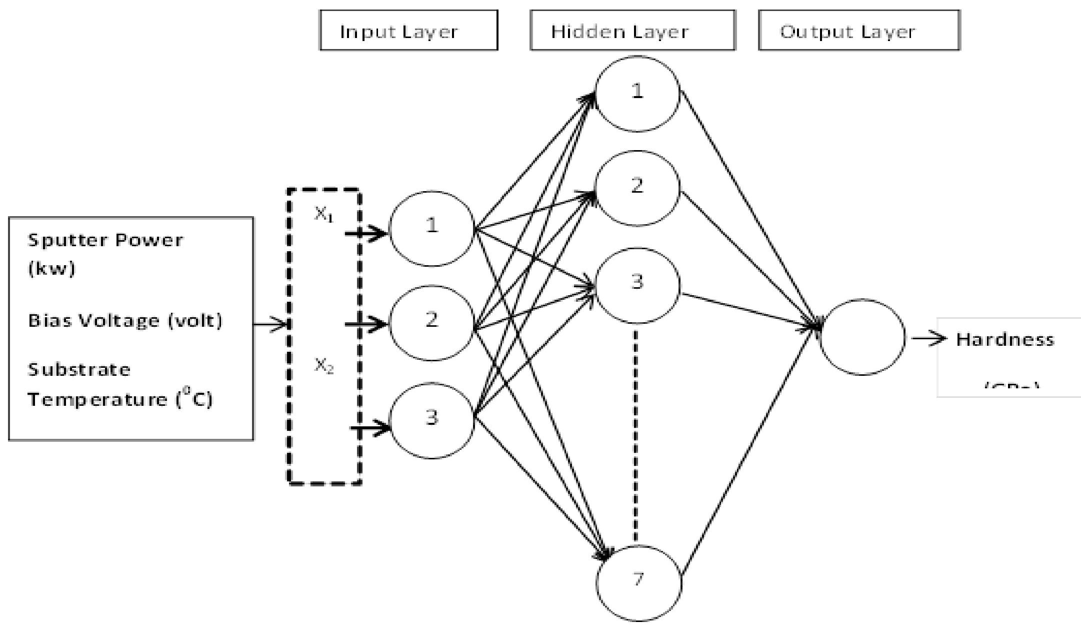

FIGURE 1: Schematic illustration of artificial neural network model for the Hardness.

4.3 Support Vector Machine

The basic theory of regression function of SVM can be express as [11-14].

$$y = f(x) = \omega. x + b \qquad (9)$$

where ω is a weight vector, b is bias, x is multivariate input and y is scalar output. By introducing slack variables, ξ and $\xi*$, the SVM model can be expressed as follows:

$$\text{Minimize} \qquad \Phi(\omega) = \frac{1}{2} \| \omega \|^2 + C \sum_{i=1}^{n} (\xi i + \xi i^*), C \geq 0$$

$$\text{Subject to} \qquad \begin{aligned} & y_i - \omega x_i - b \leq \varepsilon + \xi_i, \\ & \omega x_i + b - y_i \leq \varepsilon + \xi_i^*, i = 1, 2, .., l \\ & \xi_i, \xi_i^* \geq 0, \end{aligned} \qquad (10)$$

where C is a positive constant (regularization parameter), and ε is loss function.

$$y = f(x) = \sum_{i=1}^{n} (\alpha_i - \alpha_i^*)(x_i \cdot x) + b \qquad (11)$$

By applying the Lagrange multiplier method, the solution to above SVM model is obtained as the following equations:

$$L(\omega, b, \xi, \xi*) = \frac{1}{2}||\omega||^2 + C\sum_{i=1}^{n}(\xi_i+\xi_i^*) - \sum_{i=1}^{n} a_i(\varepsilon_i+\xi_I - y_i + \omega \cdot x_i + b) - \sum_{i=1}^{n} a*(y_i+\varepsilon_i+\xi_I - \omega \cdot x_i - b) - \sum_{i=1}^{n}(\eta_i\xi_I + \eta_i^*\xi_I^*) \quad (12)$$

where α_i, α_i^*, η_i, η_i^* are Langrange Multiplier. Hence dual problem is:

Maximize $Q(\alpha) = \sum_{i=1}^{n} y(\alpha_i - \alpha_i^*) - \varepsilon\sum_{i=1}^{n}(\alpha_i - \alpha_i^*) - \frac{1}{2}\sum_{i=1}^{n}(\alpha_i - \alpha_i^*)(x_i \cdot x_j)$

Subject to

$$\begin{cases} \sum_{i=1}^{n} y_i(a_i - a_i^*) = 0, \\ 0 \leq a_i \leq 0, \\ 0 \leq a_i^* \leq 0, \end{cases} \quad i = 1,2,\dots,n \quad (13)$$

Regression function is:

$$f(x) = \sum_{i=1}^{n}(a_i - a_i^*)(x_i,x) + b \quad (14)$$

Nonlinear regression function is:

$$f(x) = \sum_{i=1}^{n}(a_i - a_i^*)K(x_i,x) + b \quad (15)$$

When using a mapping function, the solution of $K(x_i,x)$ in the eq. (7) can be change into $K(x_i,x) = (\varphi(x_i),\phi(x))$ where K is a kernel function while b is bias and *n* is number of support vector. In SVM, kernel function enables the dot product to be performed in high dimensional feature space using low-dimensional space data input without knowing the value of ϕ. A good SVM regression model with high prediction and stability always come with a proper parameter setting [15]. The review had shown that RBF kernel function in the most common used by researchers.

Kernel function plays a crucial role in SVM and its performances. The right selection of kernel function will affect the accuracy of prediction model. Basically, the idea of kernel function is to enable the operations to be performed in the input space rather than the potentially high dimensional future space. So that, the inner products does not need to be evaluated in the future space. Function that used in SVM as a kernel function must satisfy Mercer's theorem [16, 17].

In developing SVM model, there are a few parameters that should be considered, namely, regularization parameters *C* and *gamma* value. Parameter C is the cost of the penalty [18].The C parameter will control the trade-off between margin and the slack variable size while gamma, which is a RBF kernel function parameter influences the partitioning outcome in the feature space. The choice of suitable parameters will affect the result of prediction model. Generally, there are a few steps in determining *C* and *gamma* parameter, which are trial and error implementation, grid search and feature selection approach. Grid search is a conventional way to determine parameter setting, it is an alternative method to find the best *C* and *gamma* values when using RBF kernel function. However, grid search method is time consuming [19, 20].

Kernel parameter is important in SVM. In this study, RBF kernel function is chosen to model the hardness prediction of TiA1N coating. RBF is widely used due to it generalization effectiveness and also it has universal approximation properties. Thus this function has become a first choice chosen by many researchers. In addition, RBF significantly gives the good performance in practical problem solving.

In RBF kernel function, there are two parameters that will be considered namely *C* and *gamma*. The selections of value for parameter *C* and *gamma* will affect the accuracy of prediction result. Since, there is no standard method can be applied to determine the best value of that parameters, therefore in this research we used a trial and error approach in order to obtain the best value for the parameters. For this study, in order to get the SVM model, try and error process need to be implemented accordingly with difference values of parameters. SVM regression function is used in this study in order to model the coating process parameter.

For model development, the input data was divided into training and testing dataset before the prediction process need to transform into sparse format which is accepted as data format in LIBSVM toolbox. To obtain the best prediction model, trial and error process was implemented continuously with difference values of *C* and *Gamma* parameters until we obtain highest correlation value which is considered as SVM best prediction model.

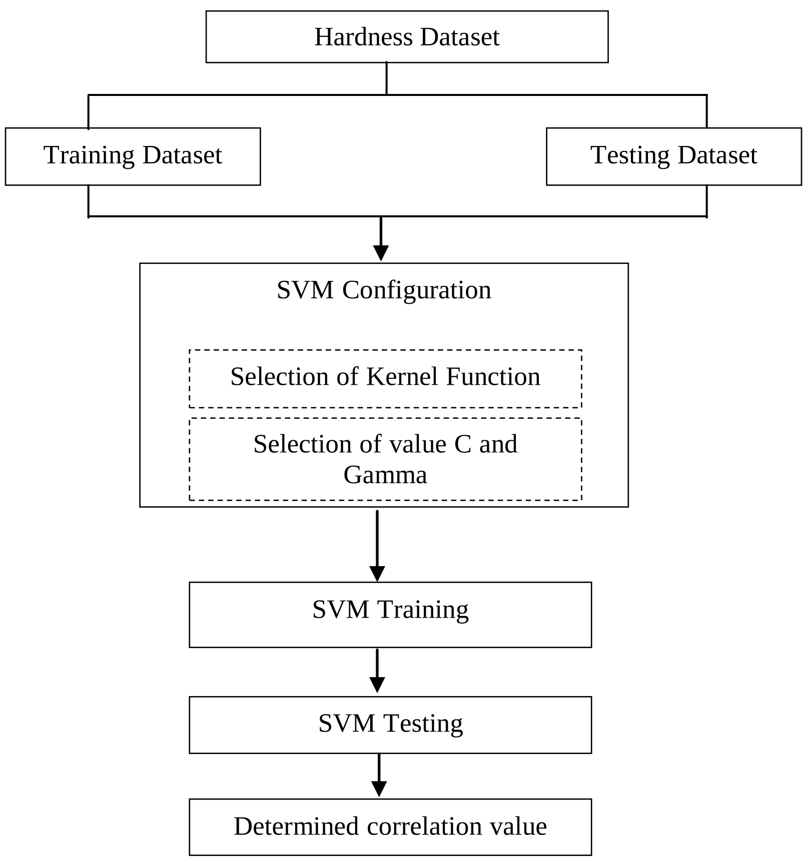

FIGURE 2: Framework of SVM Model.

5. PREDICTION RESULT

This section discussed the results obtained from SVM and ANN prediction model. The results obtained by these two models for predicting the hardness value of TiA1N coating were compared against actual experimental result. TABLE 3 shows the hardness values were generated by prediction models and the actual hardness value from the experimental result. Subsequently, FIGURE 3 illustrated the comparison of prediction result SVM and ANN against the actual experimental result for hardness TiA1N coating.

TABLE 3: Comparison of Experimental Result with SVM and ANN Model for Hardness Values.

No. of Dataset	Hardness Value (Gpa)		
	Experimental	SVM	ANN
1	3.54	3.54	3.54
2	5.27	5.27	5.27
3	13.17	13.17	13.17
4	10.96	10.97	10.94
5	8.06	8.06	8.06
6	4.33	4.33	4.33
7	4.04	4.04	4.04
8	16.12	10.97	10.94
9	7.77	10.97	10.94
10	3.53	3.53	3.53
11	9.76	9.76	9.76
12	7.48	7.48	7.48
13	15.26	15.26	15.26
14	8.91	10.97	10.94
15	22.64	22.64	14.91
16	14.14	14.14	9.99
17	8.88	8.89	13.60
18	15.69	15.69	5.67
19	11.27	10.97	10.94
20	12.34	10.97	10.94

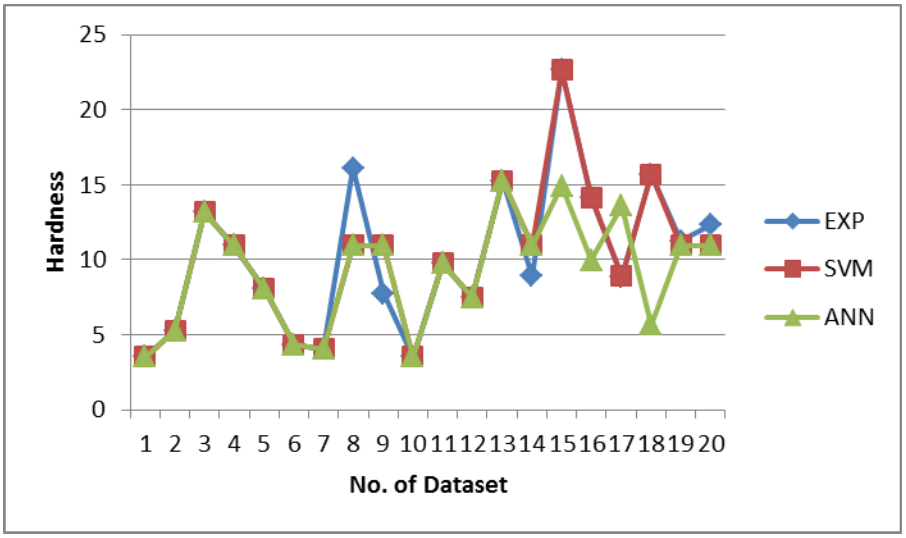

FIGURE 3: Comparison Experimental Result and SVM and ANN Prediction Result for Hardness TiA1N Coating.

6. PREDICTIVE PERFORMANCE

In this study, the following measures were used to calculate the model performances. The percentage error (δ) in (16) was used to observe the gap between actual and the hybrid models for individual value. The mean squared error (MSE) in (17) was used to quantify the difference between predicted and actual values. Meanwhile, the co-efficient determination (R^2) in (18) was calculated in order to see how well the future output response is likely to be predicted by the model. Lastly, the prediction accuracy (*A*) in (19) was computed to determine the accuracy of the models.

$$\delta_i = \left(\frac{\left|v_a - v_p\right|}{v_a}\right) \times 100\% \tag{16}$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(\left|v_a - v_p\right|\right)^2 \tag{17}$$

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{n}(v_a - v_p)^2}{\sum_{i=1}^{n}(v_p)^2}\right) \tag{18}$$

$$A = \frac{1}{n}\sum_{i=1}^{n}\left(1 - \frac{\left|v_a - v_p\right|}{v_a}\right) \times 100\% \tag{19}$$

Where n is number of testing data, v_a is experimental value and v_p is predicted value.

In validating the performances of the models, three testing dataset from separated experiment were used. From **TABLE 4**, the hardness value for the SVM, ANN and RSM-Fuzzy model were compared with actual value. Subsequently, **FIGURE 4** illustrated the comparison of prediction result between SVM, ANN and RSM-Fuzzy prediction model. From Figure 5, it can be seen that the SVM model prediction obtained better agreement between coating hardness values predicted and the actual experimental result compared to RSM-Fuzzy and ANN model. Unfortunately, the ANN model prediction shows very poor agreement between coating hardness values predicted and the actual one.

TABLE 4: Comparison of Actual Experimental Testing Result with SVM, ANN and RSM-Fuzzy Model for Hardness Values.

No. of Dataset	Input			Output			
	Power	Voltage	Temp	Actual	RSM-Fuzzy	ANN	SVM
	kW	Volt	^{0}C	Hardness(Gpa)			
1	5	100	280	5.2	6.25	5.20	4.32
2	6.5	150	350	10.3	9.92	2.64	10.61
3	7	145	450	14.2	9.66	2.64	12.74
Predictive Performance					RSM-Fuzzy	ANN	SVM
Percentage Error %					11.50	51.94	10.07
Mean Square Error (MSE)					1.09	64.09	1.00
Co-efficient Determination (R2)					0.99	-3.69	0.99
Model Accuracy %					88.49	48.06	89.93

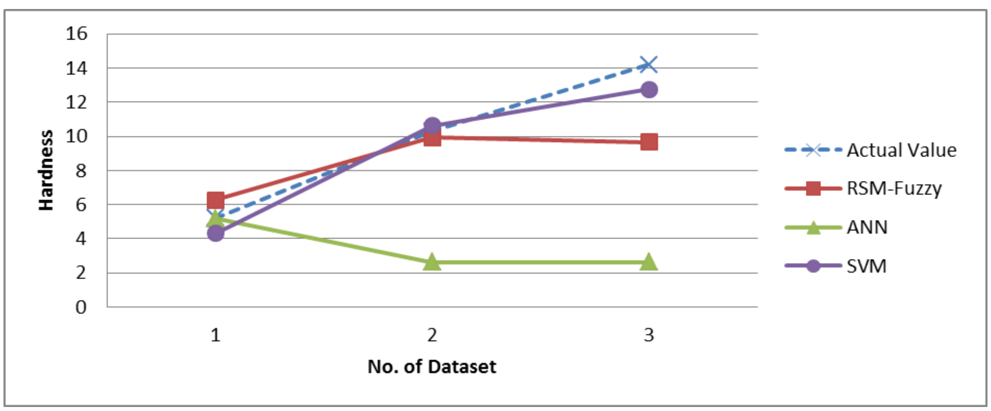

FIGURE 4: Comparison Actual Experimental Testing Result against SVM, ANN and RSM-Fuzzy Prediction Result for Hardness TiA1N Coating.

Meanwhile, FIGURE 5 shows the comparison of predictive performances between the prediction models. The percentage error was used to observe the gap between actual and the prediction model. SVM model gave the less percentage error compared to the other model with 10.07% while RSM-Fuzzy and ANN gave 11.50% and 51.46% respectively. While MSE was used to quantify the difference between predicted and actual values.The less MSE gave the better performances of the model. SVM and RSM-Fuzzy gave very less MSE compare to ANN. In term of co-efficient determination, the value of the R^2 of SVM and RSM-Fuzzy were 0.99 which means near to 1.0. So it's indicated that regression line fits the data very well. Unfortunately, ANN model obtained negative value of R^2 with -3.99 which mean the predictions which are being compared to the corresponding outcomes have not been derived from a model-fitting procedure using those data. For model accuracy, SVM model produce more accurate with 89.93% compared to the RSM-Fuzzy with 88.49%. Poorly, ANN model was outperformed by produce very less model accuracy with 48.08% only. Thus based on the result obtained, its can concluded that SVM model prediction shows the better predictive performances compared to the ANN and RSM-Fuzzy model prediction. Once again, the ANN model prediction was outperforming by obtained very poor predictive performance.

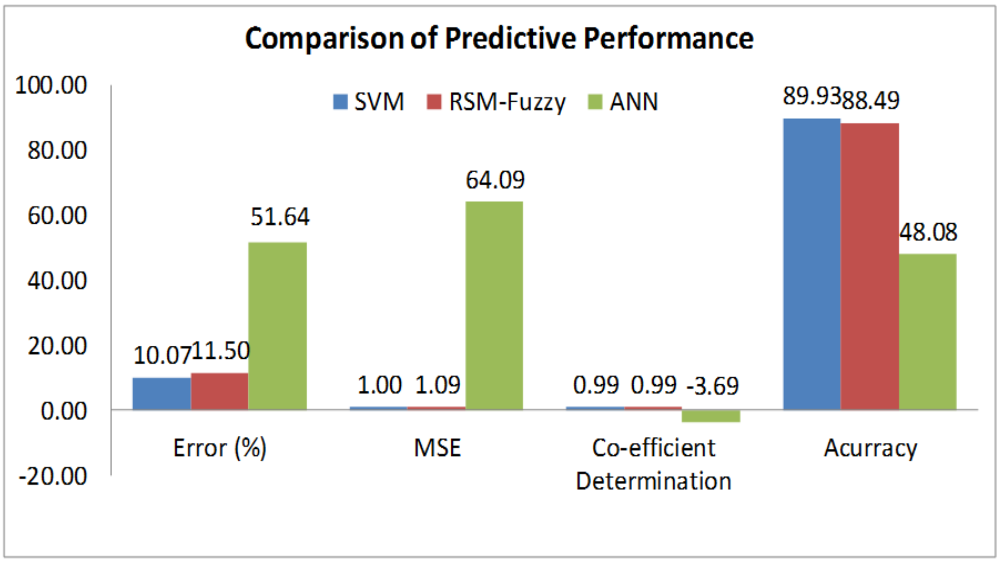

FIGURE 5: Comparison of Predictive Performance between SVM, ANN and RSM-Fuzzy Prediction Model.

7. CONCLUSION

In this paper, we have presented the computational based approach for predicting the hardness performances of TiAlN coatings. A new application in predicting the hardness performances of TiA1N coatings using a method called Support Vector Machine (SVM) and Artificial Neural Network (ANN) were implemented. The 20 experimental data were used in this study are based on previous work [7] in purpose modeling the SVM and ANN prediction. The influential factors of three coating process parameter namely substrate sputtering power, substrate bias voltage and substrate temperature were selected input while the output parameter is the hardness. These prediction models were validated using three experimental dataset in purpose validating the predictive performances of the model and the results obtained were compared against the RSM-Fuzzy model by Jaya *et al.* In terms of predictive performance evaluation, four performances matrix were applied that are percentage error, mean square error (MSE), co-efficient determination (R^2) and model accuracy. The results have shown that:

- SVM model gave the less percentage error compared to the other model.
- MSE was used to quantify the difference between predicted and actual values.The less MSE gave the better performances of the model. SVM and RSM-Fuzzy gave very less MSE compare to ANN.
- The value of the R^2 of SVM and RSM-Fuzzy were 0.99 which means near to 1.0. So it's indicated that regression line fits the data very well. Unfortunately, ANN model obtained negative value of R^2 with -3.99 which mean the predictions which are being compared to

the corresponding outcomes have not been derived from a model-fitting procedure using those data.

- In term of model accuracy, SVM model produce more accurate accuracy in prediction compared to the hybrid RSM-Fuzzy model. Unfortunately, ANN model was outperformed by produce very less model accuracy.

- Thus, based on the predictive performances, the proposed SVM model can be another alternative to predict the hardness performances of TiA1N coating other than RSM-Fuzzy found by Jaya *et al.* Even, the SVM model was better option instead of RSM-Fuzzy in cases for predicting the hardness performances of TiA1N coating.

- Unfortunately ANN model obtained very poor performances in term of predictive performances and feared cannot be an option in predicting the hardness performances of TiA1N coating.

- Thus, the result indicated that SVM model obtained better prediction performances outperform the ANN and RSM-Fuzzy model in cases of prediction of hardness performances in TiA1N coating

- As a conclusion, the SVM model is a better option for predicting the hardness performances of TiA1N coating in PVD magnetron sputtering process.

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