

# THIN FILM ROUGHNESS OPTIMIZATION IN THE TIN COATINGS USING GENETIC ALGORITHMS

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## ABSTRACT

Optimization is important to identify optimal parameters in many disciplines to achieve high quality products including optimization of thin film coating parameters. Manufacturing costs and customization of cutting tool properties are the two main issues in the process of Physical Vapour Deposition (PVD). The aim of this paper is to find the optimal parameters get better thin film roughness using PVD coating process. Three input parameters were selected to represent the solutions in the target data, namely Nitrogen gas pressure ( $N_2$ ), Argon gas pressure (Ar), and Turntable speed (TT), while the surface roughness was selected as an output response for the Titanium nitrite (TiN). Atomic Force Microscopy (AFM) equipment was used to characterize the coating roughness. In this study, an approach in modeling surface roughness of Titanium Nitrite (TiN) coating using Response Surface Method (RSM) has been implemented to obtain a proper output result. In order to represent the process variables and coating roughness, a quadratic polynomial model equation was developed. Genetic algorithms were used in the optimization work of the coating process to optimize the coating roughness parameters. Finally, to validate the developed model, actual data were conducted in different experimental run. In RSM validation phase, the actual surface roughness fell within 90% prediction interval (*PI*). The absolute range of residual errors (*e*) was very low less than 10 to indicate that the surface roughness could be accurately predicted by the model. In terms of optimization and reduction the experimental data, GAs could get the best lowest value for roughness compared to experimental data with reduction ratio of 46.75%.

**Keywords:** *Roughness, TiN coating, PVD, GAs, RSM.*

## 1. INTRODUCTION

In high speed machining, temperature on the cutting tip could exceed 800oC. This condition causes tool wear, hence reducing cutting tool performance. Thus, a cutting tool with high resistance wear is needed to deal with this crucial condition. The cutting tool with high resistance wear promises a better tool life and reduces the machining cost directly. The coating performance could be improved by applying a thin film coating on the cutting tool. The main purpose of coating is to enhance the surface properties while maintaining its bulks properties. The coated tool has been proved forty times better in tool wear resistance as compared to the uncoated tool [1]. Hard coatings, such as Titanium Nitride (TiN)

coating are usually used in metal cutting industry due to its coating performances, such as hardness and resistance to wear.

Two main techniques in depositing coating on cutting tool are the physical vapour deposition (PVD) and chemical vapour deposition (CVD). The main difference between the two processes is the vapour source. The PVD process uses a solid target as a source material which vapourises in atom particle to create a thin film coating. However, the CVD process uses a chemical source as coating material. In the PVD coating process, sputtered particle from the hard material embedded on the cutting tool results in the presence of reactive gas. A process in PVD technique, called magnetron sputtering is a well-known technology in hard coatings industry, and it is able to sputter many hard materials, such as titanium to coat

cutting tool.

In PVD coating process, many factors are reported to have significant influence to the coating characteristics, including the coating roughness [2-4]. Surface roughness is one of the important characteristics that influence machining performances. It affects the friction level and material pick-up behaviour of cutting tool upon sliding with workpiece material [5]. Some researches claimed that the N<sub>2</sub> pressure, argon pressure and turntable speed have significant effects on the deposited surface roughness and surface morphology [6-8]. To our knowledge, this study is the first to optimize the values of synthesis factors (N<sub>2</sub> pressure, Ar pressure and turntable speed) on the coating roughness in the TiN coating on tungsten carbide cutting tool using PVD coating process.

The implementation of PVD coating process brings about manufacturing and cutting tool properties' customization costs such as the required cares for tool and equipment, material usage, labor, and the need of decreasing machining time. Also, coated cutting tools' properties customization for usages like in milling, drilling and turning are some of common customization leading requests. However, the best coating characteristics have no direct formulas but are defined only out of trial and error in testing series. Additional experiments are usually required to compare optimum values and their corresponding characteristics [9, 10]. Therefore, it is highly recommended to apply a suitable integration between modeling and optimization to meet the cost and customization issues to improve sustainable manufacturing. This research is important to be used as a guideline for manufacturers to meet such issues and to reduce experimental run in the TiN coatings for the cutting tools.

Modeling and optimization are an adequate ways to address the coating process issues such as cost and customization. A model may be used to predict the coating performance value and indicate the optimum combination of input parameters to find best result. Many techniques have been applied to model coating works. Experiment-based approaches such as Taguchi [11], full factorial, and RSM [12] have been reported in designing model with minimum experimental data [13]. Intelligence based approaches such as fuzzy logic [14], neural network [15, 16], and ANFIS [17] have been also used to predict coating performance. However,

some limitations of the approaches have been discussed. The Taguchi approach has difficulties detecting the interaction effect of a nonlinear process [18] and the full factorial method is only suitable for optimization purposes [19]. A neural network needs a large amount of training data to be robust [20], and a significant amount of data as well as powerful computing resources are necessary [21].

Researchers use RSM to study relationships between measured response functions [16, 22, 23]. RSM is a collection of mathematical and statistical methods used to model and analyze significant parameters that affect the output responses [24, 25].

Genetic algorithms (GAs) are among the common methods used to improve many solutions of optimization complex problems. In the materials domain, GAs have provided an excellent insight to a large number of problems [26]. It has been demonstrated that GAs optimization are today's most implemented techniques in optimizing machining process parameters [27]. It have assisted surface roughness based machining coating researches for long time ago. In result forecasting, GAs are able to map out and match the interaction between input and output to gather less data with well-designed experiments [22]. Therefore, the application of GAs to optimize surface roughness of TiN coating has been discussed in this work.

In this paper, an integration between modeling and optimization methods are presented. The RSM approach was used to identify the most significant parameters to the coating roughness and to generate the fitness function, and optimization of the coating parameters was done using GAs technique.

The next four sections are organized as follows: experimental design is discussed in Sect. 2. Sect. 3 and 4 include modeling methodologies and experimental result. An introduction about GAs and its settings are discussed in Sec. 5. Result and discussion are described in Sect. 6. Finally, Sect. 7 concludes the paper.

## 2. EXPERIMENT

### 2.1 Materials and Methods

The experiment was run in an unbalanced PVD magnetron sputtering system made by VACTEC Korean model VTC PVD 1000. The PVD coating chamber was fixed with a vertically mounted titanium (Ti) target. The surface of tungsten carbide inserts was cleaned with alcohol bath in an ultrasonic cleaner for 20 minutes. The tungsten carbide inserts were loaded

in the rotating substrate holder inside the coating chamber. An inert gas called argon was used to produce electron in coating chamber for sputtering process. The cutting tool inserts were coated with the Ti in the presence of nitrogen gas. Table 1 shows the details setting of the coating process. In this process, the N<sub>2</sub> pressure, argon pressure and turntable speed were selected as variables.

**2.2 Experimental Design**

In this study, the experimental matrix was designed based on a Centre Cubic Design (CCD), using the Design Expert version 8.0 software. It was designed based on 8 factorial points, 6 axial points and 3 central points. The extreme points (operating window) were set as +/- Alpha value, and based on that points, the software dispensed the high and low settings for the factorial points.

The role of the extreme points is to ensure the characterization could be performed in a wide range of operating window.

**2.3 Atomic Force Microscopy**

Surface roughness values of the TiN coatings were inspected by using a scanning force microscopy (AFM) method. The method determined the morphology of the surface based with less requirement of sample preparation and non-destructive testing. The AFM XE-100 model was operated at room temperature. Non-contact mode detection approach using a commercial cantilever was used, and the scanning area was set to 25×25 microns (625 μm<sup>2</sup>). Then, XEI software was used to analyze the surface image to get the surface roughness reading.

Table 1. Process of the PVD Coating

Variables	Unit	Experiment			
		Phase 1	Phase 2	Phase 3	Phase 4
		Alcohol Bath	Ion cleaning	TiN deposition	Cooling
• Equipment	-	Ultrasonic bath cleaner	magnetron sputtering PVD		
• Sputtering power	kW	-	-	4.0	-
• Ion source power	kV/A	-	0.24/0.4	0.24/ 0.4	0.24/ 0.4
• Substrate temperature	°C	-	300	400	400-60
• Argon pressure	×10 <sup>-3</sup> mbar	-	-	3.66-4.34	4.0
• N <sub>2</sub> pressure	×10 <sup>-3</sup> mbar	-	-	0.16-1.84	-
• Substrate bias voltage	V	-	-200	-200	-200
• Duration	min	20	30	150	60
• Turntable speed	rpm	-	4.0	4.0-9.0	4.0

**3. MODELING METHODOLOGIES:**

**3.1 Determination of Polynomial Equation Using RSM Model of Tin Coating Roughness**

From previous study in [28], Determination of suitable model to represent relationship of roughness and process factors is based on model analysis. Sequential model sum of square (SMSS) analysis, lack of fit test, and model summary statistic have been analyzed to select the appropriate model. Based on that, the quadratic polynomial equation may represents the relationship of TiN coating roughness and input variables.

Based on the modeling work, a quadratic polynomial equation as shown in Eq. (1) represents

the relationship between input PVD coating process parameters and roughness is developed as the following:

$$\begin{aligned}
 \text{Roughness} = & -1265.15 + 2145.43P_{N_2} + 388.44P_{Ar} + \\
 & 174.30\omega_{TT} - 569.10P_{N_2}P_{Ar} - 333.37P_{N_2}\omega_{TT} - \\
 & 55.44P_{Ar}\omega_{TT} + 23.81P_{N_2}^2 + 2.68\omega_{TT}^2 + 86.33 P_{N_2}P_{Ar} \\
 & \omega_{TT} \tag{1}
 \end{aligned}$$

where P<sub>N<sub>2</sub></sub> is nitrogen pressure, P<sub>Ar</sub> is argon pressure, and ω<sub>TT</sub> is Turntable Speed.

In the same study [28], a validation process was done using residual error and prediction accuracy. Residual error as shown in Eq. (2) is used to measure the difference between the predicted and the actual value for each dataset. Residual error is the simple

performance measure that used in many studies [29-32]. Equation for residual error,  $e$  as the following:

$$e = \frac{vp - va}{vp} \quad (2)$$

where  $vp$  is predicted value and  $va$  is actual value.

### 3.2 Model Validation

To validate the resulted model (objective function), three set of data were conducted in three different experimental run. In validation runs, the actual surface roughness fall within 90% prediction interval ( $PI$ ). The absolute range of residual errors ( $e$ ) was very low at 4.08 to 8.62 to indicate that the surface roughness could be accurately predicted by the model.

## 4. EXPERIMENTAL RESULT AND DISCUSSION

Coating roughness values from the seventeen experimental runs ranging from 44.83 nm to 104.92 and shown in Table 2.

### 4.1 Effect of Argon Pressure

Fig.1. shows the interaction between Ar gas pressure and surface roughness. Coating roughness increases from 59.17 nm to 67.21 nm as Argon gas pressure increases from  $4.0 \times 10^{-3}$  mbar to  $4.2 \times 10^{-3}$  mbar. However, surface roughness is supported at lower Ar gas pressure and becomes smoother when the TT and N<sub>2</sub> pressure are set to 6.5 rpm and  $1.0 \times 10^{-3}$  mbar respectively.

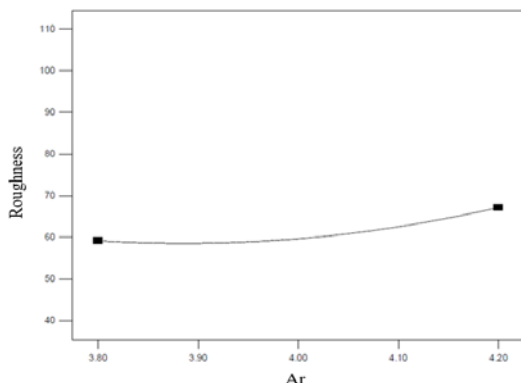


Figure 1: Interaction between Argon Gas Pressure and Coating Roughness.

### 4.2 Interaction between Turntable Speed and Nitrogen Gas Pressure

This result indicate that there is a strong interaction between coating process parameters (N<sub>2</sub> and TT). As N<sub>2</sub> gas pressure increases from  $0.5 \times 10^{-3}$  mbar to  $1.5 \times 10^{-3}$  mbar at low TT speed, 5.0 rpm, TiN coating roughness decreases from 86.47 nm to 62.76 nm. However, higher TT speed at 8.0 rpm increases the TiN coating roughness from 64.9 nm to 78.9 nm as N<sub>2</sub> gas pressure increases from  $0.9 \times 10^{-3}$  mbar to  $1.5 \times 10^{-3}$  mbar.

### 4.3 Interaction between Turntable Speed and Argon Gas Pressure

Coating roughness value increases at higher Argon pressure and higher TT speed. As TT speed is high at 8.0 rpm, and Ar gas pressure increases from  $3.8 \times 10^{-3}$  mbar to  $4.2 \times 10^{-3}$  mbar, the coating roughness increases from 56.12 nm to 82.70 nm. However, surface roughness decreases from 76.38 nm to 65.89 nm by reducing the speed of TT to 5.0 rpm while Ar pressure increases from  $3.8 \times 10^{-3}$  mbar to  $4.2 \times 10^{-3}$  mbar.

## 5. GENETIC ALGORITHMS (GAs)

GAs are an Artificial Intelligence algorithms techniques for process optimization, and are capable of extracting some of strategies in the nature uses successfully, Then derived strategies can be changed and used into theories of mathematical optimization searching for a global optimum within a time space. In the process, GAs in Fig. 2 applies three fundamentals rules in its process of learning and search for global optimum within a time space. These are selection, crossover, and mutation. An illustration for GAs methodology application in optimization process is given in Fig. 3. For implementation and based on existing literatures including [33] works, after assigning appropriate parameters for the GAs, the process parameters are encoded as follows:

- First, encode the process parameters as genes by binary encoding.
- Combine a genes set for a chromosome that execute GAs basic operations (crossover and mutation).
- Parent chromosomes exchange to generate new offspring using crossover operation.
- Apply mutation operation to create small randomness with a new chromosome.

- Evaluate each chromosome by decoding parameters from other chromosome for performance measures prediction in machining.
- For optimization process, to get the fitness or objective value, objective function is the criterion to select the new population in the next generation.
- After completing all iterations at some conditions, the optimal result is derived by comparing the objective values among all individual solutions (chromosomes).

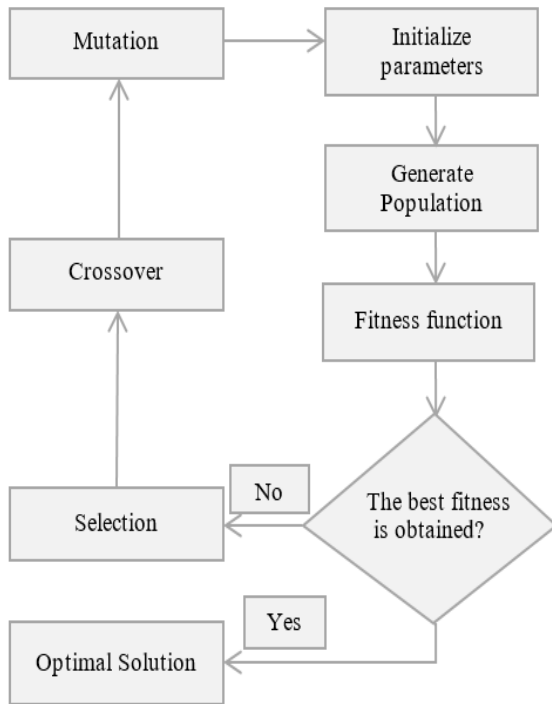


Figure 2: Optimal Solutions Flow of GAs [34]

**5.1 GAs Parameters Limitation Constraints**

For coating process experiment, Eq. (3-5) are subjected the limitation constraints for the optimization fitness function of GAs as follows:

**Nitrogen pressure:**

$$0.16 \leq N2 \leq 1.84 \tag{3}$$

**Argon pressure:**

$$3.66 \leq Ar \leq 4.34 \tag{4}$$

**Turntable speed:**

$$3.98 \leq TT \leq 9.02 \tag{5}$$

**5.2 GAs Optimization Setup and Programming**

To get the optimal solution using genetic algorithms, we take some criteria into consideration. Considering the flow of GAs to search about the optimal solutions given in Fig. 2, include initial population size of GAs parameters, the selection function type, and rates of crossover and mutation. Per prior researches, there are no optimum setting values produced as a guideline for GAs parameter combination in order to reach the optimal result. In terms of optimization using MATLAB toolbox, many combinations choices to set values were validated to get the best solution, such as the selection function type (Stochastic uniform, Remainder, Uniform, Roulette).

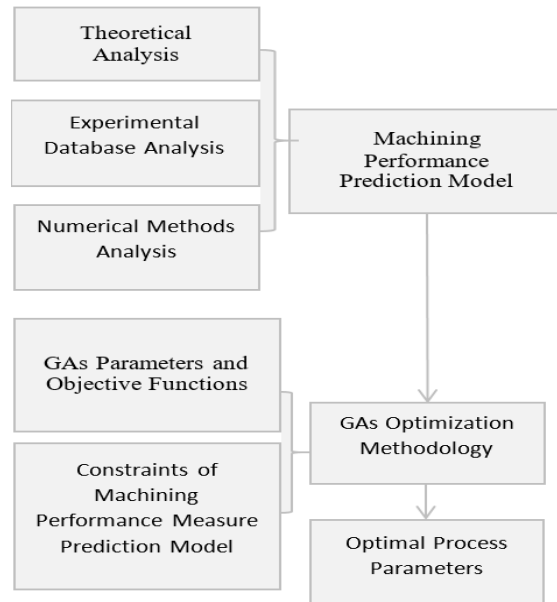


Figure 3: GAs Optimization Methodology

The best setting values of the GAs parameters combination to achieve the optimal solution were set to 100 chromosomes (solutions), roulette wheel, rank, heuristic, and uniform for the population size, selection function, scaling function, crossover function, and mutation. The cross over and mutation rate were 0.8, and 1.0, respectively [35].

**6. RESULT AND DISCUSSION**

Considering optimization objective function in Eq. (1), a combination of GAs parameter in Table 3, and the limitation constraints of the optimization in Eq. (3-5), the implementation results for the optimal value are represented in the Fig. (4-6) to minimize the coating roughness. Per Fig. 4, the minimum roughness value could be reached by setting the

optimal coating condition values for N<sub>2</sub> pressure, Ar pressure, and TT to  $1.778 \times 10^{-3}$  mbar,  $3.66 \times 10^{-3}$  mbar, and 9.02 rpm, respectively. Fig.5 draw the fitness scaling plot. Fig. 6 shows the value of the mean fitness at 45.86 nm, with the best fitness value = 23.87nm. Moreover, in this experiment and by referring to Fig. 1, the GAs findings demonstrate that low Ar rates was found to be better for coating roughness, while N<sub>2</sub> rate and TT speed were found better to be at high rate.

The optimization result in this research reveals that GAs are very effective in optimization TiN

coating roughness with reduction ratio of 46.75%. And this value is considered as a very high ratio compare to the experimental dataset.

However, some limitations have been reported in this research. One important limitation is related to machine run which gets different result in each trial for the same input parameters, and this is clear in the last three data in the dataset. On the other hand, more trials in GAs programming setting might get better result toward minimum coating roughness.

Table 2. TiN Coating Roughness Result by Actual Experiment

Run	N <sub>2</sub> pressure [ $\times 10^{-3}$ mbar]	Ar pressure [ $\times 10^{-3}$ mbar]	Turntable Speed [rpm]	Roughness [nm]
1	1.84	4	6.5	83.03
2	1	3.66	6.5	69.35
3	1	4.34	6.5	75.17
4	0.16	4	6.5	81.19
5	1.5	3.8	5	79.57
6	0.5	3.8	5	80.67
7	0.5	4.2	5	100.92
8	0.5	4.2	8	73.43
9	1.5	4.2	5	44.83
10	1	4	9.02	81.54
11	1.5	3.8	8	50.8
12	0.5	3.8	8	67.91
13	1.5	4.2	8	104.92
14	1	4	3.98	83.22
15	1	4	6.5	67.41
16	1	4	6.5	54.64
17	1	4	6.5	56.09

### 6.1 GAs Iteration Number Evaluation

Fig. 6 illustrates the number of progressive iteration which has been generated by GAs to obtain the minimum value of roughness. The roughness values have decreased sharply until generation number 15, and then fluctuating until iteration 72 to

get optimal results (iterations) depending on the parameters setting up the combination.

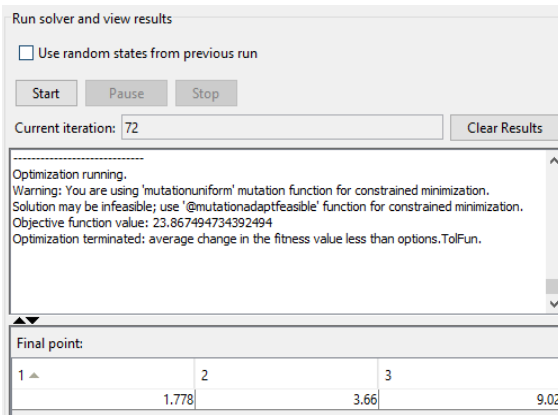


Figure 4. GAs Optimal Solutions for Roughness

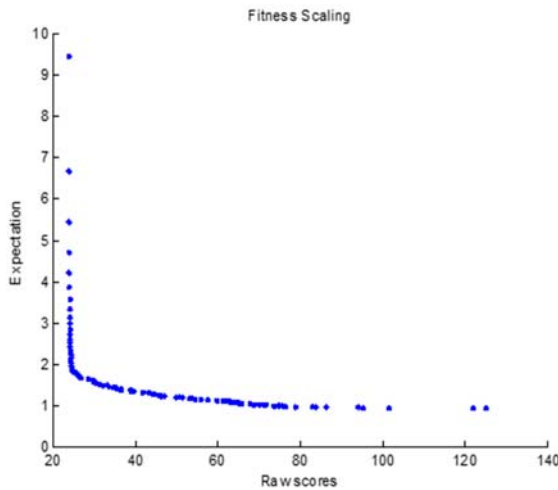


Figure 5. Fitness Scaling for Roughness

From the experimental dataset we note that the lowest value of roughness is 44.83nm. The best optimized roughness value has been reached by using GAs compare to the experimental dataset with reduction of 20.96nm at high ratio of percentage=46.75%.

This optimal reduction ratio is much higher than previous studies for GAs application in machining and coating parameters optimization. [36] revealed that GAs decreased the minimum surface roughness value of the experimental data by about 25.7 %. [35] Also applied GAs for minimizing coating grain size and found the reduction ratio was 6%.

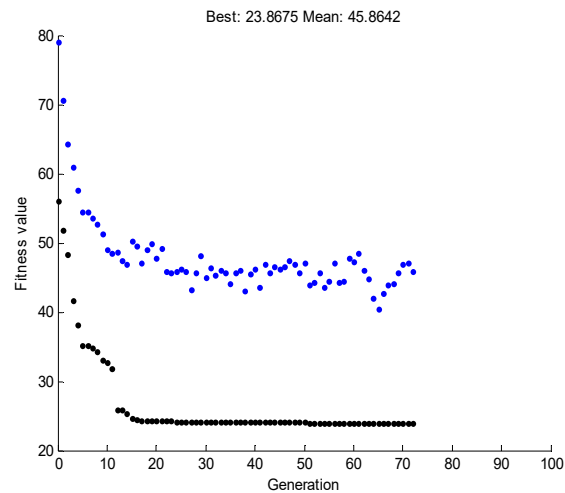


Figure 6. GAs Plot Functions for the Optimal Solution for Roughness among Generations

## 6.2 GAs Model Validation

The validation process was done by comparing the new optimal data to the experimental dataset and analyzing the number of progressive iterations for optimal solutions estimated by those approaches. The calculation for validating results can be made by the previous Eq. (1). To evaluate and prove the results depending on the equation; we need to transfer the obtained values of optimum coating parameters in GAs into this equation, and then we expect to get the same value between result using MATLAB and transformation process result. Fig. 4 indicates that we can reach the minimum roughness value by setting the optimal cutting condition values to  $1.778 \times 10^{-3}$  mbar for Nitrogen pressure,  $3.66 \times 10^{-3}$  mbar for Argon pressure, and 9.02 rpm for the Turntable Speed. After passing the obtained optimal parameters from MATLAB toolbox into Eq. (1), we found that the output is 23.87nm. By comparing this value with the MATLAB result in Fig. 4 we can observe the two values are same.

## 7. CONCLUSION

In machining, cutting tool efficiency is important to achieve high quality product, TiN is an effective material for coating process due to wear resistance and hardness. PVD vapours the target to be deposited as a thin film on substrate at different levels of three input parameters ( $N_2$ , Ar, and TT). Thus using harder cutting tool with TiN increase the quality of last product as desired toward sustainability. In this paper, the objective function for coating roughness was developed based on RSM technique. Using genetic algorithms, an objective fitness function for three input parameters has been passed and implemented. The results have been discussed in details. Prediction interval and residual error have been evaluated to validate the result.

The new presented model could get better coating roughness than actual data as follows:

• The collected data using RSM approach can be applied to develop the parameters for limitation constraints of genetic algorithms, even with a small amount of data.

• Optimal values for coating roughness have been developed using GAs with 23.87nm at  $1.778 \times 10^{-3}$  mbar for Nitrogen pressure,  $3.66 \times 10^{-3}$  mbar for Argon pressure, and 9.02 rpm for Turntable Speed.

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