Application of artificial neural networks in properties modelling of PVD and CVD coatings

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ABSTRACT

Purpose: The aim of this paper is to describe the application of artificial neural networks in development of a model, which describes the influence of PVD and CVD coatings properties on the cutting edge durability from sintered carbides covered with these layers.

Design/methodology/approach: The input data used for the artificial neural networks were PVD and CVD coatings microhardness, thickness, grain size and their adhesion to the substrate. On the network’s output is the durability of the PVD and CVD coatings coated on sintered carbide blades determined in technological cutting trials of grey cast iron.

Findings: Research results shows, that the greatest influence on the durability of coated sintered carbide blades is adhesion to the substrate. Smaller influence on blades durability has the size of grains. Other properties have a minor influence on the cutting tool.

Practical implications: The presented results indicates, that the coating material selection and design of PVD and CVD coatings deposition process should be implemented with taking into consideration in the first place the best coating’s adhesion to the substrate.

Originality/value: The application of artificial neural networks for influence determination of PVD and CVD coatings microhardness, grain size, thickness and adhesion to the substrate on the durability of the sintered carbide blades covered with investigated coatings.

Keywords: Analysis and modelling; Computational Material Science; Working properties of materials and products; Mechanical properties; Thin and thick coatings

Reference to this paper should be given in the following way:
1. Introduction

In recent years, in scientific and industrial environment an increasing interest in the production and application of multifunctional composites, and nanostructure gradient tools and machine parts coatings can be observed. Although the coating on the cutting tools blades are used for many years, their rapid development has occurred in the last decade. Currently, modified PVD (Fig. 1) and CVD (Fig. 2) coatings methods enable the production of machine parts and tools covered by these coatings with extreme tribological properties [1-7].
The dynamic development of research in the field of surface engineering is often aided by computerised techniques for data collecting and processing and for numerical simulations. Literature also provides many examples of materials computer science in surface engineering [14-18].

2. Methodology

The investigations were performed on sintered carbide cutting edges coated with PVD and CVD coatings, which are described among others in [1,19,20]. To build a model with use of artificial neural networks such properties as coating thickness, microhardness, grain size and adhesion to the substrate were used.

Coating thickness was measured by kalotest method. Microhardness was examined using a dynamic method Vickers method. Grain size was estimated with use of Scherrer method. The measure of coating adhesion to the substrate is the critical load [N], was determined by Scratch Test (Fig. 3).

Fig. 3. Acoustic emission (AE) and friction force Ft as a function of the load Fn for Ti(C,N)+Al2O3+TiN coating obtained by CVD method on sintered carbides

In Table 1 applied ranges summary of coating thickness, microhardness, grain size and the critical load is presented.

For the coatings ranking in terms of inserts cutting ability coated with investigated coatings technological cutting trials on grey cast iron were performed. During the cutting process, the mean width of flank wear VBh was measured. The tests were stopped when the VBh value obtained the assumption criterion VBh = 0.20 mm. Tool life T is determined by time of continuous machining (determined by minutes) close to a threshold VBh. Operations were carried out with a cutting speed vc of 180 m/min; feed rate f=0.2 mm/rev tooth; depth of a cut ap=1 mm. The range of cutting ability is presented in Table 2.

![Table 1](image_url)

<table>
<thead>
<tr>
<th>Thickness, µm</th>
<th>Microhardness HV 0.05</th>
<th>Grain size, nm</th>
<th>Critical load, N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min. value</td>
<td>1.8</td>
<td>2500</td>
<td>9.8</td>
</tr>
<tr>
<td>Max. value</td>
<td>8.4</td>
<td>3861</td>
<td>27.2</td>
</tr>
</tbody>
</table>

For the construction of artificial neural networks the software package called Statistica Neural Network was used. Created numerical model of PVD and CVD coatings on sintered carbides was developed. Two sets of descriptive vectors were obtained during data collection processes. The input set consists of four input descriptors, which are PVD and CVD coatings microhardness, thickness, grain size and their adhesion to the substrate.

The corresponding output set contains the durability of the PVD and CVD coatings coated on sintered carbide blades determined in technological cutting trials of grey cast iron. The whole set of collected vectors was divided into three subsets. First set, which was used for artificial neural networks training, was build of a half of available vectors.

A quarter of vectors was placed in a validation set used for neurons weight modification in the training process. Remaining vectors were used as testing set after teaching processes. The kind of the problem was determined as the standard, which means, that every vector is independent from another vector. The assignment of vectors to training, validation or testing set was random. Different architectures such as linear networks, radial base functions (RBF), regressive networks (GRNN) and multilayer perceptron (MLP) were applied in the training process. Best results was obtained for multilayer perceptron with four input neurons, one hidden layer and one output neuron. This architecture (4:4-6-1:1) is presented on (Fig. 4).
- standard deviation ratio - standard deviation of errors for the output variable;
- Pearson correlation - the standard Pearson-R correlation coefficient between measured and predicted output values of the output variable. In Table 3 accepted evaluations of correlation forces are presented.

Table 3. Evaluation of correlation force

<table>
<thead>
<tr>
<th>$R$</th>
<th>Correlation force</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 ~ 0.2</td>
<td>none</td>
</tr>
<tr>
<td>0.2 ~ 0.4</td>
<td>small</td>
</tr>
<tr>
<td>0.4 ~ 0.7</td>
<td>medium</td>
</tr>
<tr>
<td>0.7 ~ 0.9</td>
<td>strong</td>
</tr>
<tr>
<td>0.9 ~ 1.0</td>
<td>very strong</td>
</tr>
</tbody>
</table>

3. Results

The paper presents the application of artificial neural networks to assess the impact of PVD and CVD coatings properties on the durability of carbide blades covered with these coatings. The average absolute error, standard deviation ratio and Pearson correlation coefficient for the training, validation testing sets are summarised in Table 4 shows, that all property models build with use of artificial neural networks are correctly simulated. The sensitivity analysis between input and output data (Table 5) shows that the blade durability has the greatest influence on coating adhesion to the substrate. In addition, the analysis of 3D charts shows, that the change of critical load, which is a measure of coating adhesion to the substrate has the greatest influence on the change of blades cutting ability (Figs. 5-14). Other properties, such as microhardness, coating thickness and grain size have a lesser impact on tested blades durability changes. However, it should be noted, that, among other properties, changing the grain size affects the most intensively the blade durability. In addition, the blade durability is inversely proportional to grain size. Change of microhardness and thickness of tested coatings have a minor influence on the cutting blade durability.

4. Summary

Based on experimental examinations results of multi-point inserts coated with PVD and CVD coatings computational model of the relationship between coating properties and inserts’ cutting ability covered by these coatings have been developed using artificial neural networks. The model includes the impact of properties such as hardness, adhesion to the substrate, grain size and thickness of the coating on the durability of coated blades. The results are presented in 3D graphs. It was found that the greatest impact on the durability of the blades covered with coatings has the adhesion to the surface. Significant influence has also the grain size change. Other properties, hardness and thickness have small influence on the examined coated multi-point inserts stability. In addition, developed tool life models may be useful for prediction of coatings’ operational properties based on knowledge of coatings' mechanical properties, without having to perform expensive and time-consuming cutting ability examinations.

Table 4. Regression statistics of artificial neural network trained for prediction of PVD and CVD coatings properties deposited onto sintered carbides

<table>
<thead>
<tr>
<th>Network architecture</th>
<th>Regression statistics</th>
<th>Training Set</th>
<th>Validation Set</th>
<th>Testing Set</th>
</tr>
</thead>
<tbody>
<tr>
<td>MLP3 4:4-5-1:1</td>
<td>Average absolute error</td>
<td>4.68</td>
<td>4.38</td>
<td>4.32</td>
</tr>
<tr>
<td></td>
<td>Standard deviation ratio</td>
<td>0.31</td>
<td>0.27</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td>Pearson correlation</td>
<td>0.95</td>
<td>0.97</td>
<td>0.93</td>
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Table 5. Results of sensitivity analysis of input data for output data of artificial neural network trained for prediction of PVD and CVD coatings properties deposited onto sintered carbides

<table>
<thead>
<tr>
<th>Data sets</th>
<th>Statistics</th>
<th>Microhardness HV 0.05</th>
<th>Critical load $L_c$</th>
<th>Grain size</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Training</td>
<td>Range</td>
<td>4</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>Error</td>
<td>5.57</td>
<td>22.14</td>
<td>6.63</td>
<td>6.38</td>
</tr>
<tr>
<td></td>
<td>Ratio</td>
<td>0.92</td>
<td>3.66</td>
<td>1.10</td>
<td>1.05</td>
</tr>
<tr>
<td>Validation</td>
<td>Range</td>
<td>4</td>
<td>1</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Error</td>
<td>4.25</td>
<td>20.49</td>
<td>6.80</td>
<td>7.12</td>
</tr>
<tr>
<td></td>
<td>Ratio</td>
<td>0.86</td>
<td>4.13</td>
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<th>Critical load Lc</th>
<th>Grain size</th>
<th>Thickness</th>
</tr>
</thead>
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<tr>
<td>Training</td>
<td>Range 4 1 3</td>
<td>Error 5.57</td>
<td>Ratio 0.92</td>
<td>&lt; 60</td>
<td>22.14</td>
</tr>
<tr>
<td>Validation</td>
<td>Range 4 1 2</td>
<td>Error 4.25</td>
<td>Ratio 0.86</td>
<td>&lt; 60</td>
<td>20.49</td>
</tr>
</tbody>
</table>

Fig. 5. Evaluation of the PVD and CVD coatings critical load and the microhardness influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks at a fixed coating thickness 2.5 microns and particle size 9.8 nm

Fig. 6. Evaluation of the PVD and CVD coatings critical load and the microhardness influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks at a fixed coating thickness 2.5 microns and particle size of 420 nm

Fig. 7. Evaluation of the PVD and CVD coatings critical load and the microhardness influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed thickness of 2.5 microns and coating microhardness 3600 HV 0.05

Fig. 8. Evaluation of the PVD and CVD coatings particle size and the critical load influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed thickness of 2.5 microns and coating microhardness 2300 HV 0.05
3600 HV 0.05
neural networks with a fixed grain size of 9.8 nm microhardness
coated with PVD and CVD coatings determined by artificial
the critical load influence of tool life T for sintered carbide tools
Fig. 9. Evaluation of the PVD and CVD coatings thickness and
and grain size influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 11. Evaluation of the PVD and CVD coatings microhardness
3600 HV 0.05
coated with PVD and CVD coatings determined by artificial
neural networks with a fixed grain size of 9.8 nm microhardness
Fig. 10. Evaluation of the PVD and CVD coatings thickness and
and grain size influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 12. Evaluation of the PVD and CVD coatings microhardness
350 nm grain size and microhardness
coated with PVD and CVD coatings determined by artificial
Fig. 13. Evaluation of the PVD and CVD coatings microhardness
2355 HV 0.05
neural networks with a fixed thickness of 1.8 microns and the
critical load Lc = 35 N
coated with PVD and CVD coatings determined by artificial
Fig. 14. Evaluation of the PVD and CVD coatings thickness and
and grain size influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 15. Evaluation of the PVD and CVD coatings microhardness
3600 HV 0.05
networks with a fixed thickness of 2.5 microns and the
coated with PVD and CVD coatings determined by artificial
Fig. 16. Evaluation of the PVD and CVD coatings microhardness
100 N
networks at a fixed and microhardness of 3600 HV and the
critical load Lc = 100 N
networks with a fixed critical load Lc = 100 N and particle
coated with PVD and CVD coatings determined by artificial
Fig. 17. Evaluation of the PVD and CVD coatings thickness and
and the thickness influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 18. Evaluation of the PVD and CVD coatings microhardness
9.8 nm
coated with PVD and CVD coatings determined by artificial
networks with a fixed grain size of 350 nm and microhardness
Fig. 19. Evaluation of the PVD and CVD coatings thickness and
the critical load influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 20. Evaluation of the PVD and CVD coatings microhardness
2.5 microns and the
coated with PVD and CVD coatings determined by artificial
Fig. 21. Evaluation of the PVD and CVD coatings microhardness
100 N
networks at a fixed and microhardness of 3600 HV and the
critical load Lc = 100 N
networks with a fixed critical load Lc = 100 N and particle
coated with PVD and CVD coatings determined by artificial
networks with a fixed grain size of 9.8 nm microhardness
Fig. 22. Evaluation of the PVD and CVD coatings thickness and
and grain size influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 23. Evaluation of the PVD and CVD coatings microhardness
350 nm grain size and microhardness
neural networks with a fixed thickness of 1.8 microns and the
critical load Lc = 35 N
coated with PVD and CVD coatings determined by artificial
Fig. 24. Evaluation of the PVD and CVD coatings microhardness
2355 HV 0.05
neural networks with a fixed thickness of 2.5 microns and the
coated with PVD and CVD coatings determined by artificial
Fig. 25. Evaluation of the PVD and CVD coatings microhardness
3600 HV 0.05
networks at a fixed and microhardness of 3600 HV and the
coated with PVD and CVD coatings determined by artificial
Fig. 26. Evaluation of the PVD and CVD coatings thickness and
and grain size influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 27. Evaluation of the PVD and CVD coatings microhardness
9.8 nm
coated with PVD and CVD coatings determined by artificial
networks with a fixed grain size of 350 nm and microhardness
Fig. 28. Evaluation of the PVD and CVD coatings thickness and
and grain size influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 29. Evaluation of the PVD and CVD coatings microhardness
2.5 microns and the
coated with PVD and CVD coatings determined by artificial
Fig. 30. Evaluation of the PVD and CVD coatings microhardness
100 N
networks at a fixed and microhardness of 3600 HV and the
critical load Lc = 100 N
networks with a fixed critical load Lc = 100 N and particle
coated with PVD and CVD coatings determined by artificial
networks with a fixed grain size of 9.8 nm microhardness
Fig. 31. Evaluation of the PVD and CVD coatings thickness and
and grain size influence of tool life T for sintered carbide tools
coated with PVD and CVD coatings determined by artificial
Fig. 32. Evaluation of the PVD and CVD coatings microhardness
350 nm grain size and microhardness
neural networks with a fixed thickness of 1.8 microns and the
critical load Lc = 35 N
coated with PVD and CVD coatings determined by artificial
Fig. 33. Evaluation of the PVD and CVD coatings microhardness
2355 HV 0.05
neural networks with a fixed thickness of 2.5 microns and the
coated with PVD and CVD coatings determined by artificial
Fig. 34. Evaluation of the PVD and CVD coatings microhardness
3600 HV 0.05
networks at a fixed and microhardness of 3600 HV and the
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Additional information

Selected issues related to this paper were presented at the 18th International Scientific Conference on Achievements in Mechanical and Materials Engineering AMME’2010.

References


