Journal of Achievements in Materials and Manufacturing Engineering

VOLUME 24
ISSUE 2
October
2007

Modelling of properties of the PVD coatings using neural networks

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Received 11.04.2007; published in revised form 01.10.2007

Analysis and modelling

ABSTRACT

Purpose: The goal of this work is to develop the neural network model for prediction of properties Ti+TiN, Ti+Ti(C,N) and Ti+TiC coatings obtained in the PVD process.

Design/methodology/approach: Neural network models were developed based on the experimental results multifractal analysis of the examined coatings were made basing on measurements obtained from the AFM microscope, using the projective covering method.

Findings: Investigations carried out confirm that the fractal dimension and parameters describing the multifractal spectrum shape may be used for prediction of coatings obtained in the PVD processes.

Research limitations/implications: Investigation or relationship between parameters describing the multifractal spectrum and physical properties of the examined materials calls for further analyses.

Originality/value: The presented in the paper research results indicate that neural networks can be applied for modeling the properties of PVD coatings on the base of multifractal parameters.

Keywords: Computational material science; PVD coatings; Multifractal geometry; AFM

1. Introduction

The fractal and multifractal analysis used to describe the structure of the surface has become more and more popular lately and it is more broadly applied to many fields of science including material engineering. The analyses conducted, focus not only on the description of the processes themselves but also on their relation to the parameters of the definite materials.

In the case of the coatings obtained in the PVD processes numerous physical qualities depend on the structure and the chemical composition. The coatings are also characterised by specific geometric properties to describe which such concepts as morphology, topography and shape are used. The results of the research indicate that there is a relation between the morphology of the surface of the coatings and the technology used in the process. It is extremely important to define the kind of relation as the morphology of the surface is crucial for such properties of coatings as: roughness parameter, coefficient of friction, hardness and wear resistance [1]. The contemporary methods used to describe the topography of the surface of the coatings make it possible to define the relation between the parameters of the technology applied to obtain the coatings, their structure, usable properties and their fractal dimension and multifractal characteristics [2, 3].

Investigation results are presented in [4, 5] of the possibility of employing the artificial neural networks and fractal analysis for description of the analysed surface roughness. Results of the own research [6-9] on the coatings properties and fractal methods of their description induced authors to begin work on investigating the relationships between the PVD coatings service properties and the fractal and multifractal parameters [10-16], using the artificial neural networks.

2. Experimental procedure

The tests were carried out on the samples made of high-speed sintered steel of the ASP30 type containing 1,28% C, 4,2% Cr, 5,0% Mo, 6,4% W, 3,1% V i 8,5% Co. The samples underwent the heat treatment in the salt bath furnaces with the austenitizing in the temperature of 1180 ºC and the triple tempering in the temperature of 540 ºC. The samples were introduced into the one-chamber vacuum furnace with the magnetron to the ionic sputtering built-in. The samples were placed at the distance of 95 mm from the disc of the magnetron. It was carried out in the atmosphere containing 100% N_2, 50% CH_4 and 50% N_2 and 100% CH_4 in the temperature of 460, 500 and 540 ºC. The TiN, Ti+Ti(C,N) and TiC PVD coatings were deposited on the surfaces of the samples in 60 minutes.

The microhardness tests of coatings were made on the SHIMADZU DUH 202 ultra microhardness tester. Test conditions were selected so that the required and comparable test results would be obtained for all analysed coatings. Measurements were made at 0.05 N load, eliminating influence of the substrate on the measurement results.

Erosion resistance of the applied coatings was determined basing on the erosion test, carried out on the Falex Corporation Falex Air Jet Eroder device, representing the air jet type devices, in which the erodent leaving the nozzle at a particular pressure hits the examined specimen surface positioned at a given angle in respect to the nozzle [1].

Examinations of the topography of the deposited coatings were made on the scanning electron microscope and using the atomic force microscopy method (AFM) on the Digital Instruments Nanoscope E instrument. Scanning ranges were 5 and 2 µm respectively.

The detailed methodology of the fractal and multifractal analyses was presented in [2-3].

The artificial neural networks were employed for modelling the relationships between the parameters defining the multifractal spectrum (Ds, α_{min}, α_{max}, $\Delta\alpha$, $F(\alpha_{min})$, $F(\alpha_{max})$ and $\Delta F(\alpha)$) and their properties. All calculations were carried out using the Statistica Neural Network program. Therefore, the standard regression statistics calculated by the program were assumed to be the base evaluation characteristics of the developed neural networks: average error, standard deviation of the output variable error, quotient of standard deviations for errors and data, R-Pearson correlation coefficient value for the assumed value and the one obtained at the output and relative error value (expressed in %).

It was assumed that the following relationships will be determined:

- between the roughness and the multifractal parameters,
- between the micro-hardness and erosion resistance, and the multifractal parameters,
- between erosion resistance of PVD coatings and α_{min}, α_{max}, $F(\alpha_{min})$, $F(\alpha_{max})$ parameters,
- between micro-hardness of PVD coatings and Ds, α_{min}, α_{max}, $F(\alpha_{min})$, $F(\alpha_{max})$ parameters,
- between roughness of PVD coatings and Ds, α_{min}, α_{max}, $F(\alpha_{min})$, $F(\alpha_{max})$ parameters.

The RBF (networks with the radial base functions) and MLP networks (multilayer perceptrons) with one and two hidden layers were analysed as network types. The number of the hidden layers and the number of neurons in the hidden layers was selected automatically by the program. In each case several thousand to a dozen thousand of various networks were analysed, and in case of analysis of the assumed network quality coefficients the best one was selected.

3. Results and discussion

Fractal dimension of the analysed coatings deposited onto the ASP 30 high-speed sintered steel was determined using the projective covering method.

Table 1.
The detailed results of the fractal and multifractal analysis and of the roughness parameter R, micro-hardness and erosion resistance (Er) results

Coating	Temperature°C	Ds	R µm	α_{max}	α_{min}	$\Delta\alpha$	$f(\alpha_{max})$	$f(\alpha_{min})$	Δf	Er	HV
Ti+TiC (2000nm)	460	2.0183	0.2530	2.0080	1.9320	0.0760	1.8710	0.4600	-1.4110	7.7	3100
	500	2.0191	0.2200	2.0120	1.8370	0.1750	1.8890	0.0340	-1.8550	7.1	3200
	540	2.0486	1.1120	2.0620	1.7750	0.2870	1.5760	0.1760	-1.4000	10.9	3400
Ti+Ti(C,N) (2000nm)	460	2.0259	0.2800	2.0160	1.8600	0.1560	1.8110	0.2090	-1.6020	9	2800
	500	2.0120	0.2180	2.0060	1.9890	0.0170	1.9720	0.6820	-1.2900	2.7	2300
	540	2.0335	0.2070	2.0150	1.8910	0.1240	1.8200	0.4680	-1.3520	5.4	2700
Ti+TiN (2000nm)	460	2.0299	0.3920	2.0170	1.8140	0.2030	1.8260	0.0650	-1.7610	10.5	2800
	500	2.0260	0.1710	2.0120	1.8750	0.1370	1.8620	0.2310	-1.6310	5.4	2600
	540	2.0153	0.2580	2.0090	1.9340	0.0750	1.8820	0.6010	-1.2810	5.3	2500
Ti+TiC (5000nm)	460	2.0122	0.4300	2.0050	1.9340	0.0710	1.9230	0.4170	-1.5060	7.7	3100
	500	2.0237	0.2640	2.0100	1.8450	0.1650	1.8980	0.0680	-1.8300	7.1	3200
	540	2.0679	0.9690	2.0440	1.7600	0.2840	1.6610	0.1400	-1.5210	10.9	3400
Ti+Ti(C,N) (5000nm)	460	2.0273	0.3710	2.0110	1.8640	0.1470	1.8540	0.1510	-1.7030	9	2800
	500	2.0016	0.2080	2.0020	1.9650	0.0370	1.9630	0.7830	-1.1800	2.7	2300
	540	2.0317	0.4100	2.0140	1.8950	0.1190	1.8320	0.4000	-1.4320	5.4	2700
Ti+TiN (5000nm)	460	2.0275	0.5220	2.0180	1.8330	0.1850	1.8170	0.1990	-1.6180	10.5	2800
	500	2.0245	0.3980	2.0120	1.8710	0.1410	1.8520	0.0360	-1.8160	5.4	2600
	540	2.0207	0.3420	2.0080	1.9020	0.1060	1.8930	0.1470	-1.7460	5.3	2500

The determined A(δ) values are presented in bilogarithmic plots and the auxiliary plots were made which show changes of the fractal dimension value, determined basing on two consecutive points of the bilogarithmic diagram make their correct selection easier. Based on the multifractal analysis spectra of the generalised fractal dimensions were determined for all scanning ranges and their corresponding multifractal spectra of the analysed coatings (Fig. 1). Measurements carried out using the AFM atomic force microscope (Fig. 2) made it also possible to determine parameter R characterising the analysed surface roughness according to [3]. The detailed fractal and multifractal analysis summary results and the obtained R parameter and mechanical properties results are presented in Table 1.

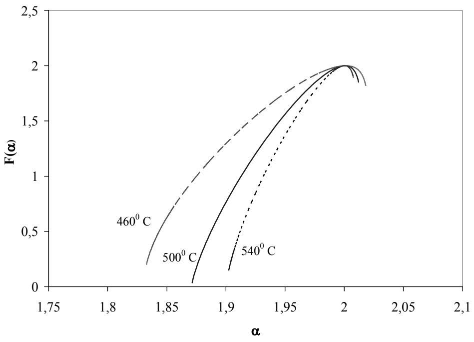

Fig. 1. Multifractal spectra of the analysed surface (Ti+TiN coatings, scanning range 5000nm)

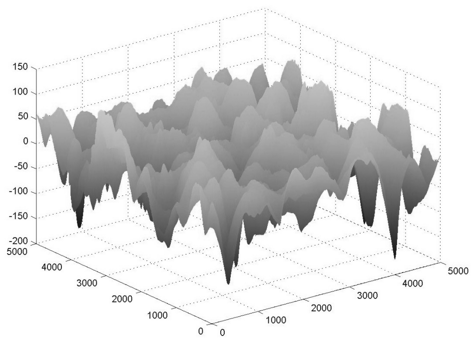

Fig. 2. Topography of the analysed surface (AFM, Ti+TiN coating, 500°C, scanning range 5000nm)

Test results presented in Table 1 were used for development of the neural networks models describing relationships between the coatings properties and the fractal parameters. The experimental data set was split into three subsets: training, validation, and the test one. Cases from the training subset were used for modification of the network weights in the training set and those from the validation subset for evaluation of the prediction errors in the training process. The test subset was used for the independent assessment of the network efficiency when its development procedure was completed. Splitting the input data set into the particular subsets was carried out at random. The following proportions of case numbers in the subsets were used: training – 50%, validation – 25%, test – 25%.

Types, structures of the particular networks, and assessment coefficients of the neural network efficiency are listed in tables 2-4.

Analysis of the effect of the parameters describing the multifractal spectrum on the erosion resistance of the coatings, presented in figure 3 was carried out as an application example for the developed neural networks.

Table 2.
Type, structure of particular neural networks and quality coefficients for calculating the multifractal parameters on the basis of roughness

Parameter	Type/ structure of the network	Data set	Relative error E, %	Quotient of standard deviations	Pearson correlation coefficient
α_{max}	RBF	Testing	7.1	0.38	0.93
	1-1-1-1	Average	6.6	0.51	0.83
α_{min}	MLP	Testing	20.3	0.66	0.76
	1-31-1	Average	16.9	0.75	0.65
$\Delta\alpha$	MLP	Testing	20.2	0.66	0.76
	1-31-31-1	Average	17.0	0.75	0.65
$f(\alpha_{max})$	MLP	Testing	13.8	0.51	0.87
	1-1-6-1	Average	11.0	0.60	0.91
$f(\alpha_{min})$	MLP	Testing	27.1	0.96	0.31
	1-1-1-1	Average	22.7	0.91	0.47
Δf	MLP	Testing	>40	-	-
		Average	>40	-	-

Table 3.
Type, structure of particular neural networks and quality coefficients for calculating the multifractal parameters on the basis of micro-hardness and erosion resistance

Parameter	Type/ structure of the network	Data set	Relative error E, %	Quotient of standard deviations	Pearson correlation coefficient
α_{max}	MLP	Testing	8.1	0.54	0.99
	2-8-1	Average	4.6	0.44	0.91
α_{min}	RBF	Testing	6.6	0.99	0.99
	2-6-1	Average	4.6	0.24	0.97
$\Delta\alpha$	MLP	Testing	3.8	0.13	0.99
	2-28-10-1	Average	3.3	0.13	0.99
$f(\alpha_{max})$	MLP	Testing	6.8	0.37	0.98
	2-31-21-1	Average	4.5	0.39	0.93
$f(\alpha_{min})$	MLP	Testing	22.1	0.76	0.83
	2-47-1	Average	13.1	0.64	0.79
Δf	MLP	Testing	24.2	0.84	0.56
	2-31-1	Average	25.3	0.77	0.60

4. Conclusions

In the paper there have been presented the examples of applying artificial neural networks for modeling the interrelations between the selected properties of PVD coatings like roughness, microhardness and erosion resistance, and the parameters describing the multifractal spectrum of those coatings. Using the results of research, the proper models of neural networks have been worked out that allow for determining the interrelations between the mentioned parameters.

Table 4.
Type, structure of particular neural networks and quality coefficients for calculating the properties of the PVD coatings on the basis of multifractal parameters

Property	Type/ structure of the network	Data set	Relative error E, %	Quotient of standard deviations	Pearson correlation coefficient
Erosion resistance	MLP 4-1-1-1	Testing	11.6	0.31	0.96
		Average	14.3	0.49	0.86
Micro-hardness	MLP 5-13-11-1	Testing	13.5	0.42	0.92
		Average	12.1	0.52	0.85
Roughness	MLP 5-47-1	Testing	12.0	0.32	0.95
		Average	9.7	0.48	0.85

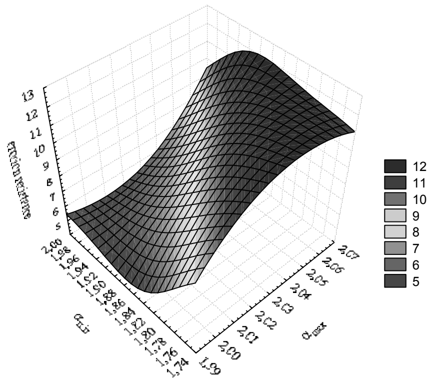

Fig. 3. Effect of α_{max} and α_{min} multifractal parameters on the erosion resistance (for $f(\alpha_{max})$=1,845 and $f(\alpha_{min})$=02,93)

Quality coefficients of the worked out neural networks have been presented in tables 2-4. In the case of modeling parameters defining the multifractal spectrum on the basis of the roughness of coatings, the obtained results are not satisfactory as show quality coefficients (a big relative error) and quotient of standard deviations as well as a small value of R-Paerson correlation coefficient. Only in the case of α_{max} parameter, the calculation results are satisfactory. In the case when calculations are done on the base of micro-hardness and erosion resistance (Table 3), a firm improvement of conformity of results for α_{min}, α_{max}, , $\Delta\alpha$, $f(\alpha_{max})$ parameters, have been obtained. For $f(\alpha_{max})$ and $\Delta\alpha$ parameters, the quality coefficients do not allow for defining the existence of interrelations between these parameters and micro-hardness and erosion resistance of the analysed PVD coatings.

The most interesting results are when the properties of the coating are being calculated (erosion resistance, micro-hardness and roughness) on the basis of multifractal parameters. Then, the quality of the worked out neural networks are satisfactory (Table 4) and enable the analysis of the influence of selected parameters on the properties of the coatings, what has been presented in Fig. 3.
The presented in the paper research results indicate that neural networks can be applied for modeling the properties of PVD coatings on the base of multifractal parameters, what will be the subject of future detailed examinations.

Acknowledgements

Investigations were financed in part within the framework of the research project KBN 3 T08C 019 28 headed by Dr. W. Kwaśny.

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