The neural networks application in predicting the geometrical parameters of coatings formed on a steel substrate by laser alloying

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Abstract. A mathematical model for predicting the geometric parameters of boron and aluminum-based coatings formed on a steel substrate by laser alloying is presented in the work. The model combines the principles of the theory of experiment planning with an artificial neural network (ANN) apparatus. Coatings were formed by means of laser heating of the steel surface with a pre-applied treatment paste. The ANN was built, trained and tested for the prediction of the width and depth of the molten bath on a steel substrate. The prediction results of the obtained neural network were compared with the corresponding linear models. The efficiency of the considered approach and the possibility of its application for predicting the values of laser treatment of steel parts of machines subjected to surface hardening are shown. The presented approach allows to use one mathematical model for predicting several parameters, thereby reducing the number of experiments.

1. Introduction
Nowadays combined processes of thermal-chemical treatment (TCT) and high energy fluxes have been effectively applied in surface engineering technologies of machine parts for surface (local) hardening [1-3]. In particular, laser radiation can modify a metal surface in a short time, compared to traditional TCT methods [1]. It is possible to obtain coatings with the same phase composition as traditional treatment, but different microstructure.

For practical application in order to build a computer system for predicting the results of laser reflow diffusion layers, interesting mathematical models that summarize experimental data, which are obtained in the form of a regression equation or in the form of power relations. Currently, one of the most effective methods of experimental data processing is the apparatus of artificial neural networks [4].

Artificial neural networks (ANN) is a mathematical model, as well as its software implementation, in which the process of transforming information is aimed at accumulating experimental knowledge and presenting it for further processing [4-6]. Interpreted information has a digital representation that allows to use ANN as a model of an object with unknown characteristics.

However, the capabilities of neural network models are limited by their learning method. The most well-known method of ANN teaching is the error propagation algorithm [4]. The disadvantages of this method are the unpredictability of the result as well as the duration of the learning process. The duration of training can be the result of a non-optimal choice of the step length and the size of the
training sample, and the problem in learning usually occurs for two reasons: network paralysis and falling into a local minimum.

To improve the efficiency of the models based on the use of the mathematical apparatus of the ANN, it is important to reduce the number of experiments to obtain training pairs. The training set should adequately describe the process of diffusion hardening, i.e. contain maximum information about the effect of laser alloying parameters on the geometric parameters of the melting zone. From this point of view, it is of interest to use the results of mathematical experiments planning (MEP) or experimental design [7].

The purpose of this work is the ANN synthesis of predicting the geometric parameters of the coatings (width and depth of the molten bath) based on boron and aluminum, formed on a steel substrate using laser heating based on experimental data.

2. Regression models of the geometric parameters and the algorithm of the ANN application
The profiles investigation of the formed laser tracks on the surface of carbon steel showed that a two-layer structure is formed, consisting of a remelted zone (RZ) and a heat-affected zone (HAZ) (figure 1) [8].

![Figure 1](image)

(a) (b)

Figure 1. The scheme of the laser alloying (a), where 1 is the RZ, 2 is the HAZ, 3 is the base metal (substrate); and macrostructure of the laser track cross-section (b), where $L$ is the RZ width, $h$ is the RZ depth.

HAZ is formed due to the rapid heat removal from the RZ to the substrate and is up to 50 μm thick. It will be not taken into account when the geometric parameters modeling of coatings.

The values of geometrical parameters ($L$ and $h$) depending on the modes of laser heating are given in table 1.

| Velocity $V$ (mm min$^{-1}$) | focus $Z = -2.9$ mm | focus $Z = -0.9$ mm |
|-----------------------------|--------------------|--------------------|
| 200                         | ![Image](image)     | ![Image](image)     |
| 500                         | ![Image](image)     | ![Image](image)     |

Table 1. Geometric parameters of the RZ (μm).

The initial data preparation and the construction of a mathematical model for predicting the geometric parameters dependence on the scan speed and focal length values were presented in previous research [8]:

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\[ h = 302.38 - 0.06 \cdot V + 40.7 \cdot Z + 0.04 \cdot V \cdot Z, \]  
(1)

\[ L = 242.46 + 0.19 \cdot V - 234.05 \cdot Z + 0.24 \cdot V \cdot Z. \]  
(2)

All ANN data about the task is collected in a set of examples. Therefore, the quality of the neural network training depends on the number of examples in the training sample, to what extent these examples describe the task. The experimental results are being used as the training sample for both ANN and the construction of generalized mathematical models. To supplement the training sample, generalized models (1) and (2) are being used to increase the number of training pairs without increasing the number of experiments. Thus, the construction sequence of the ANN prediction consists of the following steps: 1) preparation the initial data; 2) the construction of a mathematical model using the MEP; 3) preparation of factor space for ANN learning on the basis of the initial data and the obtained polynomial mathematical model; 4) building a model of the ANN; 5) ANN training.

Two types of networks are suitable for solving the forecasting problem: a multilayer perceptron (MLP) and a network of radial basis functions (RBF) [4]. RBF networks provide more accurate results, but require a large amount of experimental data. With a relatively small dimension of the training sample, which is typical for this study, the MLP-type ANN is more effective. The main task at ANN building is to determine the number of neurons in the hidden layer. Figure 2 shows a graphical representation of the architecture of a synthesized neural network consisting of input, internal and output layers.

Figure 2. The topology of the ANN prediction, where: \( \omega_{ij} \) is the weight of the neuron connection of the previous layer with the next one.

ANN training was conducted using the error back-propagation method where its mathematical interpretation goes to the functional dependency [4, 5]:

\[ F : F(X_i) \rightarrow y_i, i = 1, 2...132, \]

where \( X_i \) is the \( i \)-th row of the matrix of \( X \) input values; \( y_i \) is the \( i \)-th row of the matrix of \( Y \) output values (the \( i \)-th element of the column vector).

This is achieved by minimizing the objective function of the neural network error, calculated by the least squares method:
\[ MSE(\{\omega_{ij}\}) = \frac{1}{2n} \sum_{k=1}^{n} (r_k - y_k)^2, \]

where \( r_k \) is the value of the \( k^{th} \) output of the ANN, \( y_k \) is the target value of the \( k^{th} \) output of the ANN, \( n \) is the neurons number of the output layer, \( \omega_{ij} \) is the connection weight linking neurons \( i \) and \( j \).

### 3. Modeling of coatings geometric parameters using ANN

It is necessary to form training sets before building neural networks. The generated data matrix consisting of 50 examples obtained from equations (1) and (2) as well as previously conducted experiments will be used as a file of experimental data [8].

**Table 2.** Training and test sets for ANN.

| No. | Velocity \( V \) (mm min\(^{-1} \)) | Laser focus \( Z \) (mm) | RZ depth \( h \) (μm) | RZ width \( L \) (μm) |
|-----|--------------------------------|---------------------|-----------------|------------------|
| 1   | 200                            | -2.9                | 149.15          | 820              |
| 2   | 500                            | -2.9                | 96.35           | 668.21           |
| ... | ...                            | ...                 | ...             | ...              |
| 49  | 287                            | -1                  | 232.98          | 462.16           |
| 50  | 230                            | -1                  | 238.68          | 465.01           |

ANN modeling was performed using the Artificial Neural Network tool of Scilab package choosing the best network topology.

The simulation results are presented in figure 3.

**Figure 3.** The regression coefficient R of the ANN training: (a) for a network with a 2-2-2 topology; (b) for a network with topology 2-5-2; (c) for a network with a 2-8-2 topology.

The best performance in terms of the correlation coefficient was shown by a network with the architecture of 2-8-2, where it equals to 1. There is an exact linear relationship between the ANN output and the target value at \( R = 1 \), if \( R \) is close to zero, then there is no linear relationship between these values [4, 5]. The results comparison of the calculations of the diffusion layer depth using the ANN and the model obtained using the MEP are presented in table 3.
Table 3. Comparison of the calculations results of the RZ parameters: width and depth.

| Velocity $V$ (mm min$^{-1}$) | Focus $Z$ (mm) | RZ depth $h$ (μm) | RZ width $L$ (μm) (MEP) | RZ depth $h$ (μm) (ANN) | RZ width $L$ (μm) (ANN) |
|-----------------------------|---------------|-------------------|------------------------|------------------------|------------------------|
| 200                         | -2.9          | 149.15            | 820                    | 149.16                 | 819.24                 |
| 500                         | -2.9          | 96.35             | 668.21                 | 96.58                  | 668.24                 |
| 200                         | -0.9          | 247.41            | 447.2                  | 246.57                 | 448.3                  |
| 500                         | -0.9          | 219.92            | 438.34                 | 217.83                 | 440.16                 |

4. Conclusion

The ANN prognostic model based on experimental data and the results of MEP is able to distinguish functional relationships between the geometrical parameters of coatings and laser processing modes. The efficiency of this mathematical tool in the subject area is shown.

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