Use of neural networks for modelling the mechanical characteristics of epoxy composites treated with electric spark water hammer

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Abstract

The main research area of this article is the analysis and modelling of the physical and mechanical characteristics of epoxy composites. The value of internal stresses was investigated using artificial neural networks. The results of the modelling studies of these parameters obtained by the authors are in good agreement with the experimental data of other scientists.

It was found that the correlation coefficient in the presented test sample is 0.98. For these features in the test samples, the prediction error when using artificial neural networks is 0.35% for aluminium oxide filler, 0.55% for chromium oxide, and 0.12% for carbon black.

It is shown that neural networks are able to analyse data and use them for the next stage of research - training. Therefore, modelling the properties of materials by neural networks provides an increase in the accuracy of experimental studies of the main physical and mechanical features of materials based on epoxy composites activated by electrospark water hammer containing dispersed fillers.

Keywords

Machine learning, neural networks, composite, test sample, internal stresses

1. Introduction

The current development of the global industry involves the widespread use of new materials with predefined characteristics for various functional purposes. From both a scientific and practical point of view, the use of composite materials, including coatings based on polymer composites [1-7] and moulded using advanced methods with the use of gas-thermal spraying [8-24], is perspective. Also, composite materials created on the basis of technologies using the external influence of mechanical force fields that regulate their structure and, as a result, determine their properties have become widely used [1-5,7].

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Composites based on cold-cured epoxy diane resins demonstrate high performance features. [3-6]. Such materials are technologically advanced when used as coatings on long-dimensional surfaces of complex profiles. When creating and studying composites, a necessary condition is the use of systems for automated processing and analysis of research results, namely neural networks.

Artificial neural networks are a promising tool for predicting processes with many variables and complex interactions of various factors [25,26]. Such networks are designed like the neural structures of the human brain, which processes information using a large number of neuronal connections. In the last few years, there has been a steady increase in the use of neural network modelling for analysis in various fields of science to predict the properties of an object both at the stage of its formation and at the next stage of processing the results of experimental studies [27-30]. In particular, the use of artificial neural networks is effective in the study of polymeric composite materials based on reactoplastics, where a number of factors should be taken into account both in their formation and in the study of properties. It is worth noting that the chosen parameters of neural networks affect the accuracy of the systems in research [31-33]. In general, the properties of polymer composites can be accurately modelled using machine learning algorithms. The advantage of this approach is the opportunity to obtain research results using the proposed non-destructive testing method. In this case, the effects on the structure change in the composite, which is crucial for the control of their features, are not only in the formulation of the composite, but also in the study of their properties. [25-27].

The main task of modern polymer composite materials technology is to ensure high technological and operational properties.This is achieved by targeted control of the structure of polymeric materials.This approach is based on the general theoretical understanding of the structure formation processes and their impact on the properties of composites, and the analysis of empirical data when studying the characteristics of the developed materials.A number of complex requirements are imposed on composite materials (CM) with optimal performance characteristics at the stage of their formation. This is primarily true for the polymer matrix as the basis for the composite materials. It should have high physical, mechanical, adhesion and thermal characteristics and sufficient technological properties. This is achieved by selecting the ingredients of the polymer binder, modifiers, plasticisers, catalysts, fillers, etc. [1,3-5,7]. The processing of composite materials by electric spark water hammer is also interesting from a scientific and practical point of view. It is known that the treatment of oligomers by electric arc spark discharge provides cracking of binder macromolecules [1]. This, in turn, increases the level of cross-linking of the material during moulding in the composite, and thus improves the cohesive characteristics of the materials. The main requirements for these composites and coatings based on them are a targeted complex improvement of their structural and mechanical characteristics. This leads to experimental studies to determine the dynamics of the CM structure formation processes under different modes and specifically selected stages of material formation. It should be noted that the most important properties of CMs are low residual stresses, high adhesive and cohesive strength, corrosion resistance, and processability when applied to parts of complex profiles of various technological equipment. This is achieved by introducing fillers of different nature into the polymers and adjusting the temperature and time regimes of crosslinking of the CM [3]. It is known that one of the ways to reduce internal stresses in CM is to regulate the relaxation processes at the polymer-base, polymer-filler interface, due to the creation of a homogeneous ordered structure in the coatings [2,7]. In addition, new methods of mechanical and thermodynamic activation of physicochemical processes have been developing most intensively recently, which are associated with the possibility of controlling the structure formation of composites by changing the physicochemical interaction between the components of the system [1-3,7].

In particular, a necessary condition for obtaining composites with high technological and operational properties is to ensure a strong and long-term connection between the active centers on the filler surface and the binder macromolecules. The change in the value of internal stresses should be explained on the basis of the basic principles of physical and chemical surface effects, and in particular, the active influence of the surface of dispersed particles on the crosslinking processes of the matrix in the surface layers.

In view of the above, the use of artificial neural networks in the study of internal stresses, which is an important feature of the mechanical properties of epoxy composites, is an important problem of modern materials science. However, modern scientists have not yet paid enough attention to modelling the physical features, specifically the internal stresses of epoxy composite materials, with neural networks. It is important to study the internal stresses of materials at different stages of the formation of epoxy composites filled with aluminium oxide, chromium oxide and carbon black by neural networks based on a matrix activated by electric spark water hammer.

2. Method of research with neural networks

Artificial neural networks (ANNs) have emerged as a new branch of computing that can be used in a wide range of experimental studies. Many studies have been published on predicting the properties of composites [31,33-35]. ANNs are based on the neural structure of the human brain, which processes information between many neurons, and in the last few years there has been a steady increase in interest in neural network modelling in various fields of materials science [36-38]. The basic unit in the ANN is a neuron. Neurons are connected to each other by a weighting factor that determines the existing and strength of interconnections and thus affects the performance of the next groups of neurons. ANNs can be trained to perform a function by adjusting the values of the weights between neurons either based on information from outside the network or by the neuron itself in reaction to input data. This is the key point of the ability of ANNs to learn and record research results. The multilayer neural network (MLP) is the most widely used in most experimental studies[25-27]. A backpropagation algorithm can be used to train these multilayer feedforward networks with a differential transfer function for approximation, pattern matching, and pattern classification. The term ‘backpropagation’ refers to the process by which the derived network errors in terms of network weights and biases can be calculated and taken into account in later stages of the experiments.

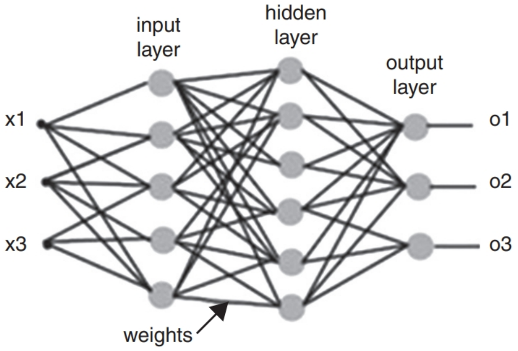

Fig. 1 – General view of a MLP network.

Fig. 1 shows a general view of an MLP network. As you can see from the figure, a multilayer perceptron (MLP) is a feed-forward artificial neural network model that maps a set of input data to a set of related output data. An MLP consists of multiple layers of units in an oriented field, with each layer fully connected to the next. Except for the input units, each unit is a neuron (or processing unit) with a nonlinear activation function. MLP uses a supervised learning technique called backpropagation to train the network. MLP is a modification of the standard linear perceptron and can distinguish between data that cannot be separated linearly [27-31].

In this research, a 2-9-1 MLP network was built for composites filled with aluminium oxide, chromium oxide and carbon black. The training algorithm was BFGS, the error function was SOS, the hidden layer activation functions were tangential for carbon black and chromium oxide, and exponential for aluminium oxide. The activation functions of the outer layer are identity for chromium oxide and carbon black filler, and tangential for aluminium oxide filler [29, 35,37,39]. It should be noted that the epoxy diane binder ED-20 pretreated with electric spark water hammer was used as a matrix. In this case, the activity of such a matrix increases when interacting with dispersed fillers of aluminium oxide, chromium oxide and carbon black, improving the degree of crosslinking of the composite as a whole.

3. Experimental approach

The main task of the modern technology of manufacturing polymeric composite materials is to study the ways of directed control of the structure of polymeric materials. The targeted control of its parameters is used to ensure high technological and operational properties[4,40,41]. This approach is based on the general theoretical understanding of structure formation processes and the analysis of the influence of the empirical data on the physical, mechanical and operational properties of the developed materials. Much attention has been paid to improving the polymer matrix to form materials with high physical, mechanical, adhesive, and thermal characteristics and sufficient rheological properties. Also, modification of compositions by external force fields is a promising direction for improving the properties of heterogeneous composites at the current stages of materials science development. The technology of activation of oligomeric compositions by magnetic, ultrasonic, ultraviolet, radiation fields and electrospark water hammer at the initial stages of material formation opens up fundamentally new possibilities for controlling the processes of interaction between components, which can be used to regulate the performance characteristics of the material [1,6,7].

Processing in external fields of both compositions as a whole and individual components under selected modes allows creating new classes of materials with a given set of performance properties. In this regard, interesting from a scientific and practical point of view, special attention was paid to the use of electrospark water hammer to activate the binder by electrospark water hammer. It is known that the treatment of oligomers by electric arc spark discharge provides cracking of binder macromolecules. [1,4,5] This increases the level of cross-linking of the material during composite forming and, as a result, increases the cohesive properties of the materials.

Changes in molecular and segmental mobility during crosslinking of oligomeric compositions due to the formation of new physical and chemical links, as well as increase in molecular weight to gelation, depend heavily on the rheological characteristics and concentration relations of the input components of the system. Therefore, in further studies, the effect of the plasticiser on the physical, mechanical, and thermal properties of the CM under optimised material forming regimes was investigated. It has been experimentally established that the introduction of aliphatic resin DEG-1 into an epoxy oligomer at a concentration of 10 wt% per 100 wt% of ED-20 provides an increase in heat resistance by 19...21%, a destructive bending stress by 63...65%, and a decrease in internal stresses by 45...52% relative to the original epoxy matrix.

The non-monotonic nature of the dependence of the physical and mechanical characteristics of CM on the concentration of the plasticiser was experimentally established. It has been found that the maximum values of the dependence of properties on the concentration of DEG-1 occur as a result of the introduction of an aliphatic resin in the amount of 10...20 wt% per 100 wt% of the modified epoxy oligomer. It should be noted that at these concentrations, the destructive stress, flexural modulus, and impact strength of the treated ED-20 resin with plasticiser increase by 1.5...1.8 times, and the internal stresses decrease by 2.1 times relative to the untreated plasticised matrix.

It is known that one of the ways to reduce internal stresses in CM is to regulate the relaxation processes at the polymer-base, polymer-filler interface, due to the creation of a homogeneous ordered structure in the coatings [1-6]. In addition, new methods of mechanical and thermodynamic activation of physicochemical processes have been developing most intensively recently, which are associated with the possibility of controlling the structure formation of composites by changing the physicochemical interaction between the components of the system. We have used the activation of polymer chains of macromolecules by cracking heterogeneous compositions with electric spark water hammer (ESWH).

It is important to study the value of internal stresses in ESWH-modified composites at different concentrations of fillers. The analysis of the research results shows that with an increase in the concentration of fillers, the internal stresses in the CM increase. This is explained by an increase in the degree of gelation and better physical crosslinking of the matrix in the surface layers with an increase in the concentration of dispersed particles in the ESWH, which allows creating a material with a more crosslinked structure. At the same time, the introduction of carbon black particles as a filler ensures the formation of CMs with minimal internal stresses compared to other composites under study. This is due to the active influence of the surface of these particles on the physical and chemical processes of interfacial interaction of active centers on the surface of the solid phase with free radicals formed during the ESWH of epoxy oligomer [4-7]. It should be noted that this effect of the filler is not only near its surface, but also extends over some distances into the polymer volume. This makes it possible to form a material with surface layers around the filler that have a significant length and high physical and mechanical characteristics. This creates the conditions for targeted control of structural parameters on the performance characteristics of the studied CMs.

In order to confirm the above-described mechanism of CM structure formation, it is important to study the dynamics of internal stress growth at different stages (including high-temperature) of the formation of epoxy composites containing selected fillers at different concentrations. It has been experimentally established that an increase in internal stresses was observed for all composite materials with increasing temperature. This is confirmed by the analysis of the results of calculating internal stresses at different stages of sample thermostatting. It should be noted that a general analysis of the kinetics of internal stress growth in all samples, without exception, shows the highest gradient of internal stress growth at the stages of CM crosslinking. The first stage is the period after heat treatment of the composites at a temperature of $T = 393 \pm 2$ K for $\tau = 2 \pm 0.1$ h. In our opinion, after heat treatment, the processes of chemical crosslinking are completed in epoxy composites, and a material with a thermodynamically balanced structure is formed. During cooling of the CM, as well as in the future, processes occur that are accompanied by the formation of physical units both between macromolecules or free radicals and the filler surface, and between the active radicals themselves, in particular at temperatures below the glass transition temperature of the polymer matrix. This, in turn, is followed by the formation of a thermodynamically unbalanced system [2-5]. We observed a sharp jump in the value of internal stresses in the CM at the last stage of the study within 12 hours after heat treatment.

In addition, it should be noted that in all the studied samples, after the EIGU matrix treatment, an increase in internal stresses in the CM was observed compared to the original composites (at the same concentrations) at all stages of composite thermostatting. The obtained results confirm the above assumption about the formation of new physical nodes after ESWH of the matrix at the last stages of material crosslinking.

The value of internal stresses was modelled using the experimental data obtained in the work by neural networks [28,29,33,34]. In particular, a sample of 28341 elements for each epoxy polymer filled with carbon black, aluminium oxide and chromium oxide was used to train the neural networks. Of this data, 80% was randomly selected for the training set, and the remaining 20% was left to evaluate the quality of the forecast. Here, the output parameter was the value of internal stresses (sint, MPa). The filler concentration (wt% per 100 wt% of binder) and temperature were considered as input parameters.

The dependences of the experimental data of internal stresses on the predicted ones obtained by the neural network method are shown in Figs. 2-4. It is proved that the prediction results are in good agreement with the experimental data obtained by the authors [30,35]. The data obtained using neural networks coincide with the input data (research results). It was confirmed that the created models adequately match the research results. This allows us to assert that neural network models can be used to predict the parameters of polymers treated with electric spark water hammer.

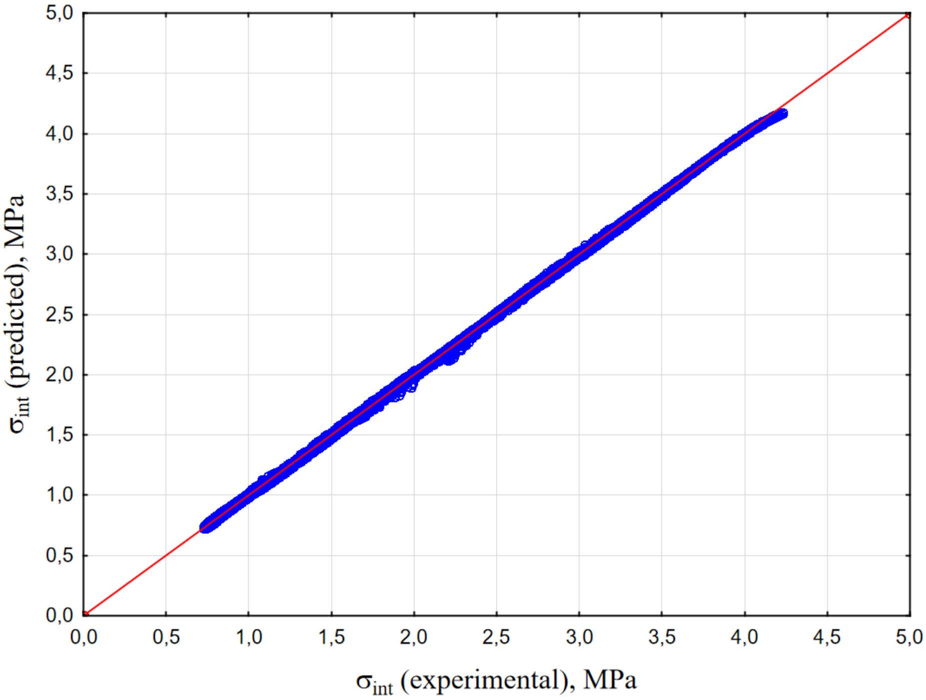

Figure 2: Predicted and experimental dependences for aluminium oxide filled composite

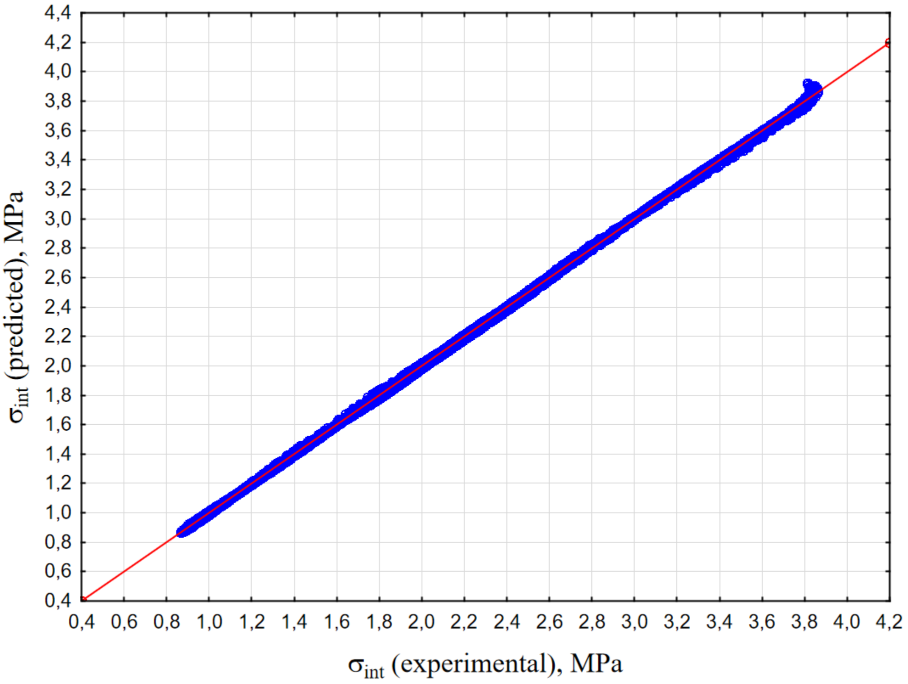

Figure 3: Predicted and experimental dependences for a chromium oxide-filled composite

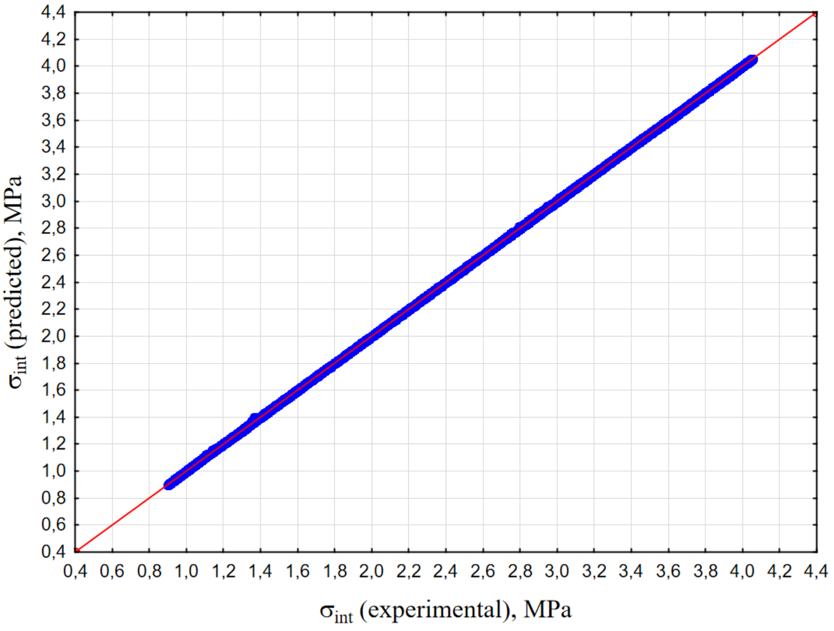

Figure 4: Predicted and experimental dependences for a composite filled with carbon black

The dependences of the predicted value of internal stresses on the filler concentration in the composite and temperature are shown in Figs. 5-7. These figures make it possible to visually assess the dependence of internal stresses on temperature and filler concentration at certain points, which allows to reduce the time and material costs for further research [36-38].

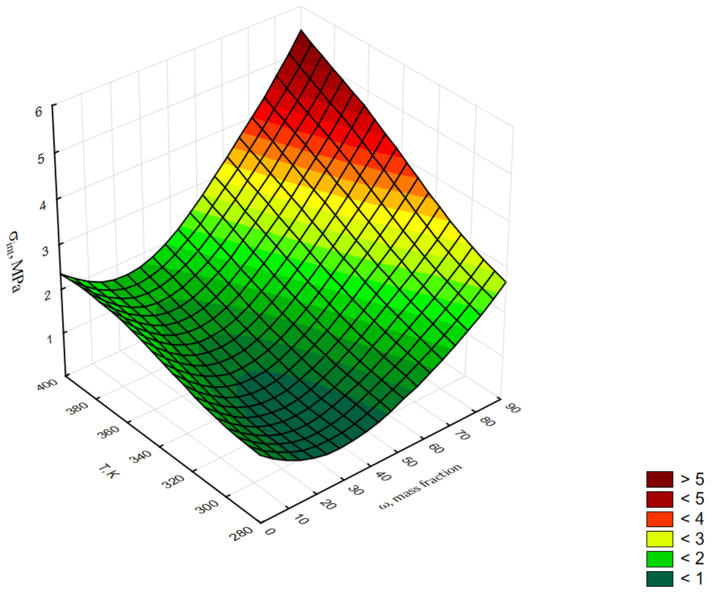

Figure 5: Temperature dependence of internal stresses of aluminium oxide-filled CM

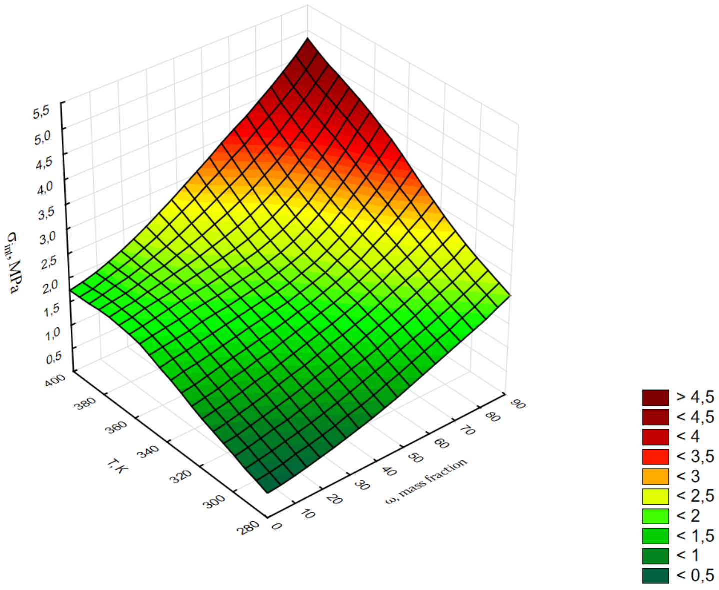

Figure 6: Temperature dependence of internal stresses in chromium oxide-filled CM

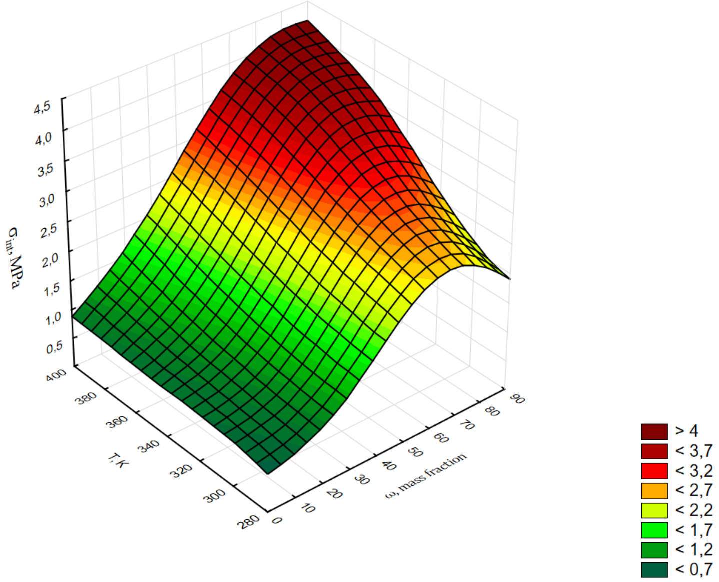

Figure 7: Temperature dependence of the internal stresses of the carbon black-filled CM

The diagrams of residual values for composites filled with aluminium oxide, chromium oxide, and carbon black, respectively, are shown in Figs. 8-10. The histogram data of the residual values shows the frequency of each value interval compared to the residual values. In particular, the residuals show the difference between the experimental and predicted values. They are found to be concentrated around zero and have a normal distribution [29,34,36,39,42].

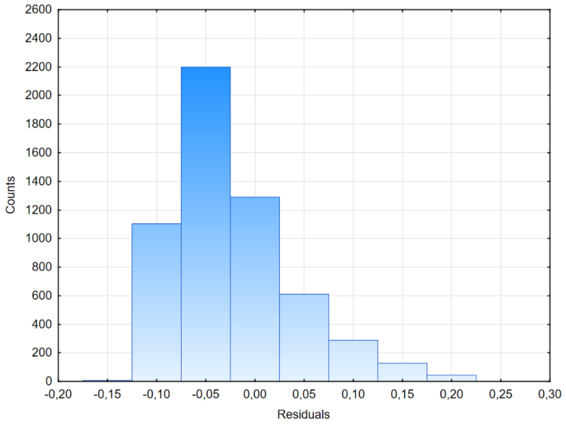

Figure 8: Histogram of residual values for aluminium oxide-filled composites

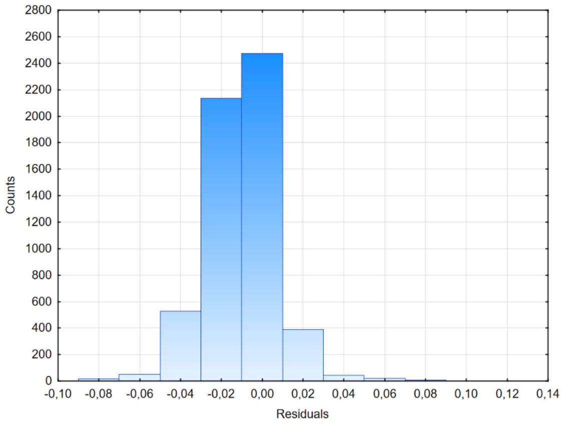

Figure 9: Histogram of residual values for chromium oxide-filled composites

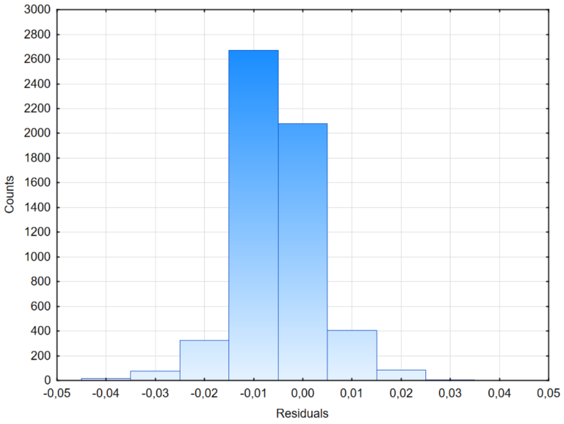

Figure 10: Histogram of residual values for composites filled with carbon black

To analyse the data, a statistical graph in the form of residual value diagrams is often used. It was found that these characteristics have a dependence close to the normal distribution law, which allows the use of statistical mathematical methods for processing the results of the experiment.

4. Conclusion

Neural networks have modelled the changes in the internal stresses of epoxy polymers filled with aluminium oxide, chromium oxide and carbon black. The results obtained are in good agreement with experimental data. The prediction error of the neural networks is 0.35, 0.55, and 0.12 % in the test samples. The obtained results will allow to create conditions for targeted regulation of physical, mechanical and thermal characteristics by controlling the structural organisation in the material. Further research is planned to optimise the processes of developing epoxy composites for various functional purposes.

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