

# Neural networks for processing experimental studies of the modulus of elasticity and hardness of epoxy composites containing $\text{Al}_2\text{O}_3$ , ZnO and PTFE<sup>\*</sup>

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## Abstract

The effect of filling with aluminum oxide, zinc oxide, and polytetrafluoroethylene on the physical and mechanical characteristics of an epoxyfuran composite was investigated. It was found that the maximum values of material hardness were achieved at a concentration of 6-8 mass fraction  $\text{Al}_2\text{O}_3$  and 12-16 mass fraction ZnO per 100 mass fraction of binder. The introduction of polytetrafluoroethylene leads to a gradual decrease in hardness. The mechanism of structure formation caused by physical crosslinking at low levels of oxide filling, which contributes to the formation of a more crosslinked mesh structure, is shown.

The dependence of the elastic modulus  $E$  and the elastic modulus above the glass transition temperature ( $T_g$ )  $E_t$  on the degree of oxide filling was investigated. At temperatures above  $T_g$ , the mechanical characteristics of the components are determined by the ratios of their characteristics. In this case, there are no physical nodes between the binder macromolecules and the active centers of the filler surface. It was found that when 11-13 mass fraction of  $\text{Al}_2\text{O}_3$  and 13-17 mass fraction of ZnO per 100 mass fraction of binder were introduced, the formation of elastic modulus maxima on the concentration curve was observed. A further increase in the concentration of fillers reduces the elastic modulus  $E$ .

Using neural networks to process the results of experimental studies, a correlation between the predicted and experimental values of the physical and mechanical characteristics of epoxy composites is established. It is proved that in this case, it is more efficient to use the Akim method to study materials, which provides a more accurate reflection of changes in the relevant material characteristics. The use of interpolation methods in combination with artificial neural networks can significantly improve the accuracy of prognostication and ensure a high level of correspondence between the experimental and calculated values of epoxy composites. The obtained research results can be used to develop composite materials with predetermined characteristics.

## Keywords

machine learning, neural networks, composite, material hardness, elastic modulus

## 1. Introduction

Improving the performance of mechanisms and machines by using new composite materials (CM) [1-2], including coatings, and technologies for their formation [3-5] is perspective for minimizing the energy and metal consumption of equipment [6-8]. Increased strength characteristics of CM improve the reliability and efficiency of equipment operation. Currently, it is also promising to use epoxy binders. Such materials have improved physical and mechanical characteristics compared to other polymers. Further improvement of these characteristics is carried out by reinforcing polymeric materials with high-modulus fillers [9-11]. Oxides, nitrides are used for filling. Such materials are selected according to the value of surface energy, which, in turn, causes their different effects on the strengthening of epoxy-furan composites [12].

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The development of antifriction materials involves increasing the strength characteristics of composites by structuring them with fillers. In the process of frictional interaction, a local temperature increase occurs, which causes the CM coating to heat up. Upon reaching the glass transition temperature (T<sub>g</sub>), which for an epoxy binder is 130-132 °C, a decrease in the instantaneous elastic modulus by an order of magnitude was observed. In the highly elastic state, which is characteristic of temperatures above T<sub>g</sub>, the material wear intensifies. The decrease in the wear resistance of polymeric CM under such conditions is due to an increase in both the mechanical (deformation) and adhesive components of friction in the friction contact zone [13]. To reduce the mechanical component of friction, high-modulus fillers are added to the epoxy matrix. The elastic modulus increases, which reduces the deformation characteristics of the material. Even a slight increase in E, E<sub>t</sub>, and H reduces local deformations in the functional contact zone, which in turn helps to reduce the wear rate. One of the most important parameters that determines the wear resistance of CM is the hardness of the material. An increase in hardness helps to reduce deformations in the contact zone and increase resistance to mechanical damage. It is known that composite materials with higher hardness are characterized by a lower wear rate under the same high-speed friction conditions. Due to reduced deformation of the surface layer. The optimal combination of hardness and elasticity allows to realize a positive gradient of mechanical properties between the friction surfaces in a pair. The introduction of high-modulus fillers, such as dispersed particles of aluminum or zinc oxides, allows to increase the hardness and at the same time provide a sufficient level of material strength. At the same time, the effect of surface activity, including physical crosslinking, of the filler on the physical and mechanical properties of epoxy composites has not been sufficiently studied. In connection with the above, this area of research is an actual task of modern materials science.

Artificial intelligence technologies, in particular neural networks, are playing an increasingly important role in modern composite materials (CM) research. This is due to their ability to significantly improve the accuracy of predicting the mechanical characteristics of materials and automate the processing of large amounts of experimental data. Neural networks effectively model complex multidimensional relationships, allowing them to take into account the influence of numerous factors such as temperature, load, sliding speed and filler type. At the same time, traditional mathematical methods such as spline interpolation and the Akeem method allow for accurate smoothing of experimental dependencies without distortions caused by local fluctuations. The integrated application of these approaches provides a comprehensive and reliable analysis of CM properties under various operating conditions.

The purpose of this work is to use neural networks to develop materials with enhanced physical and mechanical characteristics to protect friction surfaces from wear by additional structure formation through physical interaction between binder macromolecules and active centres on the surface of Al<sub>2</sub>O<sub>3</sub>, ZnO, and PTFE fillers.

## **2. Research materials and methods**

An epoxy oligomer ED-20 was chosen for the study. For its crosslinking, a polyethylene polyamine hardener was used. The samples were formed by the method of hydrodynamic combination of components. Aluminium oxides, zinc oxides, and polytetrafluoroethylene were used as fillers. Their concentration was set in wt% per 100 wt% of the binder.

In modern research on polymeric CMs, artificial intelligence technologies, in particular neural networks [14-16], are becoming increasingly important, as they can significantly improve the accuracy of predicting their characteristics [17-20]. Neural networks are a promising tool for predicting the mechanical characteristics of epoxy CM. These systems are able to effectively handle nonlinear dependencies, automate data analysis [21-23], optimise the composition of materials and adapt to new conditions [24-26]. The properties of CMs determine the behavior during frictional interaction, since their mechanical properties depend on a number of factors, such as temperature, load, sliding speed, and filler type. Traditional mathematical methods often do not take into

account the complex correlations between these parameters. This makes it difficult to accurately predict material characteristics. Neural networks, especially deep architectures, are capable of modeling multidimensional relationships between parameters, which significantly improves the accuracy of predicting the performance of CM under various conditions [27-28]. Automation of experimental data analysis provided by neural networks reduces the influence of the human factor, which is important for obtaining accurate and reproducible results. Machine learning algorithms detect hidden trends and patterns in experimental data, which provides more objective conclusions and predictions without the need for operator intervention.

Various mathematical methods are used to analyze and process the results of the characteristics of polymer composite materials. Among the most common approaches are spline interpolation [29-30] and the Akim method [31-33], which provide an accurate reproduction of the dependencies between experimental data and allow obtaining smoothed functions for further analysis. Spline interpolation is an approximation method that allows you to build a smooth curve that passes through the specified points. It is based on dividing an interval into smaller subintervals.

The Akeem method is an interpolation method that avoids excessive oscillations typical of some other approximation methods, such as high-order polynomial interpolation. The basic idea of the method is to use special algorithms to determine the derivatives at key points, which allows for a smooth transition between curve segments. Due to this, the Akeem method gives more accurate results, especially in cases where the original data have an irregular distribution or contain local peaks. These methods are used to process experimental research results where it is necessary to obtain smoothed dependencies without unwanted fluctuations that can distort the real picture of friction and wear processes.

One of the most effective neural network architectures for analyzing mechanical characteristics is multilayer perceptron (MLP) [34-36]. They consist of an input layer, several hidden layers, and an output layer, where each neuron processes the received information and transmits it to the next level. The use of such architectures makes it possible to work effectively with large amounts of experimental data, to analyze the influence of various factors on the performance properties of polymer CM. The use of neural networks in predicting the mechanical characteristics of polymer CMs increases the accuracy of the analysis, automates data processing to optimize the composition of the CM. The use of spline interpolation, the Akeem method, and artificial intelligence elements allows for an integrated approach to the analysis of mechanical characteristics.

### **3. Discussion of the results**

High-modulus additives are commonly used to reinforce polymers, but the effect of the surface energy of fillers on the physical and mechanical properties of epoxy composites has not been studied sufficiently. The research used fillers with different surface energies: aluminum and zinc oxides, and polytetrafluoroethylene (PTFE). The introduction of oxides causes the formation of boundary layers with low molecular mobility around the filler particles. The intensity of linear wear, microhardness, and curing activation energy of epoxyfuran composites depend on the content of metal oxides, which indicates their influence on the formation of the binder's mesh structure. The process of CM formation is affected by the topology of the filler's hard surface. Selective adsorption of components is possible, which causes local enrichment of the layers located in close proximity to the interface with the binder. This contributes to the formation of a material with a different degree of crosslinking of the polymer matrix. This process is facilitated by the formation of physical nodes between the filler and binder surfaces. Such nodes remain until the phase transition of the glass transition temperature (T<sub>g</sub>).

The minimum activation energy of curing is observed at the content of 10 mass fraction per 100 mass fraction of aluminum oxide binder, which is due to the formation of a material with a more cross-linked mesh structure in the material. The latter provides high physical and mechanical characteristics of the CM. The shift of the minimum towards higher concentrations on the concentration curve for aluminum oxide compared to zinc oxide is explained by the difference in

their surface energy. It has been proven that the introduction of both aluminum and zinc oxides and fluoroplastic reduces the degree of curing of the binder. At low levels of oxide filling, additional structure formation occurs due to physical crosslinking, which contributes to the formation of a material with a tighter grid structure.

The monotonic decrease in hardness when filled with PTFE indicates the absence of physical crosslinking. It has been proven that this is due to the chemical inertness of the filler and the absence of active centers on the PTFE surface in relation to the epoxy binder. This limits or completely prevents the formation of physical bonds between the filler and the binder. The lower wear rate and friction coefficient are explained by the formation of PTFE transfer films with low shear stress on the friction surfaces.

A binder with a content of 5-10 mass fraction of aluminum oxide and 15-20 mass fraction of zinc oxide per 100 mass fraction of binder is used for the manufacture of liquid filler composites. At a higher degree of filling of 80-120 mass fraction of aluminum oxide and 60-80 mass fraction of zinc oxide per 100 mass fraction of binder, CM is used in the form of a paste-like composite.

Further study of the crosslinking mechanism was carried out by analyzing the elastic modulus ( $E$ ) below and ( $E_t$ ) higher than the temperature ( $T_{gt}$ ) of the polymer matrix. The presence of two extremes in the dependence of the elastic modulus on the filler content was established: at low concentrations up to 20 mass fraction and at high filling of 70-80 mass fraction of metal oxides, the fillers were brought to 100 mass fraction of the binder. The study of the elastic modulus ( $E_t$ ) at a temperature above the glass transition temperature ( $T_{gt}$ ) demonstrated its monotonic increase with increasing filler content.

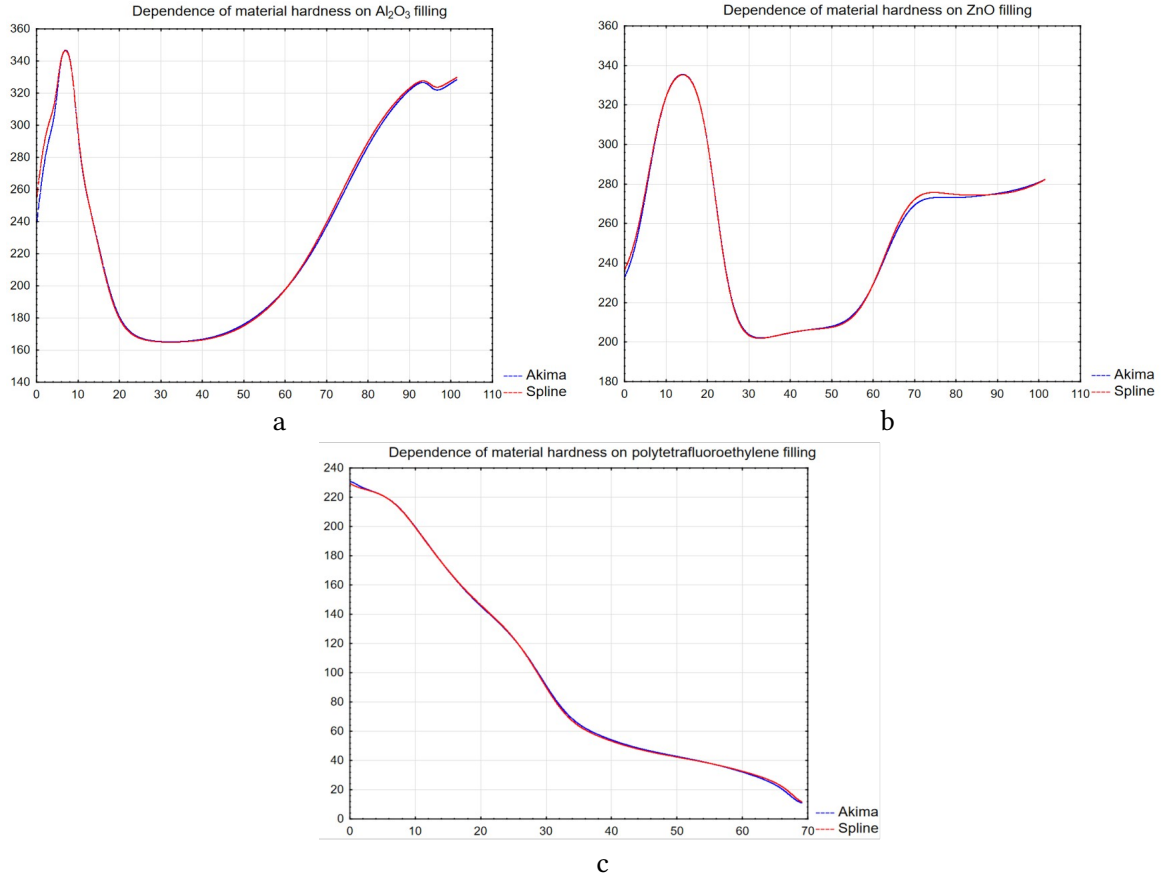
The next step in the study of mechanical characteristics is the use of neural networks to process experimental data. To model the results of hardness in PTFE and ZnO material, we used MLP 1-9-2 multilayer perceptron networks (one hidden layer, nine neurons, and two output neurons), and MLP 1-7-2 for the Al<sub>2</sub>O<sub>3</sub> filler. For the three above-mentioned fillers, error functions of the SOS type (sum of squared deviations) were used. The activation of neurons in the hidden layers was carried out using the Logistic functions for ZnO and Al<sub>2</sub>O<sub>3</sub> and the Tanh function for PTFE. For the output layers, we chose the Identity (ZnO) and Logistic (Al<sub>2</sub>O<sub>3</sub> and PTFE) functions.

The strength analysis of materials was performed on the basis of pre-processed data using artificial neural networks. The use of neural networks has significantly increased the accuracy and reliability of the results obtained, which is important in the study of mechanical characteristics of materials. Artificial neural networks significantly reduce the impact of interference in experimental studies. They reveal hidden nonlinear dependencies between strength parameters. The integration of neural networks with classical interpolation methods, such as the Akeem method and splines, ensures optimization of approximation parameters and adaptation to specific material properties [37-39]. Machine learning helped to achieve a high level of correlation between experimental data and predicted values, which contributed to the reliability of the research results. In addition, the use of neural networks made it possible to harmonize different interpolation methods, which contributed to a comprehensive analysis and minimization of deviations in complex nonlinear sections of graphs [40-42].

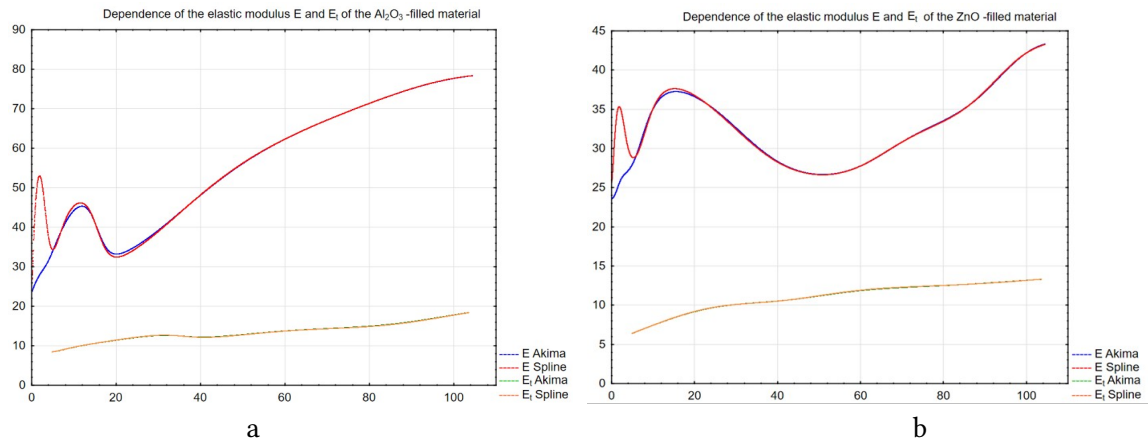
The dependence of the hardness of the epoxy-furan composite material on the degree of filling with Al<sub>2</sub>O<sub>3</sub> and ZnO is shown in Fig. 1(a, b). The study showed that the maximum hardness of the material (335-437 MPa) was achieved at 6-8 mass fraction Al<sub>2</sub>O<sub>3</sub> filling and 334-336 MPa at 12-16 mass fraction zinc oxide filling per 100 mass fraction binder. With further increase in the content of fillers, the hardness of the material decreases. At the values of 25-45 mass fraction of Al<sub>2</sub>O<sub>3</sub> filler and 30-55 mass fraction of ZnO, a minimum hardness of 163-166 MPa for aluminum oxide and 202-211 MPa for zinc oxide was found. With increasing filler concentration, the hardness monotonically increases to 325-330 MPa (90-100 mass fraction Al<sub>2</sub>O<sub>3</sub>) and 275-282 MPa (73-100 mass fraction ZnO). It should be noted that with an increase in the content of polytetrafluoroethylene-based filler, a gradual and monotonous decrease in the hardness of CM was observed [43-46].

Based on the experimental data after interpolation by the Akeem and spline methods and interpolation processed by the artificial neural network, it was found that although the deviations

are not significant in both cases, the Akeem method more accurately reflects changes in the value of physical and mechanical characteristics in the CM. Also, Akeem's method reflects more detailed modeling of the characteristics, which is confirmed by the results of processing with an artificial neural network.



**Figure 1:** Dependence of the hardness (H) of epoxyfuran composite on the filling: (a) -  $\text{Al}_2\text{O}_3$ ; (b) - ZnO; (c) – PTFE.



**Figure 2:** Dependence of the modulus of elasticity E below and  $E_t$  above the glass transition temperature of a material on the degree of filling with aluminum oxide (a) and zinc oxide (b).

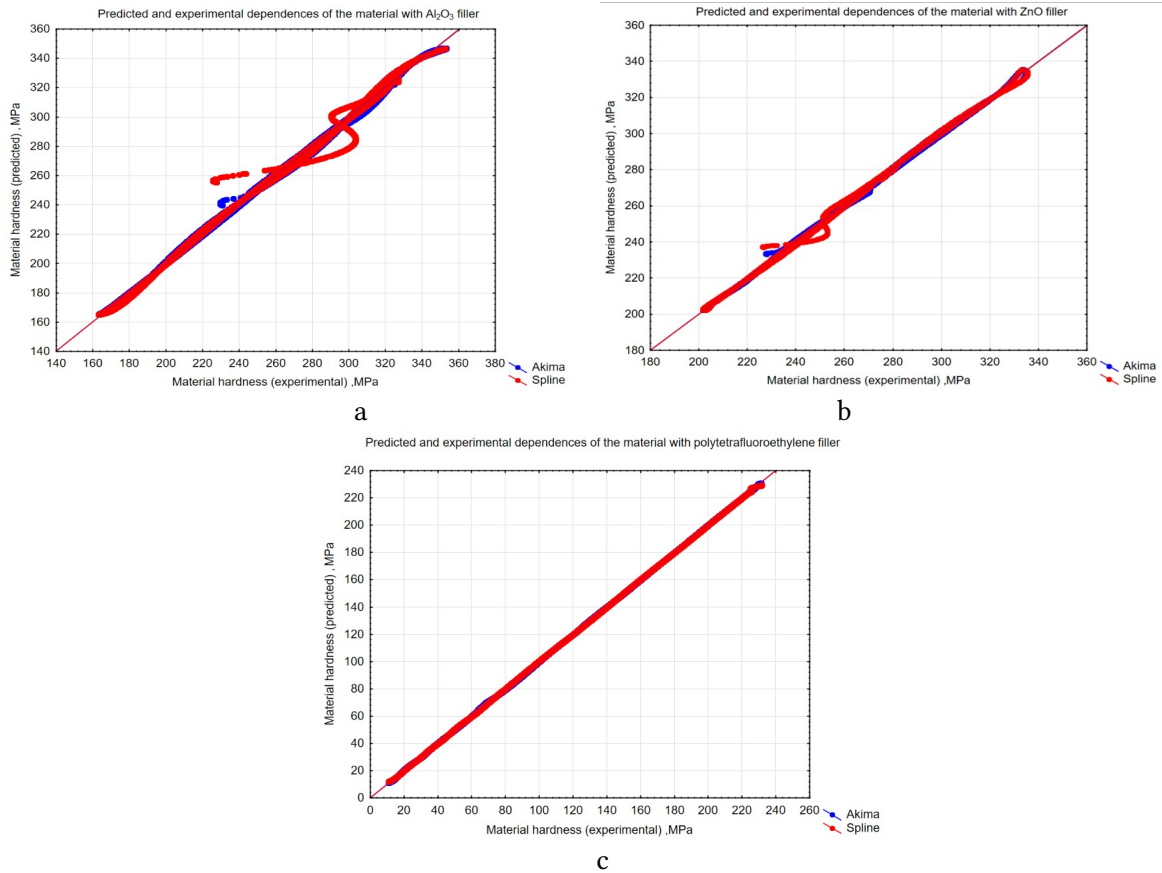
The results of experimental studies (Fig. 2 a, b) showed that the introduction of a relatively small amount of filler (in the range of 11-13 mass fraction for  $\text{Al}_2\text{O}_3$  and 13-17 mass fraction for ZnO) at a temperature below the glass transition temperature contributes to the formation of local

maximums of the material's elastic modulus. A further increase in the concentration of fillers leads to a decrease in this parameter.

The analysis of the data obtained using various interpolation methods made it possible to establish that for more accurate modeling of the elastic modulus of an epoxy material at a temperature below the glass transition temperature, it is advisable to use the Akim interpolation method. This method provides high approximation accuracy and allows for adequate reproduction of the changes in the elastic modulus in this temperature range. At the same time, when analyzing the behavior of the material at temperatures higher than the glass transition temperature, no significant advantages were observed between the considered methods. This is probably explained by the absence of sharp changes in the value of the elastic modulus in this temperature range, which reduces the need to use specific interpolation algorithms to accurately describe the material's behavior.

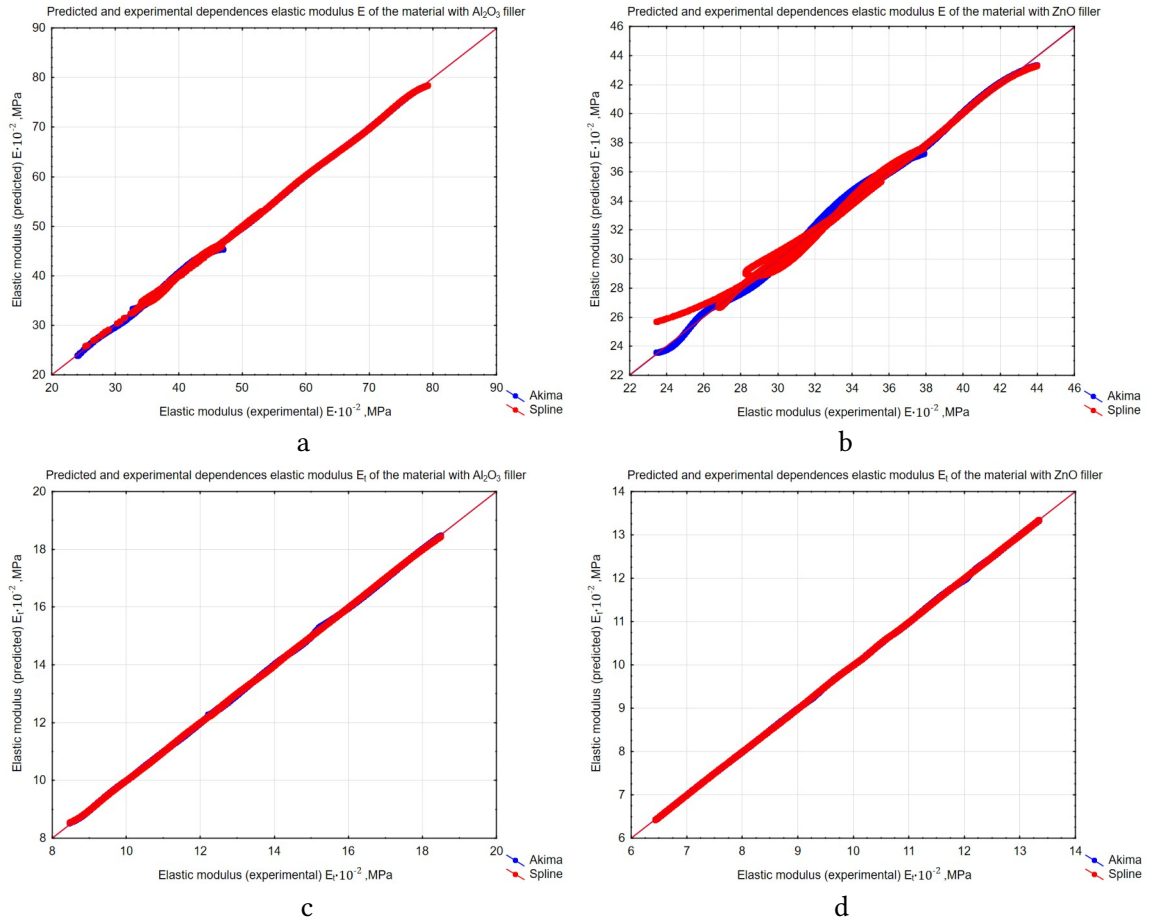
Based on the research, it can be concluded that the introduction of low concentrations of oxides ( $\text{Al}_2\text{O}_3$  and  $\text{ZnO}$ ) provides additional structure formation due to physical crosslinking. This helps to form a more cross-linked polymer network, which improves the mechanical characteristics of the material, in particular, increases its hardness and elastic modulus. The monotonous decrease in hardness when filling PTFE indicates the absence of physical crosslinking. Obviously, this is due to the chemical and physical inertness of polytetrafluoroethylene, as well as the absence of functional groups in its structure both in the material volume and on its surface. As a result, the epoxy matrix does not form physical nodes at the intermolecular level. The mechanical strength of the composite material as a whole is reduced.

The obtained experimental results confirm the influence of filler surface activity in the processes of structure formation of epoxy materials and can be used for targeted modification of polymer compositions where it is necessary to achieve an optimal balance between mechanical strength and other performance characteristics.



**Figure 3:** Predicted and experimental dependences of the hardness of an epoxy-furan composite filled with (a) -  $\text{Al}_2\text{O}_3$ ; (b) -  $\text{ZnO}$ ; (c) - PTFE.

Building dependencies between predicted and actual values is an important tool for assessing the accuracy of models created using artificial neural networks and helps to identify the presence of systematic errors. Analyzing correlations between predictions and actual values helps to assess the level of generalization ability of a neural network, which is important for ensuring its effective functioning on new data. It is also important to assess the distribution of errors, which helps to identify areas where the model does not work with sufficient accuracy and allows for adaptive adjustment of its structure or training algorithms. A comparative analysis of different neural network architectures is performed, choosing the optimal parameters and training algorithms that minimize forecasting errors. The stability, accuracy, and reliability of the model are improved, which is a prerequisite for its application in real-world problems, in particular in predicting the characteristics of CM.



**Figure 4:** Predicted and experimental dependences of the elastic modulus  $E$  of the material filled with (a) -  $Al_2O_3$ ; (b) -  $ZnO$  at a temperature lower than the glass transition temperature, and the elastic modulus  $E_t$  of the material filled with (c) -  $Al_2O_3$ ; (d) -  $ZnO$  at a temperature higher than the glass transition temperature.

The analysis of the results shows that it is more expedient to use the Akim method to study the properties of a composite material whose characteristics undergo drastic changes under the influence of the nature and concentration of the filler (Fig. 3a, b; Fig. 4a, b), since this method is able to more accurately reflect changes in material characteristics. At the same time, the advantages of the Akim method over the spline method were not observed in monotonic dependencies without sharp changes in physical and mechanical characteristics (Fig. 3c; Fig. 4c, d).



## Conclusions

The dependence of the hardness (H) of the epoxyfuran composite on the filling with aluminum oxide, zinc oxide, and polytetrafluoroethylene was investigated. It was found that the maximum hardness of the material was achieved when filling with 6-8 mass fraction of  $\text{Al}_2\text{O}_3$  and 12-16 mass fraction of zinc oxide per 100 mass fraction of binder. Additional structure formation caused by physical cross-linking between the binder and the surface of the fillers was proved. With an increase in the content of polytetrafluoroethylene-based filler, a gradual, monotonous decrease in the hardness of the CM was observed.

The dependence of the elastic modulus E and the elastic modulus above the glass transition temperature  $E_t$  of the material on the degree of filling with aluminum oxide and zinc oxide was investigated. The results of experimental studies have shown that the introduction of a relatively small amount of filler (11-13 mass fraction for  $\text{Al}_2\text{O}_3$  and 13-17 mass fraction for ZnO per 100 mass fraction of binder) at a temperature below the glass transition temperature of the epoxy matrix contributes to the formation of local maxima of the material's elastic modulus. A further increase in the concentration of fillers leads to a decrease in this parameter.

A correlation between the predicted and experimental values of physical and mechanical characteristics was established. It is proved that to study the properties of a composite material, the characteristics of which change radically under the influence of the type and concentration of the filler, it is more expedient to use the Akim method, which more accurately reflects the behavior of the material. The application of the interpolation method in combination with the post-processing of the results using artificial neural networks helps to significantly improve the accuracy of the original data and provides a high level of correlation between the experimental and predicted values. The obtained regularities can be used to develop composite materials with predetermined characteristics.

## Declaration on Generative AI

The authors have not employed any Generative AI tools.

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