Comparison of interpolation methods for modelling the characteristics of oxide-containing epoxy composites

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Abstract
Modern scientific research is increasingly using mathematical methods for planning, forecasting and modelling the processes of studying the properties of materials. The development of this area is promising for the study of polymer composite materials, especially epoxy composites with high specific characteristics.
The paper considers the influence of dispersed oxide fillers on the mechanical and structural-dynamic properties of epoxy composite materials. Al_2O_3 and ZnO, which have been studied in detail by many scientists, were selected as fillers. An interpolation analysis of experimental data was performed using cubic spline and Akima interpolation methods in order to form an extended sample for further processing of interpolated experimental data in neural networks. It was proven that Akima interpolation provides a better fit to empirical dependencies, especially in areas of uneven distribution of points or rapid changes. Multilayer perceptrons were used to predict the physical and mechanical characteristics of materials, which made it possible to evaluate the effectiveness of the selected processing methods. It was found that spectral bias in neural networks determines the choice of interpolation strategy, which affects the accuracy of predicting the selected characteristics. The results obtained confirm the feasibility of integrating interpolation methods and machine learning algorithms to improve the accuracy of modelling composite properties.

Keywords
interpolation, neural networks, epoxy composite, Akim method, spline interpolation

1. Introduction

The efficiency of mechanisms and machines is improved through the use of modern composite materials, in particular in the form of protective or functional coatings [1-3]. The creation of these materials involves the development and use of new approaches through the development and improvement of their forming technologies [4,5]. This approach opens up prospects for reducing the energy and material intensity of industrial equipment [6,7]. Improved composite characteristics contribute to increased operational reliability and economic feasibility of their use [8,9]. At the present stage, special attention is paid to epoxy binders, which are characterised by higher physical and mechanical properties compared to other polymer composites that can be used as coatings [10]. Further improvement of the properties of such materials is achieved by reinforcing them with high-modulus fillers [11,12]. Oxides, carbides and nitrides are commonly used as fillers, the choice of which is based on their surface energy, which determines the multidirectional effect on the implementation of the mechanisms of the composite material (CM) strengthening process.

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The process of creating anti-friction materials is focused on improving the strength characteristics of composites through structural modification, which was achieved by introducing functional additives. The decrease in the wear resistance of polymer composite materials under such conditions is caused by an increase in both mechanical and deformation components of friction and a decrease in the adhesive component of friction in the friction interaction zone [13-15]. To minimise the mechanical friction component, high-modulus fillers are introduced into the epoxy matrix, which increases the modulus of elasticity and reduces the material's ability to deform under cyclic loads.

Even a slight increase in the elastic modulus of CM significantly reduces localised deformations in the friction contact zone. This, in turn, reduces wear intensity by limiting mechanical destruction under cyclic loads. One of the key factors determining the wear resistance of polymer composites is their hardness, which plays an important role in reducing contact stresses during deformation of friction surfaces and ensures the material's resistance to abrasive and adhesive wear. Increased hardness contributes to the formation of a more stable surface layer of the friction surface, which is less susceptible to plastic deformation and destruction under loads. It is known that composites with higher hardness values demonstrate lower wear rates under the same friction conditions, which is explained by a decrease in deformation changes in the surface layer. A balanced ratio between hardness and elasticity allows a positive gradient of mechanical characteristics to be formed in the contact zone, which minimises the accumulation of residual stresses and prevents the formation of cracks in the coating material during frictional interaction of friction surfaces. The use of high-modulus fillers, in particular dispersed particles of aluminium and zinc oxides, is an effective approach to simultaneously increase hardness and maintain the required level of strength and deformation resistance of the composite matrix.

The use of the electron paramagnetic resonance (EPR) method will allow obtaining quantitative information about the mobility of macromolecular links and evaluating their behaviour under the action of external mechanical loads. The analysis of the relative mobility of a paramagnetic probe is of current scientific interest in the context of studying the structural and dynamic characteristics of polymer composite materials. This parameter is an informative indicator of molecular mobility within the polymer matrix, allowing the degree of cross-linking of the material to be assessed based on the interaction between the components of the composite. A decrease in the mobility of the paramagnetic probe in the presence of fillers indicates an increase in the degree of polymer network cross-linking, which is directly related to the improvement of the mechanical properties of the material, in particular, an increase in its strength, stiffness and stability. At the same time, structural changes caused by a decrease in the material's ability to deform contribute to a decrease in the coefficient of friction and wear intensity, which is important for the effective functioning of anti-friction composite systems. Thus, the results of EPR analysis can be used as an effective tool for predicting the operational behaviour of composites under cyclic loads.

Improving the accuracy of experimental data and reducing the number of studies required to obtain it is an important task in modern materials science. Most modern experiments are costly and can be lengthy, which significantly complicates the assessment of the influence of various factors, such as force fields [16,17], modifiers [18] and fillers [19] on the structure of the material. This greatly complicates the study of the characteristics of epoxy composite materials and the development of new materials based on them.

The growing complexity of structural organisation and the multifactorial nature of the influence of component composition on the operational characteristics of CM make it necessary to improve methods for their modelling and prediction. In this area of research, artificial intelligence technologies, in particular artificial neural networks, are becoming particularly relevant, opening up new opportunities for improving the accuracy of assessing the mechanical properties of composites. Thanks to their ability to effectively reproduce complex nonlinear dependencies, perform automated analysis of large-scale data arrays, and adapt to changes in system parameters, neural networks have proven themselves to be a promising tool for predicting the characteristics of polymeric CM, including epoxy CM. Their use contributes to the optimisation of material composition and allows the development of composites with predetermined properties that meet the requirements of specific operating conditions.

The aim of the study is to improve the efficiency of predicting the physical and mechanical characteristics of epoxy composite materials through a comparative analysis of interpolation methods (cubic spline and Akim method) with subsequent use of interpolated data for training artificial neural networks capable of forming models for further analysis and prediction of CM characteristics, which makes it possible to significantly reduce the volume of experimental research, reduce the time and materials required for the development of composites with specified performance characteristics.

2. Materials and Investigation Procedure

The binder for creating composites was selected based on the operating conditions of the components. Epoxy composites as coatings have sufficiently high adhesion strength to the working surface. An important characteristic of these materials is low residual stress during product formation. In view of the above, ED-20 epoxy-dianic resin and polyethylene polyamine hardener were selected. The amine hardener (PEPA) allows the material to be formed at room temperature on long surfaces with a complex profile. The following fillers were used for research: aluminium oxide (Al2O3) and zinc oxide (ZnO). These fillers were selected for the formation of epoxy composites. Such materials have been well researched and are used to model the properties of epoxy composites [20,21].

In modern materials science, particularly in research on epoxy matrix composites, there is a growing need for accurate and reliable methods of analysis and processing of experimental data [22-25], in particular the modulus of elasticity, hardness and mobility of macromolecules as parameters of the structural organisation of epoxy composites. These properties determine the functional capabilities of composites and coatings based on them. Usually, regression approaches are used to analyse the dependence between the structural and mechanical parameters of a material, in particular the least squares method [26,27], which requires a significant amount of experimental data. However, in conditions of limited sample size or experimental complexity, there is a need for methods that allow the construction of a smooth function that passes exactly through all available data points.

In this context, special attention is paid to interpolation methods, in particular cubic spline interpolation and Akim's interpolation method [28-29]. These methods allow visualising experimental dependencies and expanding the data sample by generating intermediate points, which is especially important for the further use of machine learning methods. Cubic spline interpolation ensures the continuity of the function itself, as well as its first and second derivatives over the entire interval of definition. This approach is extremely important for the correct modelling of the mechanical behaviour of composite materials, in particular when evaluating their modulus of elasticity and hardness. At the same time, it should be emphasised that the Akima method, based on local weighted slopes, allows for better preservation of local features of material behaviour, reducing oscillations that can distort the physical interpretation of the results.

In this study, cubic spline and Akima methods were used to interpolate experimental data in order to expand the sample of points required for training artificial intelligence models. The sample formed on the basis of the interpolated data was used to train multilayer perceptrons (MLP) [30-32], which are used to predict the characteristics of epoxy composite materials (Fig. 1).

Multilayer perceptrons consist of an input layer, several hidden layers, and an output layer, with each neuron processing the input information and transmitting the results of the calculations to the next level of the network. The use of such architectures allows for effective work with large volumes of experimental data [33,34], as well as analysis of the influence of various factors on the performance characteristics of polymer composite materials. The use of artificial neural networks in predicting the mechanical properties of polymer CMs increases the accuracy of assessment, facilitates data processing automation, and serves as a tool for optimising the formulation of materials [35-39]. The combination of cubic spline interpolation, Akim interpolation, and artificial intelligence technologies forms an integrated approach to the analysis and modelling of the mechanical behaviour of composites.

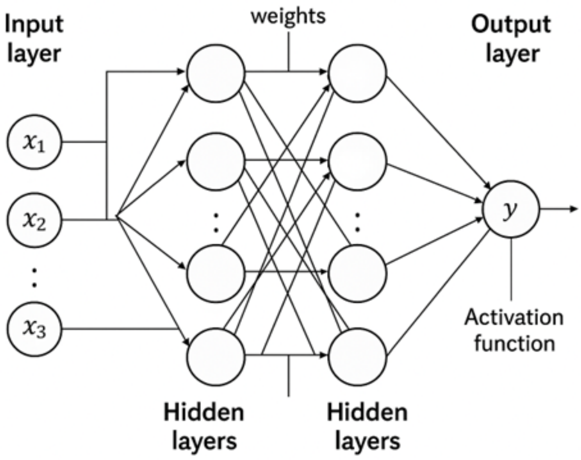


Figure 1: Diagram of a multilayer perceptron neural network (MLP).

3. Results and Discussion

When developing polymer materials, including epoxy composites, high-modulus fillers are used, which play an important role in forming the structural organisation of the composite, which is crucial for improving their mechanical characteristics. This study analyses the influence of aluminium and zinc oxides, which differ in terms of surface energy and physical and mechanical characteristics, on the properties of epoxy CMs. The introduction of oxide fillers into the polymer matrix leads to the formation of boundary layers with reduced molecular mobility in close proximity to the surface of the dispersed filler particles. An external surface layer zone (ESL) is formed. The characteristics of the ESL material differ significantly from those of the epoxy matrix. The presence of such structures affects the spatial cross-linking of the binder and determines the microhardness and wear intensity of the composite. It has been established that these effects are closely related to the morphology and topology of the solid surface of the filler, which causes local differences in structure formation. Selective adsorption of low-molecular-weight components of the binder on the surface of the filler is possible, causing local enrichment of the binder layers in the region of the phase boundary. Such heterogeneity in the distribution of components contributes to the formation of a polymer matrix with varying degrees of cross-linking. This process is further facilitated by the occurrence of physicochemical interactions in the form of physical nodes between the functional groups of the binder and the active surface of the filler particles.

At the initial stage of analysing the experimental data of the study of the elasticity, hardness and relative mobility of macromolecules, interpolation was performed using the Akim method and a spline function. The applied technique allows increasing the density of the data array by interpolation, which fills the gaps between the values obtained with a fixed measurement step and provides a more detailed visualization (Figure 2).

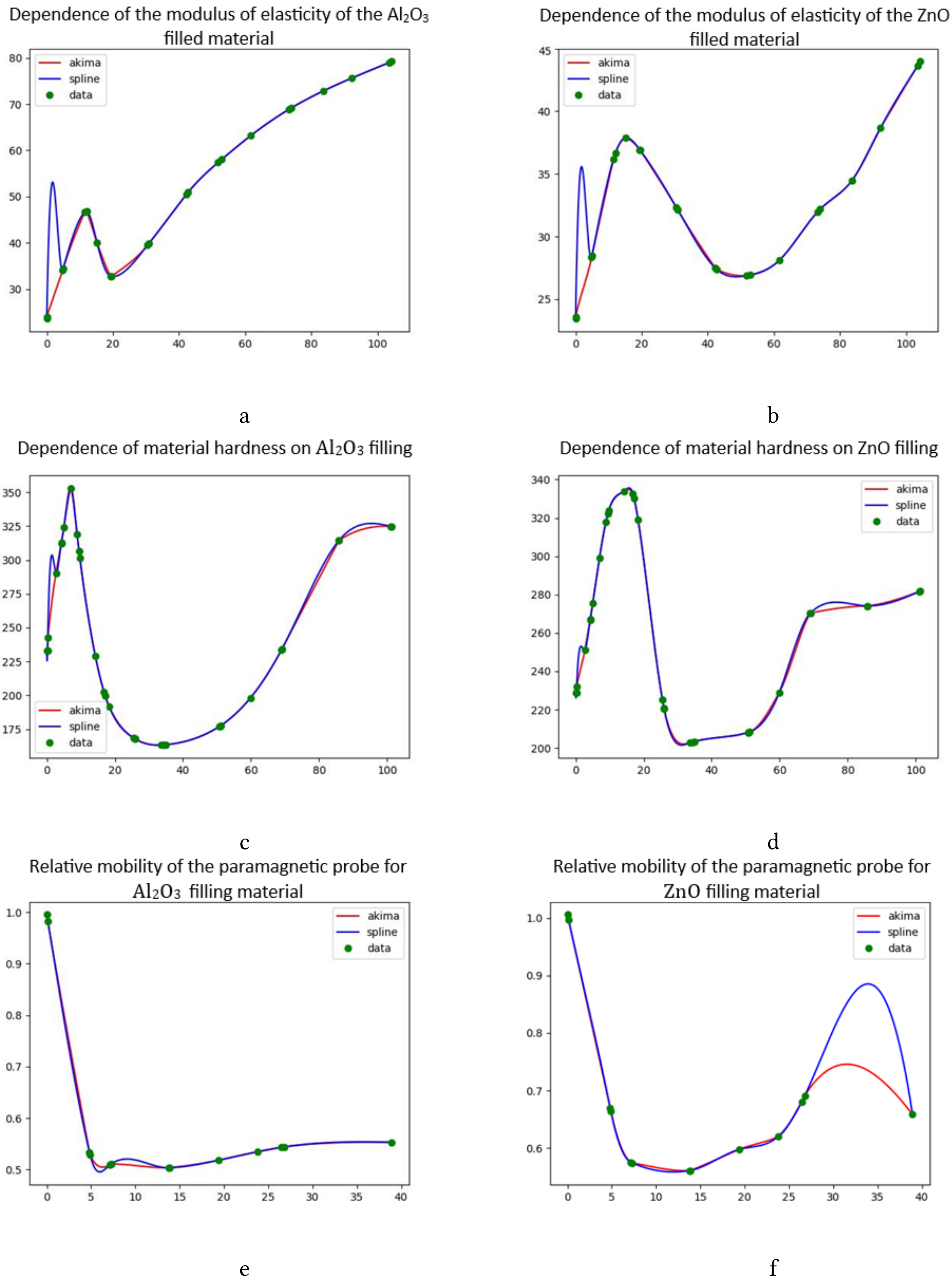


Figure 2: Results of the Akim interpolation method and spline function of the dependence of the elastic modulus (a,b), hardness (c,d) and relative mobility of the paramagnetic probe (e,f) on the filling.

After analysing the constructed curves (Figure 2), we can conclude that the Akima interpolation method better reflects the local features of the experimental data, especially in cases of sharp changes or uneven distribution of points. Unlike spline interpolation, which creates globally smooth curves, the Akima method provides more moderate smoothing without creating artificial extrema. This is especially noticeable in the graphs of the mobility of the paramagnetic probe, Where, at ZnO filling in the range of 30–40%, spline interpolation constructs an artificial extremum that does not correspond to the trend reflected by the data points (Figure 2. f) and the elastic modulus in the 0–20% filling range, where the number of points is small and the nature of the change is sharp (Figure 2. a, b) - the spline shows unwanted oscillations that are not confirmed by experimental data.

To assess the accuracy of interpolation and analyse the results obtained, the deviation of the interpolated values from the straight line connecting the corresponding pairs of points was calculated (Table 1).

Table 1.
Values of maximum deviations of physical quantities of interpolation results from values on the line connecting corresponding pairs of experimental data points.

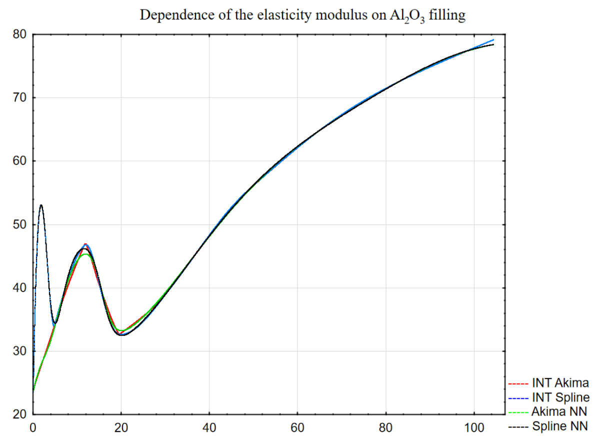
Physical value	Filler	Akima	Spline
Modulus of elasticity, MPa	Al_2O_3	1.17	26.08
	ZnO	0.29	10.37
Hardness, $E \cdot 10^{-2}$ MPa	Al_2O_3	3,65	41,37
	ZnO	7,65	12,34
Relative mobility of the paramagnetic probe, t_0/t_f	Al_2O_3	0,017	0,23
	ZnO	0,07	0,215

It has been proven that interpolation using the cubic spline method leads to significantly greater deviations compared to the Akima method. This is due to the tendency of the cubic spline method to smooth, which ensures the continuity of the first and second derivatives. It should be noted that the use of this method can also cause excessive smoothing and the appearance of oscillations between interpolation nodes, especially in cases of uneven distribution of points. In addition, the Akima method, which uses local interpolation polynomials and ensures the continuity of only the first derivative, provides better adaptation to local data changes, which reduces the deviation from the straight line between the interpolation nodes.

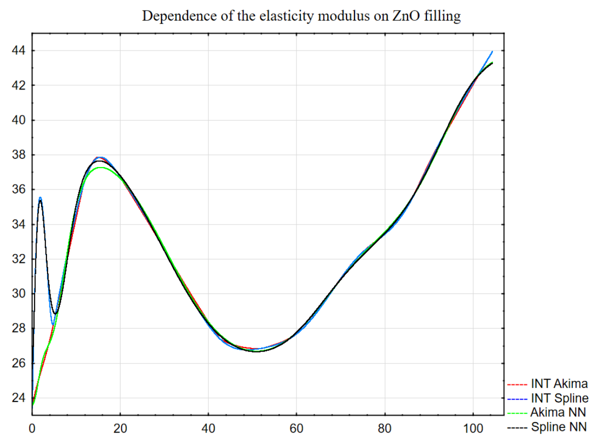
The next stage of the study was to analyse the interpolated values of the elasticity modulus, hardness and relative mobility of the binder macromolecules (based on the mobility of the paramagnetic probe) using artificial neural networks. In particular, multilayer perceptrons (MLP) were used, which consist of three main components: an input layer, one or more hidden layers, and an output layer [40-42]. In our case, the network architecture included two input neurons, several hidden layers, and one output neuron. The architecture of this network provides a high ability to approximate nonlinear dependencies between input parameters and output characteristics of the material. Thanks to its multi-level structure, MLP allows for the effective consideration of complex interrelationships in the structural and mechanical properties of composites, which is critically important in predicting and optimising their operational characteristics[43-44].

When processing experimental data, the frequency principle in neural networks is that the machine learning model automatically detects and assigns higher weight coefficients to those features, events, or patterns that have a higher frequency in the training set. The repetition of certain structures serves as a signal to the model about their potential significance, which contributes to the formation of generalisations based on statistically dominant patterns. This is especially important when analysing experimental measurements, where some of the data may be ‘noisy’, incomplete, or contain random fluctuations. Thanks to its sensitivity to regular repetitions, the neural network forms an internal representation of the data that can provide stable prediction and interpretation of key dependencies observed in the experiment.

At the same time, neural networks have exhibited a phenomenon known as spectral bias, which is closely related to the frequency principle but has a deeper theoretical basis. Spectral bias means that during training, neural networks, especially those with smooth activation functions, tend to first approximate functions with a low frequency component. The model quickly learns global, smooth dependencies between variables, while local, high-frequency variations (e.g., sharp transitions or anomalies in experimental data) are learned more slowly or may be ignored altogether. This is critical when interpreting modelling results, as it affects the accuracy of reconstructing complex physical phenomena. High-frequency information can carry important meaningful characteristics. Awareness of spectral bias allows for the judicious application of additional methods, such as pre-processing of signals, regularisation, or architectural modifications to the network, to achieve a more complete coverage of the spectrum of features inherent in the experimental data.



a



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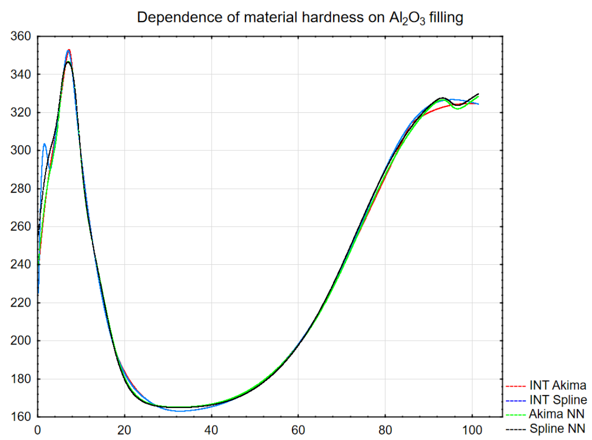

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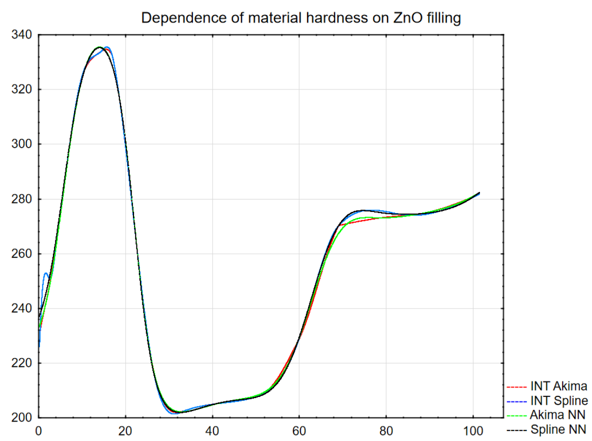

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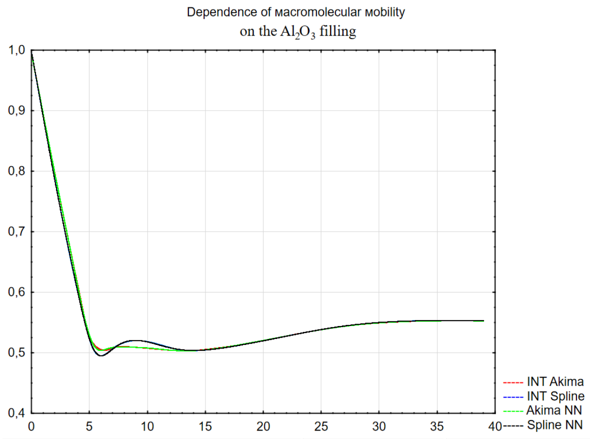

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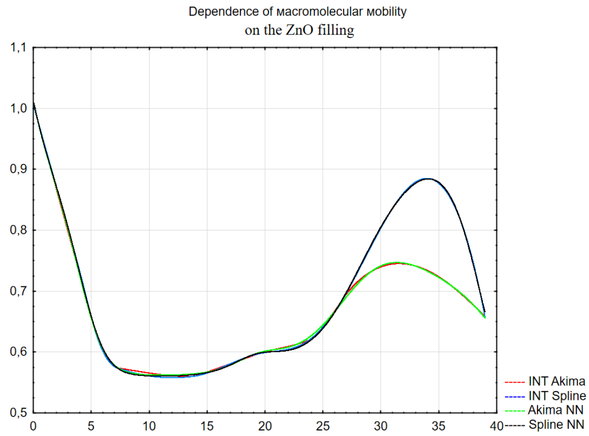

f

Figure 3: Results of processing artificial neuron networks interpolation results of the akim and spline functions for elastic modulus (a,b), hardness (c,d) and relative mobility of the paramagnetic probe (e,f) on the filling

Based on the analysis of interpolated data using a neural network, the effectiveness of the Akima interpolation method has been established. The results obtained indicate the model's ability to level out local oscillations in the input signal, ensuring a smooth reproduction of the functional dependence (Figure 3). This is due to the spectral bias of multilayer perceptrons. At the same time, it was observed that the pronounced oscillations present in the graphs of the results were not smoothed by the neural network. In the case of significant data oscillation, the model may interpret such fluctuations as informative features, leading to overfitting and a decrease in the ability to generalise. In addition, high point density combined with fluctuations contributes to the formation of false perceptions by the network regarding the significance of these variations, although they may be caused by interpolation artefacts or noise components. This highlights the need for careful pre-processing of data, in particular the use of smoothing or filtering methods for high-frequency components before feeding them into the neural network, in order to improve the stability of training and the quality of modelling.

4. Conclusions

It has been established that the selected interpolation methods—cubic spline and Akima method—demonstrate significantly different efficiency in approximating experimental dependencies of physical and mechanical characteristics of epoxy composites. In particular, interpolation using the Akima method provides a more accurate reproduction of local changes. This is especially true in areas with uneven distribution of experimental points or sharp changes in properties, which is typical for composites with a complex microstructure. Cubic spline interpolation, although it guarantees high smoothness of functions, in some cases leads to the appearance of non-physical oscillations and extrema that do not correspond to the physical processes in the material.

A detailed comparative analysis of interpolated graphs has shown that the Akima method produces a more reliable dependence curve for modelling the modulus of elasticity, hardness and relative mobility of a paramagnetic probe from the concentration of oxides in the composite. The calculated numerical deviations from the linear dependence between the experimental points confirm the higher accuracy of this method in all cases considered. This is especially important in conditions of limited sampling, when the accuracy of interpolation directly affects the subsequent stages of analysis.

In addition, models of multilayer perceptrons built on the basis of interpolated data demonstrated the ability to effectively predict key properties of composites. However, when using data with spline interpolation, overfitting of the artificial neural network was observed due to the presence of oscillations that artificially amplify local signal variations. The spectral bias detected in the MLP architecture indicates the dominance of global, smooth dependencies during training, which underline the need for smoothing the input data. This, in turn, justifies the expediency of pre-processing interpolated points — filtering high-frequency oscillations and selecting an adequate interpolation method.

The results confirm that combining the Akim method with machine learning is an effective strategy for modelling and predicting the properties of composite materials. The proposed approach makes it possible to improve the accuracy of engineering calculations, reduce the amount of experimental research, and lay the foundation for the development of new materials with predetermined characteristics.

Next, it is worth comparing Akima with physically correct schemes (PCHIP, rational splines) and evaluating how different smoothing methods affect MLP training and reduce artificial variations. It is advisable to add adaptive selection of new experimental points and uncertainty assessment, extending the modelling to multifactorial problems with simple physical constraints. It is also necessary to check the transferability of the approach to other fillers and time-thermomechanical properties and to test its resistance to sparse and noisy data.

Declaration on Generative AI

The author(s) have not employed any Generative AI tools.

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