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Application of machine learning methods to predict the optical absorption coefficient of composite ceramics based on hydroxyapatite

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Models for predicting the optical absorption coefficient of hydroxyapatite-based ceramics and composites with additives of 0.1 and 0.5 wt.% multi-walled carbon nanotubes additives in the terahertz radiation frequency range from 0.2 to 1.4 THz were constructed based on experimental data using machine learning methods. The lowest value of the mean absolute error was shown by modeling using methods of adaptive boosting (0.951 %) and neural networks (0.049 %). The results of numerical simulation confirm that the use of machine learning methods makes it possible to predict the absorption coefficient with high accuracy for ceramic materials with carbon nanotube additives in the range from 0 to 0.5 wt.% concentrations. The obtained results make it possible to optimize the composition of hydroxyapatite-based ceramics to control their optical characteristics.

Keywords: prediction, regression analysis, machine learning, neural networks, hydroxyapatite, multi-walled carbon nanotubes, absorption coefficient.

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Introduction

Today's research in the sphere of medical materials science is increasingly using the numerical modelling methods and machine learning for the analysis and prediction of materials properties [1,2]. This is caused by the complexity and cost of conventional experiments, as well as the need to find quick and effective ways to investigate the behavior of materials. The production and research of new types of implants to replace the damaged human bone tissue, stimulated by ever-increasing requirements in terms of biocompatibility and similarity of physical and mechanical characteristics with the bone tissue, led to further research on the development of predictive models that can evaluate the properties of the fabricated materials.

One of the promising research objects is ceramics based on hydroxyapatite (HA) [3,4], widely used in biomedical applications due to its biocompatibility and mechanical properties similar to the bone tissue [5]. Improving the characteristics of HA, such as the absorption coefficient of electromagnetic radiation in terahertz (THz) band, is becoming especially relevant for development of new materials for the touch devices, screens and biomedical implants [6].

By incorporating the multi-wall carbon nanotubes (MWCNTs) into HA-based composite ceramics it is possible to change the physical-mechanical properties of the material making them almost identical to the bone tissue [7–9]. However, the experimental study of the effect of different concentrations of MWCNTs additives on the optical properties of HA-MWCNTs composite is associated with difficulties due to the need to account for a large number of variables and a wide frequency range, and the susceptibility to errors due to test inaccuracies, equipment problems, or differences between manufacturers.

Knowing these limitations, researchers and specialists are increasingly using the simulation-based approaches to predict physical and mechanical properties. Conventional prediction methods mainly consist of empirical relationships developed based on statistical analysis of experimental data, where linear and nonlinear (polynomial) regression models are established [10]. In such models, analytical equations are generated through regression analysis to determine unknown coefficients that affect the relationship between the input parameter and other variables.

Machine learning methods are becoming widespread in predicting the properties of materials, including their physical, mechanical, chemical, and optical characteristics [11,12]. Machine learning is successfully used to analyze the mechanical strength of composite materials [13], to simulate thermal stability of polymers [14]. In the field of biomedical materials machine learning facilitates prediction of the implants biocompatibility [15], adhesion parameters [16], rate of biodegradation [17]. These methods also make it possible to predict a wide range of mechanical properties of materials, such as modulus of elasticity, tensile and compressive strength, etc. [18,19]. This approach contributes to a way more quick process of developing the new materials, minimizing the experimental validation costs [20]. Whereas mechanical and optical characteristics, such as refractive index and absorption coefficient, are interrelated. Porosity is the parameter which helps getting an insight into this interrelation, because porosity directly impacts both, physical and mechanical properties and optical behavior of ceramic materials. The lower is the porosity the higher is the microhardness and compression strength of HA

ceramics [4,21]. In paper [22] the interrelation between the porosity and refractive index of nano-composite materials like „semiconductor“ was shown. A decrease in the refractive index is observed with an increase in the porosity of the nanocomposite. In paper [23], an interrelation was found, among other things, between the mechanical properties and the absorption coefficient of sodium silicate glasses based on zirconium dioxide. Zirconium additives contribute to higher density and modulus of elasticity of the glasses, while the absorption coefficient decreases. Similar behavior is observed in [24], where compaction of HA-ceramics using MWCNTs additives also resulted in lower absorption coefficient. Thus, determining the effect of MWCNTs additives on optical properties will further allow to find a relation between optical characteristics and mechanical properties in ceramics.

Predicting the optical properties of HA-based ceramic composite materials with MWCNTs additives is an important research task that my ensure obtaining a wide data array to be used in experiments and further development of HA-MWCNTs ceramic materials. This study outlines the findings of numerical modelling of HA-based composite ceramics' absorption coefficient for ceramics with 0.1 wt.% and 0.5 wt.% MWCNTs in 0.2-1.4 THz frequency band. To analyze the experimental data, machine learning methods were used, including linear and polynomial regression, adaptive boosting (AdaBoost) based on decision trees, and artificial neural networks. This study is aimed at using machine learning algorithms capable of high-precision processing of nonlinear dependences of the optical absorption coefficient on terahertz emission frequencies in the range from 0.2 to 1.4 THz to build predictive models of optical absorption spectra of porous HA-based ceramics depending on the content of MWCNTs hardening additives. This opens up the possibility of obtaining a wide array of data supplementing the experiment in order to further improve the HA-based composites for controlling both, their optical and physical-mechanical characteristics.

1. Materials and research methods

The prediction of the absorption coefficient was carried out for ceramic materials based on data from experimental studies of HA without additives and with 0.1 wt.% and 0.5 wt.% MWCNTs, which was used to harden the HA ceramic matrix and control its porosity by varying additives. The experiment was carried out using terahertz time-domain spectroscopy on spectrometer T-SPEC (EKSPLA, Estonia) in the frequency range from 0.2 to 1.4THz according to the procedure described in jcite24. Cylindrical samples were tested, with thickness and diameter of (3 ± 0.1) and (8 ± 0.05) mm respectively. The experimentally obtained optical absorption coefficient spectra as a function of THz radiation frequency are shown in Fig. 1, where the dots indicate average values of the absorption coefficient, and the lines indicate confidence intervals.

To solve the problem of predicting the absorption coefficient of a ceramic composite material, as well as choosing the optimal model, both classical approximation methods and some types of machine learning were used. Regression analysis methods such as linear and polynomial regressions were used as standard methods. Regression analysis is a set of statistical methods used to study the effect of one or more independent variables on a dependent variable. At the same time, the concepts of dependent and independent variables reflect only mathematical dependence of variables [25]. For data processing, creation of regression models, as well as visualization and comparison of generated models, Python programming language was used along with Scikit-learn library that has a slew of built-in regression methods and also being well-integrated with other Python libraries such as NumPy, Pandas and Matplotlib.

Linear regression is a model of x variable versus one or several other variables with a linear dependence function [25–30], and is expressed as (1):

$$Y = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_k x_k, \tag{1}$$

where b_j — regression parameters (coefficients), x_i — regressors (model factors).

In practice, the relationship between the two variables is very often non-linear, and an attempt to use linear regression can lead to significant computational error [30].

The method of accounting for the nonlinear relationship between variables is polynomial regression, according to the equation (2) [26]:

$$Y_i = b_0 + b_1 x_i + b_2 x_i^2 + \ldots + b_n x_i^n$$

$$(i = 1, 2, \ldots, n) + \varepsilon, \tag{2}$$

where b_j — parameters (coefficients) of regression, x_i — regressor (model factor), ε — number of model factors, n — regression degree.

When the value of n power increases, the model better corresponds to the non-linearity of the estimated data, but in practice, a power of no more than 4−5 is used.. Beyond this point the model becomes too flexible and „matches“ the data, which leads to high error in the data that wasn't used for the model „training“ [30,31]. To compensate for the disadvantages of conventional linear and nonlinear regression models, the paper introduces machine learning methods as a serious candidate for predicting the properties of ceramic materials. One such method is adaptive boosting (AdaBoost), based on a random decision forest (Random Forest), which uses multiple decision trees to improve the accuracy and the generalizing ability of the model [32]. The basic element of the decision forest is a decision tree, which is a tree structure where each node corresponds to a feature, and the branches correspond to the feature values, while the „leaves“ of the trees represent classes for classification or numerical values for regression [33,34]. AdaBoost is an ensemble learning algorithm that uses an iterative approach to improve prediction accuracy by learning from the errors

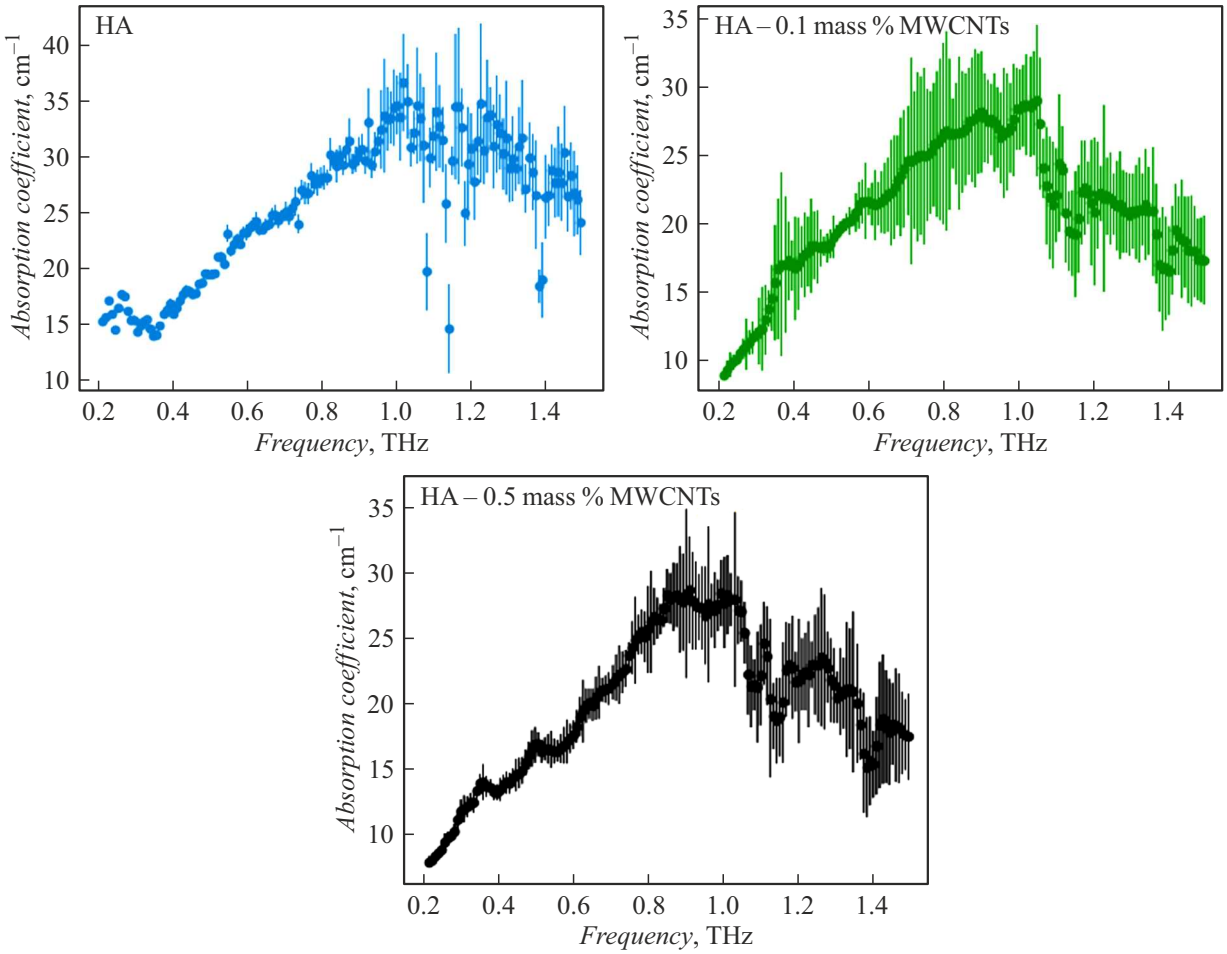

Figure 1. HA-based ceramics absorption coefficients obtained from experiments.

of previous trees. This method attributes the weights for each tree in such a way that the least accurate values get more weight, and the most accurate ones — lose weight [32–35].

The most popular and promising ML method is an artificial neural network (ANN), which is a mathematical model that is built similarly to biological neurons. ANN consists of many simple elements — artificial neurons that combine into complex structures to solve a variety of tasks such as classification, regression, image processing, etc. [36]. A multilayer perceptron — is one of the most basic types of neural networks, consisting of several layers of neurons [37], namely — the input layer that receives input data; then the second layer is triggered, receiving signals from the first layer, this layer also performs signal conversion and their further transfer to the third layer , etc. In this case, the loss function estimates the difference between the predicted outputs and the actual values. This method allows modelling functions of almost any degree of complexity, depending on the number of input and output elements used, as well as the number of hidden layers and the number of neurons in them [38,39].

TensorFlow and Keras libraries were used in this study for creation of the neural network. The main elements of a neural network are artificial neurons and activation functions. Activation functions put the models into non-linearity, the most commonly used of which are:

1) Sigmoid which transforms any input value in the range from 0 to 1, which is used in the models for probability prediction and is expressed by (3) [36]:

$$\sigma(x) = \frac{1}{1 + e^{-x}}; \tag{3}$$

2) The hyperbolic tangent (Tanh), unlike previous function, converts any input value into a range from -1 to 1, which allows to center the output values around zero and speeds up the learning process compared to the sigmoid (4) [36]:

$$\tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}; \tag{4}$$

3) ReLU (Rectified Linear Unit) allows to avoid the problem of gradient decay for positive values, at that, it doesn't require large computations but may „freeze“ the

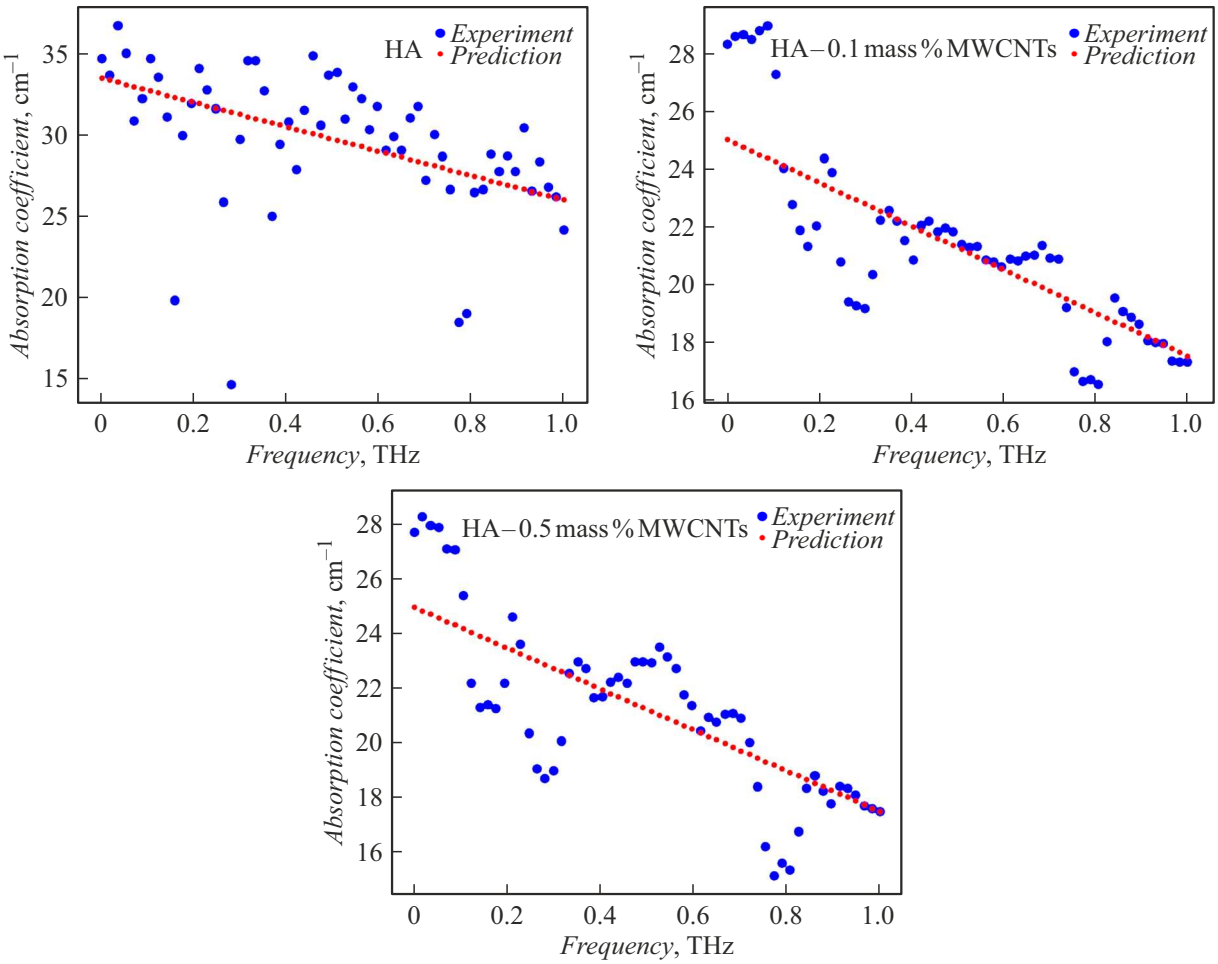

Figure 2. Data approximation by method of linear regression.

neurons, when the gradients become equal to zero and are not updated anymore (5) [37]:

$$eLU(x) = \max(0, x); \tag{5}$$

4) Leaky ReLU — this activation function reduces the risk of neurons „freezing“ allowing to get small negative values due to introduction of additional coefficient which slightly complicates a more simple type (6) [36]:

$$\text{LeakyReLU}(x) = \{\alpha \cdot x,\ if\, x < 0x, otherwise\}. \tag{6}$$

The metric of the average absolute error in percent (MAPE) was used to compare the models (7):

$$M = \frac{1}{n}\sum_{t=1}^{n}\frac{|Y_t - \hat{Y}_t|}{Y_t} \cdot 100\,\%, \tag{7}$$

where Y_t and $\hat{Y}_t$ — actual and estimated values of the target variable for t-th sampling object, n — total number of the test samples [40].

Using this metric, you can compare the effectiveness of models on different training samples. The value MAPE < 5 % indicates acceptable accuracy of the indicator prediction [41]. MAPE value in the range from 10 % to 25 % indicates lower accuracy, however this accuracy is enough to predict the data, while MAPE which is higher than 25 % goes beyond the allowable accuracy and doesn't allow using this data for prediction purposes [42,43].

2. Prediction of ceramic material absorption coefficient

To verify the accuracy of models, the experimental data on the frequency dependence of the absorption coefficient were divided into training and test data based on the Pareto principle with a ratio of 80% to 20%, respectively. Figure 2 shows the results of training the experimental data using linear regression.

This model demonstrated MAPE value of 7.293 %, which indicates insufficient accuracy in predicting the optical absorption coefficient. The high error occurs due to the nonlinear relationship between the descriptors and the dependent variable, thereby making the linear regression

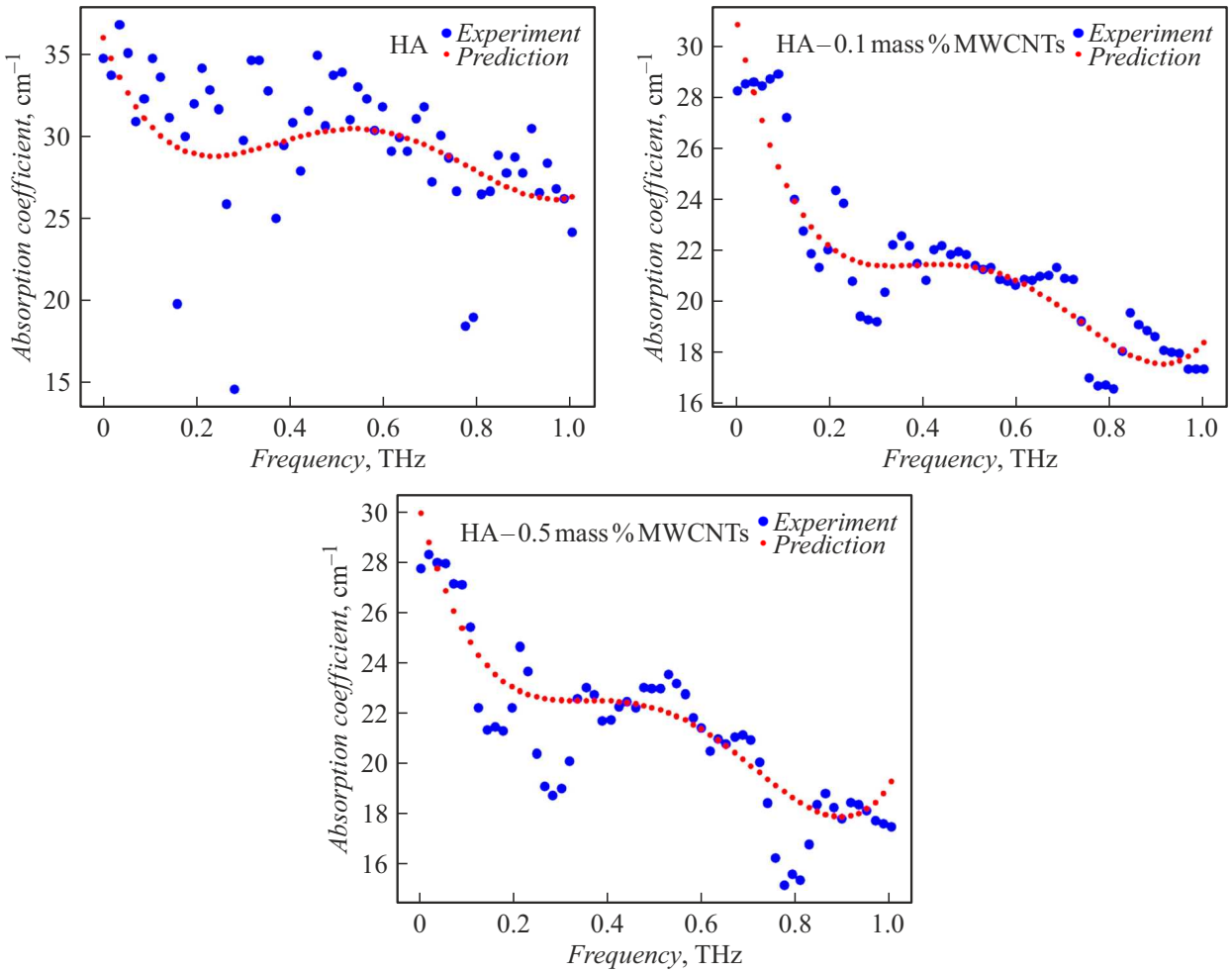

Figure 3. Data approximation by method of polynomial regression.

method unsuitable for further application. Figure 3 shows the results of data training using polynomial regression.

This model demonstrated MAPE value of 2.228,%, which is a more acceptable result compared to linear regression data. The results of absorption coefficient training were also obtained using the adaptive boosting method, which was used as a data supplement to increase the prediction accuracy using decision forest method (Fig. 4).

The results of MAPE values obtained for the adaptive boosting model (0.951 %) show significantly higher prediction accuracy compared to the polynomial regression method, which makes this method suitable for solving such problems.

GridSearchCV class of Keras library was used for building the model using neural network. For the neural network model, hyperparameters were selected from 1 to 5 of hidden layers and from 16 to 128 neurons with a step of 32 in each layer. For each layer the activation functions were selected: 'relu', 'tanh', 'sigmoid', 'selu'. Machine learning results are given in Fig. 5.

MAPE values of the prediction models compared

Model	MAPE, %
Linear regression	8.118
Polynomial regression	7.293
Adaptive boosting	0.951
Neural network	0.049

When predicting the optical absorption spectrum, the value of MAPE = 0.049 % was demonstrated, which indicates the highest accuracy of prediction by a neural network compared to other methods (see the table).

As follows from the table, the statistical indicators of the considered models reflect the noticeable advantage of ML methods compared to conventional regression models [37]. This can be explained by the ability of MO methods to accurately predict the properties of complex composite materials, where the relationship between the structure and the optical absorption coefficient is highly nonlinear.

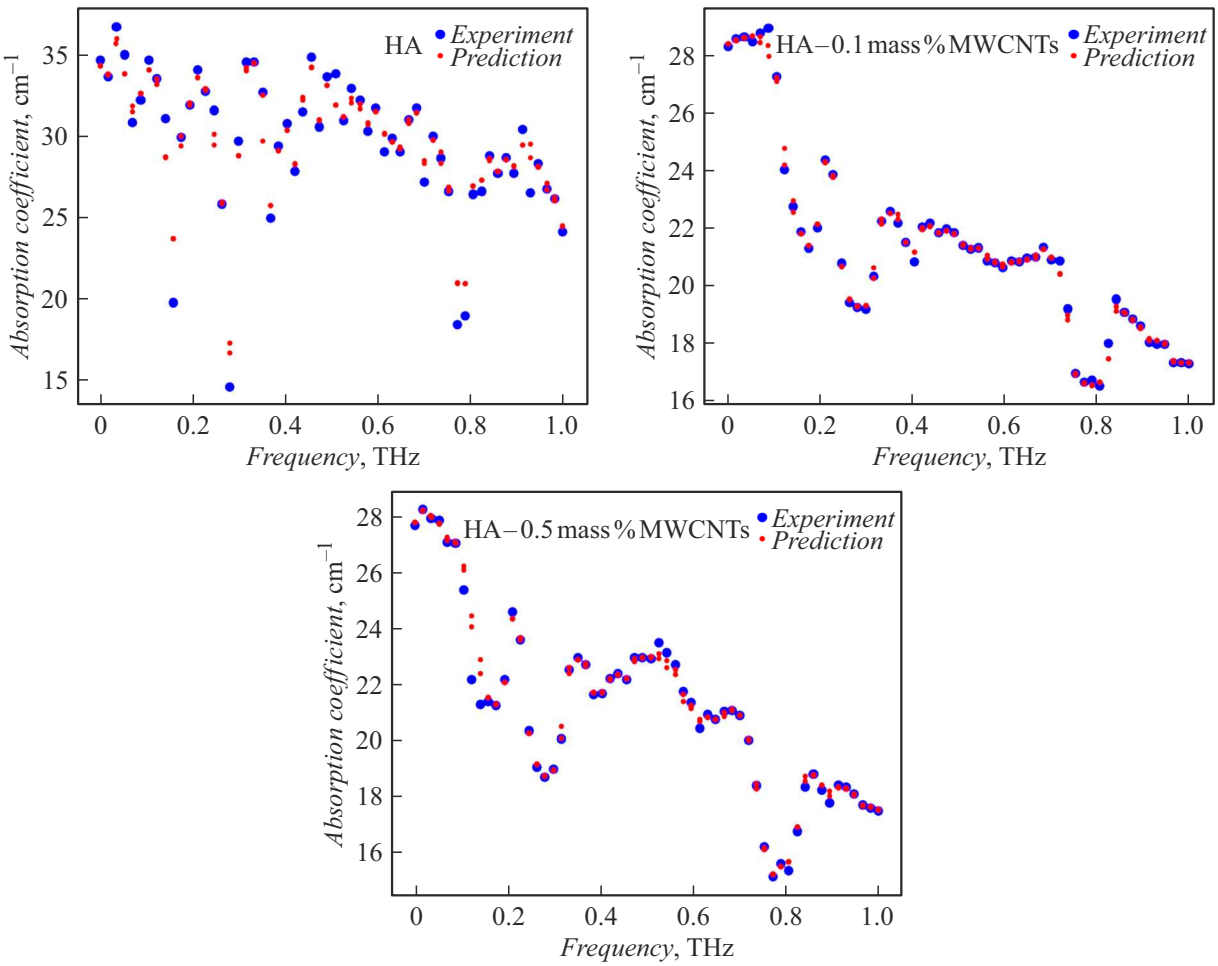

Figure 4. Prediction of absorption coefficient by adaptive boosting method.

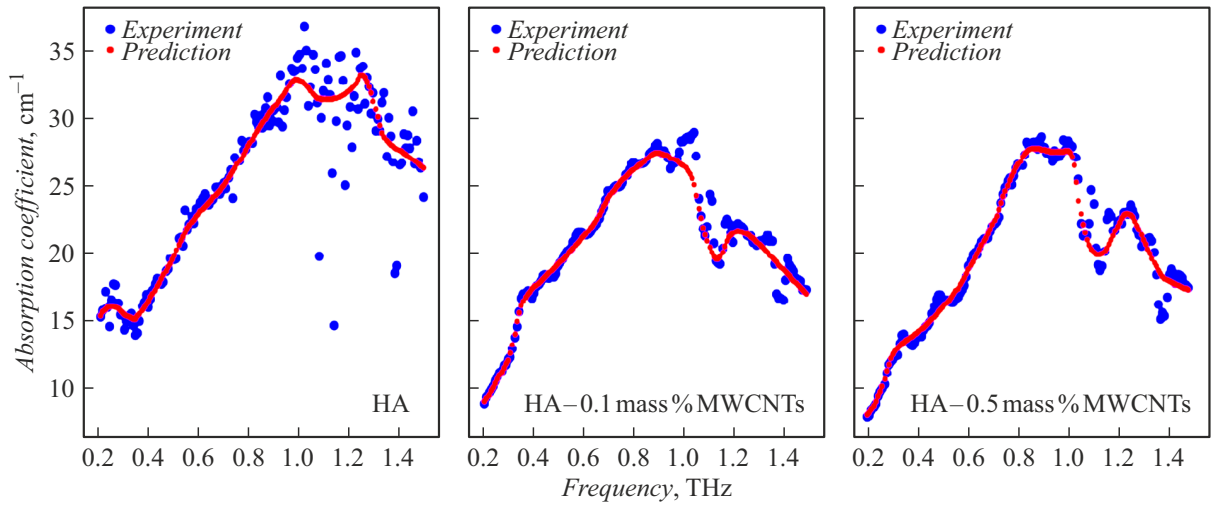

Figure 5. The result of prediction by the neural network model.

Conclusion

In this study the numerical modeling of the absorption coefficient of HA-based ceramics and composites with MWCNTs additives in 0.2–1.4 THz band was performed to predict optical parameters with concentrations of MWCNTs from 0 wt.% to 0.5 wt.%. Based on the analysis of experimental data using ML methods, qualitative and

quantitative dependences of the absorption coefficient on the radiation frequency were obtained with the addition of various concentrations of MWCNTs. The applicability of various ML methods, such as linear and polynomial regression, adaptive boosting (AdaBoost), as well as ANN, the optimal hyperparameters for which were selected using the GridSearchCV class, was evaluated. The neural network was trained on normalized and non-normalized data, where the accuracy of the model significantly dropped during normalization. To compare regression models, the metric of the average absolute error in percent (MAPE) was used, the lowest value of which was achieved by neural network processing and amounted to 0.049,%. The modelling results showed that the use of machine learning made it possible not only to effectively analyze the materials behavior, but also to accurately predict the absorption coefficient in HA-based ceramic materials with MWCNTs concentrations in the range from 0 wt.% to 0.5 wt.%. This gives opportunities to improve the content of HA-based composites to control their optical characteristics.

The results obtained are of practical importance for the development of new materials with controlled properties in the field of biomedicine, radio electronics and other high-tech industries. A promising area of further research is the use of more complex machine learning algorithms to account for additional factors affecting the properties of materials, as well as experimental verification of the generated models.

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Conflict of interest

The authors declare that they have no conflict of interest.

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