UDC 620.3

DOI: 10.20535/2523-4455.mea.287808

Using Information about Experimental Conditions to Predict Properties of Metamaterials

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***Abstract*—In this work, a method of increasing the amount of data for training neural networks is proposed using the possibility of using information about the experimental conditions of measuring the properties of metamaterials. It is shown that the method is flexible and effective. The results of predicting the transmission coefficient of the metamaterial for different angles of incidence of radiation and type of polarization are presented. Using the architecture presented in the work, a high rate of learning and generation of new data was obtained with an error that does not exceed 12% for experiments in one frequency range and does not exceed 31% if all experiments are used for training. The architecture of the neural network and the method by which it is possible to easily change the number and types of experimental conditions are presented.**

Key words — metamaterials; 3D convolutional neural network; experimental conditions.

I. INTRODUCTION

With the development of machine learning methods, it became possible to use them to obtain new materials research methods. One such method is an artificial neural network. Methods of applying neural networks in the field of materials science have been sufficiently developed [1]–[3]. A more interesting direction is the study of metamaterials using neural networks. Metamaterials are materials that have a periodic structure and have physical properties that are not observed in nature. With the help of metamaterials, it is possible to obtain structures with electromagnetic and acoustic properties that cannot be obtained naturally. In order to obtain such properties, researchers, as a rule, model the characteristics of metamaterials using numerical methods — Mie theory, finite element method, transition matrix method, etc. [4]. Researchers have also learned to use machine learning methods to predict the characteristics of metamaterials [5]–[8]. In these methods, information about the structure or physical composition of metamaterials is usually encoded in a defined format, as well as their experimental or simulated characteristics. For this, a sufficient number of training sample elements is formed, after which a test and training set is formed [9]–[12]. The test set is used to check the ability or practicality of using the formed (learned) model for specific tasks [13], [14]. Different types of neural networks are studied — fully connected, recurrent, convolutional and their combinations [15], [16]. The problem is that all these methods are limited in the study of different types of metamaterials at the same time. This means that all studies use limited information about metamaterials, and accordingly, there are no opportunities to generate new (examples of which are not in the sample) metamaterials. Another obstacle is the limitation in the formation of a sufficient amount of data for training a neural network and its practical application. In this work, a universal method of encoding information about metamaterials was presented, with the help of which it is possible to store information about the physical composition and structure of the metamaterial [17]. It is shown that any metamaterial can be represented as a set of pixels, each of which can carry any information — physical parameters, coordinates, etc. The advantages of this approach are universality and simplicity in forming a data sample. Disadvantages are the need for a sufficient number of sample elements, a long time for neural network training, and possible complexity in optimization. The prediction accuracy is sufficient to state that this approach is working and can be used for further research as well as practical applications. The need for an effective and universal mechanism for the use of experimental conditions for measuring the properties of metamaterials is an important factor. The task of implementing this need was solved in the work.

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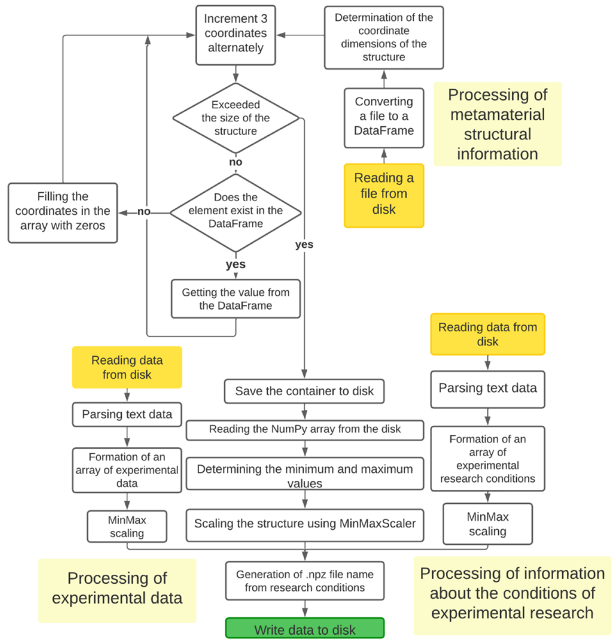

Fig. 1 Block diagram of data processing pipeline for NN training

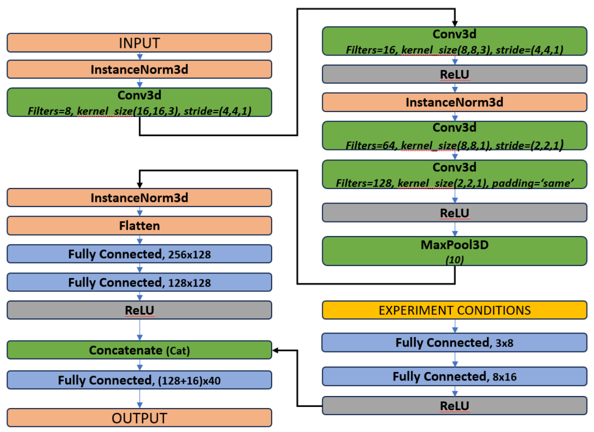

Fig. 2 Architecture of a neural network in the form of a simplified graph

II. NUMERICAL EXPERIMENT METHODOLOGY

A study where all the data were present was used to predict the transmittance based on the structure, physical composition, and experimental conditions. The following experimental conditions were used: the angle of incidence of the radiation and the type of radiation polarization. Coding of the topological structure, physical composition and experimental characteristics (dependence of the transmission coefficient on the frequency) was carried out as described in [17]. The data that was used were taken from the following works — [18]–[22]. Each structure was a set of pixels, i.e. it was defined by a 6x (number of pixels) matrix. Of the six numbers, the first three are the coordinates of the pixel, the other three are the electromagnetic pro perties of the material that was located in those coordinates. The dependence of transmittance on frequency is represented as 40×2 matrices, where forty means twenty coordinate points, and two is transmittance and frequency. That is, each graph was represented as twenty coordinate points.

In Fig. 1, a block diagram of processing information about the structures, characteristics and experimental conditions of metamaterials for its presentation in the format required for a neural network is presented. As you can see, the data goes through quite a few conversions, as the difference in formats is significant. The processing of structural information consists of several main stages — conversion to a Dataframe, addition of information about the structure to each pixel (by iterating through the xrgb file), conversion to Nmpu array and scaling to values from 0 to 1. Processing of information about characteristics consists in parsing text data, array formation and scaling to values from 0 to 1. Processing of information about the conditions of experimental studies is the same as for information about characteristics. Then all information is stored in a special .npz format, for more convenient access to all data when deploying data to a neural network.

The architecture from [17] was taken as a basis. It was further modified by changing the MaxPool layer (compressing the data by 4 times instead of 10) and adding rectification layers after each main stage (after convolutional layers as well as fully connected) and adding a vector information conversion layer and changing the kernel step from one to four (in some dimensions). These are optimization solutions that have led to improved learning and reduced neural network training time. The main input was branching information about the measurement conditions and adding its coded version to the main data vector, which is then processed by the last rectification layer of the neural network. The complete architecture is shown in a simplified form in Fig. 2.

In Fig. 2, INPUT – input block in the form of a matrix of pixels; InstanceNorm3d – normalization; Cond3d – 3D convolution; ReLU is a layer with a straightened linear node [23]; MaxPool3D – pooling operation with a value of ten units; Flatten – conversion of data into a vector; Fully Connected – a fully connected layer of the neural network; Concatenate (torch.Cat [24]) – unification of data tensors.

As shown in Fig. 2, the process of securing information about the experiment begins with the coding of this information. The conditions of the experiment were as follows: angle of incidence of radiation and type of polarization of radiation. The angle of incidence varied for the same structures from 20 to 90 degrees. There were two types of polarization — perpendicular to the required (cross-pol) and required polarization (co-pol). In all experimental studies, they refer to the same types of polarization. The angle of incidence means the angle between the beam and the plane of the metamaterial. The conditions of the experiment were presented at the beginning as three numbers, which, after several layers of the neural network, were

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connected to the main vector shown in Fig. 2. As 128 neurons of basic information and 16 about the conditions of the experiment — the last layer of the neural network. The three numbers represented two types of polarization and angles of incidence.

Advantages of this neural network — speed of operation — training takes 3-5 minutes using the Google-Colab server; flexibility in use — the number of experimental conditions can be changed as researchers need; the basic metamaterial data is a matrix of pixels, where each pixel is a vector of at least three, and can be enlarged indefinitely, due to the fact that 3D convolution can process data with an unlimited number of data channels; the output can be anything and everything will depend on what is being matched.

The disadvantages of this neural network are the need to present basic data about metamaterials in the form of a pixel matrix, which can be obtained by creating 3D objects [17] or by other methods; the need for correct coding of all data into tensors suitable for a neural network (e.g. torch. Tensor [24]); the need for significant computing power.

III. RESEARCH RESULTS AND DISCUSSION

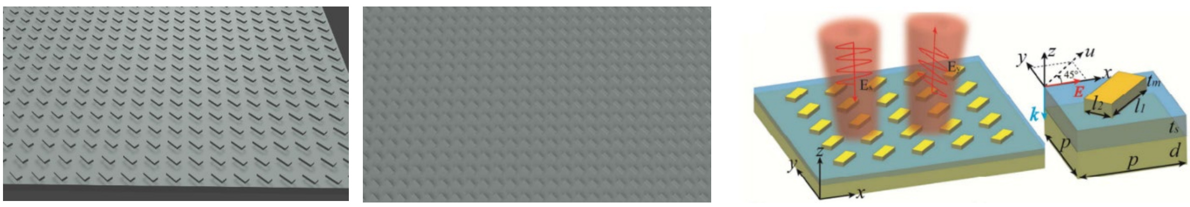
A number of numerical experiments were conducted — using experiments in the frequency range from 0.2 to 0.6 THz; experiments in the frequency range from 137 to 375 THz and all together. Each characteristic (dependence of transmittance on frequency) was represented as 40 numbers, where the first twenty numbers are the scaled frequency value, and the last twenty values are the transmittance. Frequency scaling occurred for all characteristics within the same limits (from 0.2 to 375 THz). As will be seen later, this is strongly indicated when predicting the frequency. Two characteristics were generated for each case. The distribution between training and test sets took place at the proportion of 80% : 20% of the total number.

In Fig. 3, it shows the structures that were used to test the neural network.

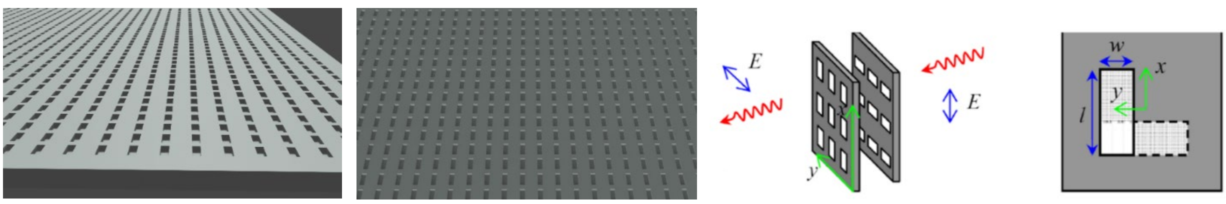
In Fig. 4, it shows the characteristics that were generated on the basis of data in the frequency range from 137 to 375 THz for the structures in Fig. 3 (a), (b).

In Fig. 5, it shows the characteristics that were generated on the basis of the structure — Fig. 3 (c) based on data in the frequency range from 0.2 to 0.6 THz.

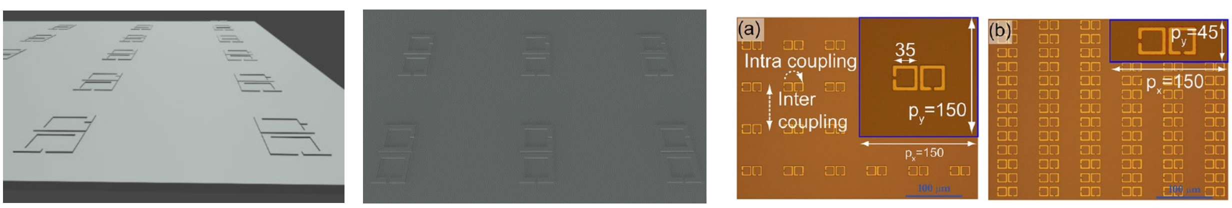
In the second graph Fig. 5, it can be seen that the deviation from the actual frequency is small (on the Y axis – from 0 to 0.05), but at the same time, the deviation in the transmission coefficient is sufficient to argue that there is not enough training data in this range to effectively predict from a practical point of view.



(*a*)



(*b*)



(*c*)

Fig. 3 Schematic view of metamaterials: (*a*) *p* = 600 nm, l_1 = 390 nm, l_2 = 165 nm, t_m = 8 nm, t_s = 110 nm, *d* = 150 nm; (*b*) *l* = 750 nm, *w* = 280 nm, *t* = 150 nm (thickness of the metal layer), *d* = 1000 nm (distance between cuts) *h* – the thickness of the dielectric layer; (*c*) All units are in micrometers. Antenna thickness: 1 µm, The thickness of the substrate: 5 µm, (a) p_y = 150 µm, (b) p_y = 45 µm.

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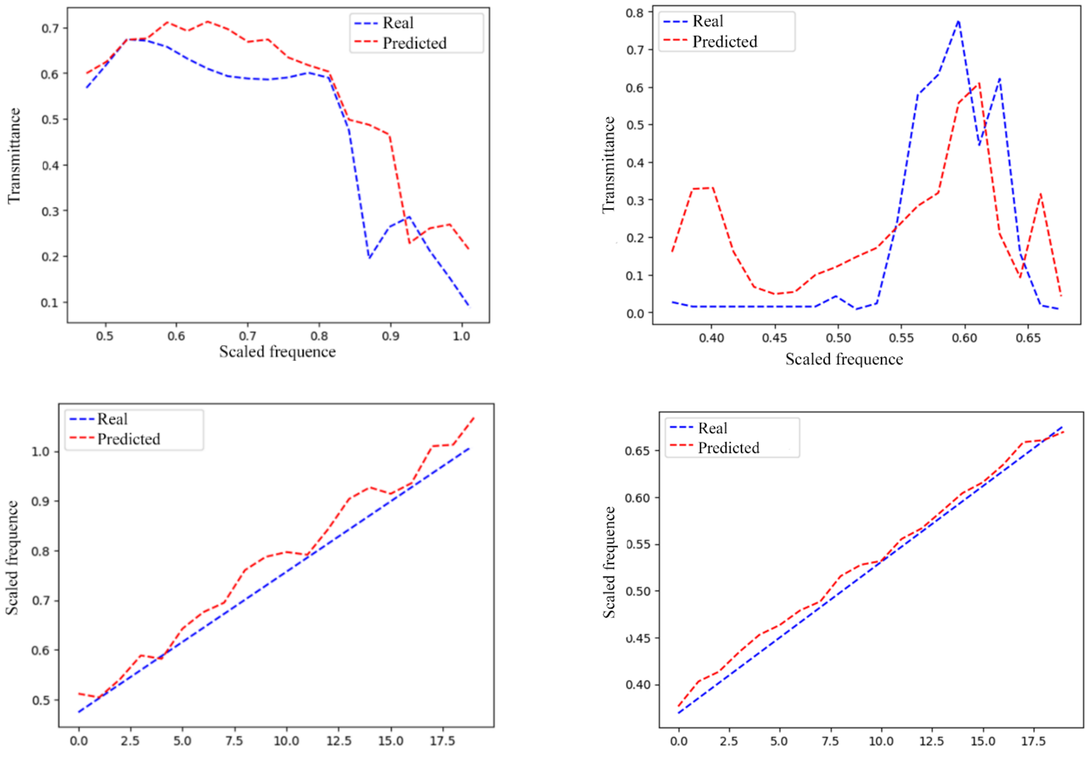

(a) (b)

Fig. 4 Real and predicted dependences of the transmission coefficient on the radiation frequency — the first graph for the transmission coefficient, the scaled frequency is the same for the real and predicted for ease of presentation; the second graph is the dependence of the frequency on the number of the output neuron. (a) For the structure presented in fig. 2 (a) with polarization – cross-pol, and the angle of incidence is 30°. (b) For the structure presented in fig. 2 (b) with cross-pol polarization and an incidence angle of 90°.

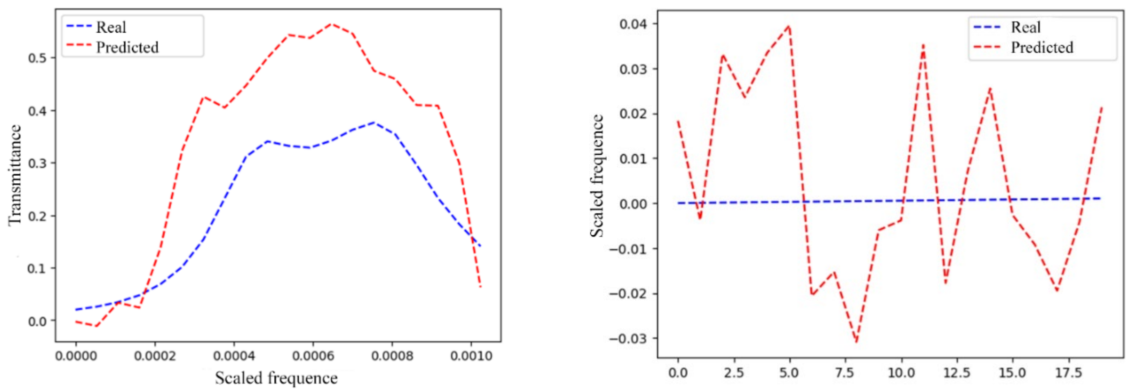

Fig. 5 Real and predicted dependences of the transmission coefficient on the radiation frequency — the first graph for the transmission coefficient, the scaled frequency is the same for the real and predicted for ease of presentation; the second graph is the dependence of the frequency on the number of the output neurons. Polarization – cross-pol and angle of incidence are 90°.

In Fig. 6, it shows the prediction of characteristics based on a neural network trained on experimental data in all ranges (from 0.2 to 375 THz). It is clear that the experimental characteristics in these ranges are affected by various effects (plasmonic effects appear closer to 1-10 THz), but the need to show the possibility of predicting characteristics in different frequency ranges is that the neural network can study physical dependencies of any nature. From one point of view, this means literally comparing numbers and letters, but from another point of view, numbers and letters are made up of the same pixels when represented as pictures. The main thing when using a neural network is to present information about the data in such a way that all the information is used.

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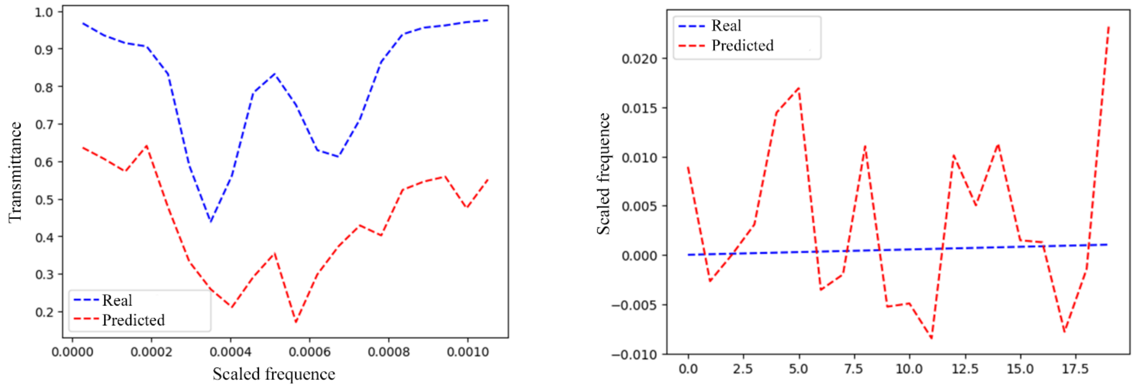
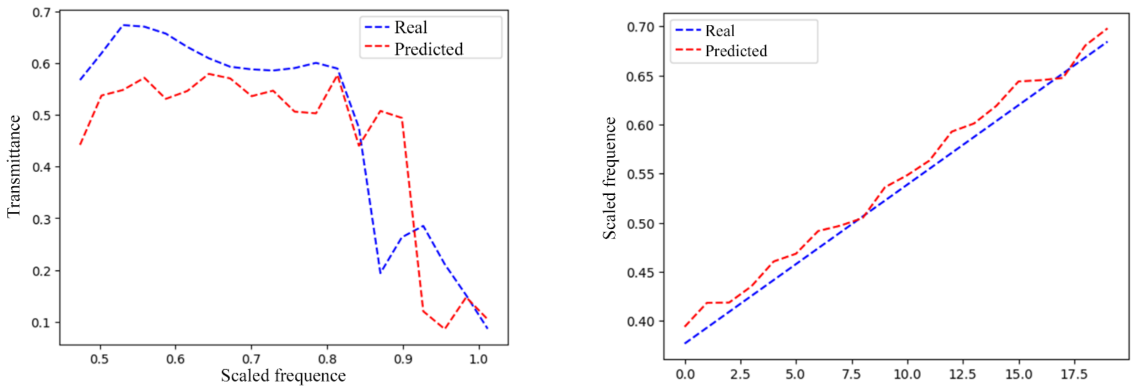


(a)



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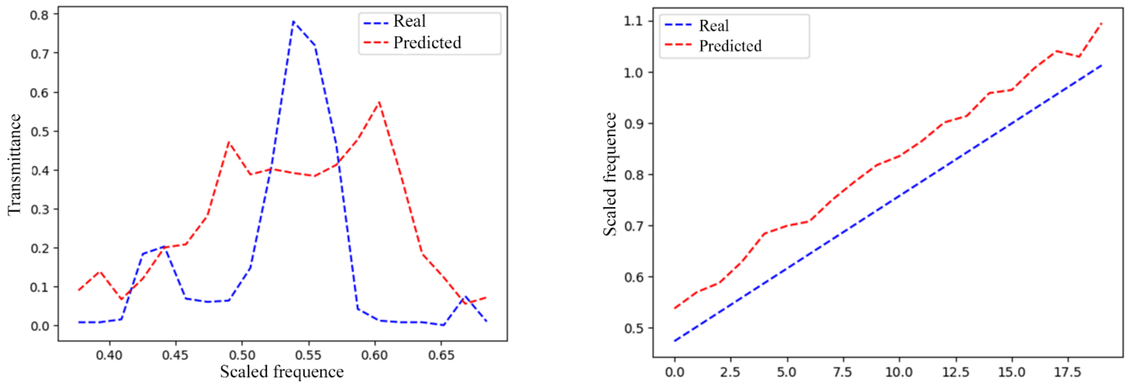

(c)

Fig. 6 Real and predicted dependences of the transmission coefficient on the radiation frequency— the first graph for the transmission coefficient, the scaled frequency is the same for the real and predicted for ease of presentation; the second graph is the dependence of the frequency on the number of the output neuron. (a) For the structure presented in Fig. 2 (c) with polarization – co-pol, and the angle of incidence is 90°. (b) For the structure presented in Fig. 2 (b) with cross-pol polarization and an incidence angle of 30°. (c) For the structure presented in Fig. 2 (a) with cross-pol polarization and an incidence angle of 90°.

As can be seen, the prediction accuracy is much lower if the total error is taken into account. The largest error is observed by Fig. 6 (a) and Fig. 6 (c). The main thing that is followed here is the preservation of the prediction of the behavior of dependencies. This means that the neural network really learns about those dependencies that are present in the data – structures with a physical composition of components and for different measurement conditions.

The great advantage of this approach is that researchers have the opportunity to determine the influence of measurement conditions on the accuracy of forecasting. That is, as was shown, the last layer of the neural network consists of two vectors — the main one (length 128)

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and the additional one (16 for measurement conditions). It is clear that the value of the additional vector can be set as needed, that is, not 16, but, for example, 128, but then it will make physical sense? Numerical experiments established that in the case of these data (which were used in the work), the ratio between the main and additional data was optimal (from the point of view of forecasting accuracy). It is clear that this ratio may be different from other data. Another advantage, as noted, is that the number of experimental conditions that need to be included can be completely different. That is, radiation intensity data could be used for that data. For example, for the same structure, the same conditions, except for the radiation intensity, have the same characteristics of the structure. In this way, we increase the amount of data.

Conclusions

A number of numerical experiments were conducted to generate dependence on transmission coefficient depending on the radiation frequency for three cases — using experimental data in two separate ranges and for all of them together. It was found that the best accuracy is observed for the case when for training uses characteristics in the range from 137 to 375 THz. The lowest accuracy is observed when combined data is used — in the range from 0.2 to 375 THz.

So, the frequency prediction error was 0.02, where the coefficient prediction error was 0.13, which of course means that this is not enough to use in practical applications with the data we have, but if we increase the amount of data, then these indicators will improve. The speed of prediction is several seconds, while the training time is several minutes, which greatly exceeds the speed of simulation (Li method, finite element method, etc.) of various characteristics with such a large amount of data about the structure and experimental conditions. The amount of data has been increased several times only due to taking into account the change in experimental conditions, which makes it possible to increase the accuracy of forecasting. A modified improved architecture of the neural network is given, with the help of which it is possible to attach information about the conditions of the experiment to the data about the metastructure. It has been analyzed that using experimental data, which are affected by various physical effects, a sufficient amount of data is needed so that the quality of forecasting and generation of new characteristics is sufficiently accurate for practical application. It is indicated that the results of numerical experiments make it possible to state that this approach to encoding information about the metastructure (topological structure, physical composition of components, target characteristics) and experimental conditions is useful material for consideration and there are prospects for the practical use of this method in applied problems.

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Надійшла до редакції 21 вересня 2023 року
Прийнята до друку 29 жовтня 2023 року

УДК 620.3

DOI: 10.20535/2523-4455.mea.287808

Використання інформації про умови експерименту для прогнозування властивостей метаматеріалів

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***Анотація*—На даний момент існує проблема збільшення кількості елементів для навчання нейронних мереж, які повинні прогнозувати властивості метаматеріалів. У даній роботі запропоновано метод збільшення обсягу даних для навчання нейронних мереж з використанням можливості використання інформації про експериментальні умови вимірювання властивостей метаматеріалів. Показано, що метод гнучкий і ефективний. Наведено результати прогнозування коефіцієнта пропускання метаматеріалу для різних кутів падаючого випромінювання та типу поляризації. Використовуючи представлену в роботі архітектуру, була отримана висока швидкість навчання і генерації нових даних з точністю, яка не перевищує 12% для експериментів в одному частотному діапазоні і не перевищує 31%, якщо для навчання використовуються всі експерименти. Представлено архітектуру нейронної мережі та метод, за допомогою якого можна легко змінювати кількість та типи умов експерименту. Для прогнозування коефіцієнта передачі на основі структури, фізичного складу і умов експерименту використовувалося дослідження, де були присутні всі дані. Було проведено ряд чисельних експериментів — з використанням дослідів в діапазоні частот від 0,2 до 0,6 ТГц; тільки експерименти в діапазоні частот від 137 до 375 ТГц і все разом. Кожна характеристика (залежність коефіцієнта пропускання від частоти) представлялася у вигляді 40 чисел, де перші двадцять чисел — масштабоване значення частоти, а останні двадцять — коефіцієнт пропускання. Масштабування частот відбувалося для всіх характеристик в однакових межах (від 0,2 до 375 ТГц). Як буде видно далі, це сильно вказується при прогнозуванні частоти. Для кожного випадку було сформовано дві характеристики. Розподіл між навчальним і тестовим наборами відбувався у пропорції 80/20% від загальної кількості. Було встановлено, що найкраща точність спостерігається для випадку, коли для навчання використовуються характеристики в діапазоні від 137 до 375 ТГц. Найнижча точність спостерігається при використанні комбінованих даних. Задана модифікована вдосконалена архітектура нейронної мережі, за допомогою якої можна прикріплювати інформацію про умови експерименту до даних про метаструктуру. Проаналізовано, що з використанням експериментальних даних, на які впливають різні фізичні впливи, необхідна достатня кількість цих даних для того, щоб якість прогнозування та генерації нових характеристик була достатньо точною для практичного застосування. Зазначено, що результати чисельних експериментів дозволяють стверджувати, що такий підхід до кодування інформації про метаструктуру (топологічну структуру, фізичний склад компонентів, цільові характеристики) та умови експерименту є робочим і є перспективи його практичного використання в прикладних задачах.**

Ключові слова — метаматеріали; 3D-згорткова нейронна мережа; умови експерименту.