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APPLICATION OF MACHINE LEARNING METHODS FOR PREDICTING THE MECHANICAL BEHAVIOR OF DISPERSION-STRENGTHENED COMPOSITE MATERIAL

Abstract. The work is devoted for creating a model for approximating the solution by the finite element method of the problem of plane deformation of a dispersion-strengthened composite material. An algorithm for constructing a parametric 2-D composite model is proposed. The processing of the parameters of the microstructure material stress-strain state occurs using a convolutional neural network. A surrogate model is used for calculations speed up and determine the overall approximations quality of such type mechanics problems.

The modern world is characterized by the processes of adapting and changing the manufacturing technology of the product to the needs of individual audiences. To meet the needs of broad markets, such products must be low cost, manufacturable, and able to change and modify quickly during production.

The dynamic development of artificial intelligence and the relevance of using machine learning methods for analyzing large data sets contributed to the decision to study the approximation of a finite element (*FEM*) solution to the problem of deformation of a plane sample of a dispersion-strengthened composite using a convolutional neural network. Using a surrogate model, it is proposed to solve the problem of accelerating the calculations of the material microstructure stress-strain state (*SSS*), as well as to determine the overall quality of the approximation of such type of mechanics problem.

The following steps are taken to achieve the goals:

1) create a computational model of deformation of a representative sample of a composite material;

2) to obtain a set of solutions for the *SSS* of a certain number of arbitrary configurations of composite material samples and the formation of a data set to create a surrogate model;

3) determine the architecture of a surrogate model based on a neural network for approximating the distribution of equivalent stresses using the *FEM*;

4) to train the neural network to obtain a surrogate model for approximating the results;

5) evaluate the error of the solutions by comparing the solutions obtained using the *FEM* and the surrogate model.

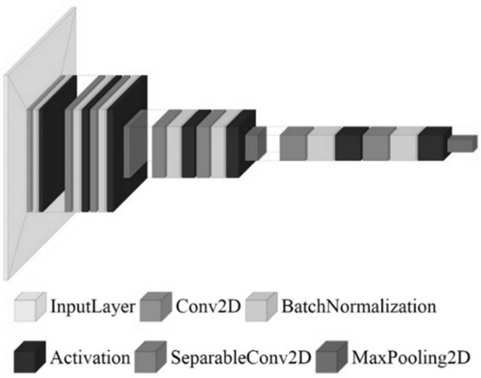
Construction of a surrogate model. The sample is a square two-dimensional plate with inclusions in the form of circles. To calculate the *SSS*, the model is fixed on two adjacent edges, and a load is applied to two opposite edges. The displacement of the ribs along the *X* and *Y* axes is taken as the latter in the work, while the magnitude of the displacements is a constant value. The calculation model is created based on the work [1-2], using ANSYS Mechanical automated design and analysis tools, using the APDL scripting tool for building models.

Data set generation. The collection and subsequent processing of the calculation results is carried out automatically. This makes it possible to form a data set for further training of the neural network. The required number of examples for training set is at 10,000. It`s known from *FEM* that the formation of the stiffness matrix is the costliest action in the process of system analysis. Therefore, the decision is made to form 1000 different samples of the composite material, and to each of them apply tension / compression in 10 different directions. The scheme is implemented using the Load Step functionality in the Ansys

Mechanical software package. At each loading step, a displacement vector is formed, which is applied to the corresponding nodes of the finite element grid. The initial bias is obtained from the uniform distribution. The *SSS* calculation is performed simultaneously for all load steps for one generated sample. After the automatic solution of the equations system, the resulting displacements of each node of the structure are used to calculate the stresses inside the finite elements.

The formation of an algorithm for constructing a computational model and subsequent processing of the results is performed using the Python programming language. The convolutional neural network algorithm takes structured matrices as input, so stress data imported into Python requires further processing. The corresponding data arrays are restructured using cubic spline interpolation. At the output, stresses are obtained in central pixels.

The neural network creation. A neural network for predicting the von Mises equivalent stress distribution under tension/compression of a two-dimensional composite sample, implemented in the Python using the TensorFlow open-source deep learning library. To achieve the purpose of the work encoder-decoder type model selected, where the encoder "compresses" the input data array into a latent space (limited in size); decoder - "reveals" the feature vector compressed into the latent space in order to obtain a modified data array at the output. The serial connection of the encoder-decoder model in combination with the algorithm for simultaneously optimizing the weights of the neurons of both networks makes it possible to obtain a neural network, which is a surrogate model for the *SSS* analysis of a composite sample. The developed neural network architecture (Fig. 1) is based on the U-NET architecture [3].



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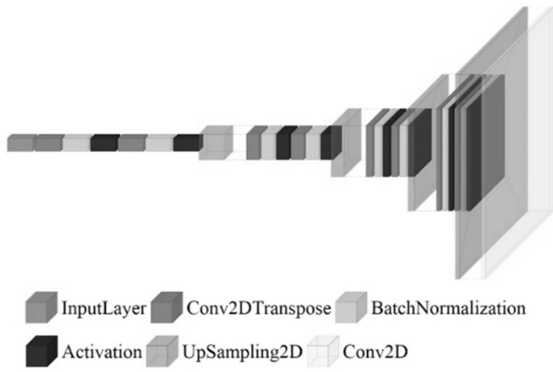

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Fig. 1 – Architecture of a neural network: a) encoder; b) decoder

After initialization of the neural network, the loss function and target metrics are determined. The loss function calculates the difference between the actual value of the target variable (in our case, the stress distribution calculated in the ANSYS software), and the value generated by the surrogate model. As a loss function, the root of the root-mean-square error (*RMSE*) over all points of the original matrix (1) is chosen:

$$RMSE = \sqrt{\frac{1}{256 \times 256}\sum_{i=1}^{256}\sum_{j=1}^{256}\left(y_{ij} - \widehat{y_{ij}}\right)^2}. \quad (1)$$

Thus, the training of the neural network occurs by minimizing the *RMSE*. At each iteration of network training, the values of the functions are also calculated: the root of the root-mean-square difference of the maxima of equivalent stresses ($RMSE_{max}$) and the root-mean-square error for 80% of the quantile ($RMSE_{80\%}$). The considered metrics are defined as the difference between the actual and model-generated stress values.

Using the first-order gradient local optimization method (ADAM) [4], the loss functions is optimized. At each iteration of the network weights optimization, the method takes into account the exponential damping of the gradient and the square of the gradient in previous iterations.

A sample of 10,000 examples for training a neural network is divided into three sub-samples: training for network training (6000 elements), validation - for controlling the cost function and metrics (2000 elements), test sub-sample - for the final assessment of the quality of the model (2000 elements). The network is trained over 30 epochs. This corresponds to 30 passes of the test data set through the network. Each epoch takes an average of 270 seconds, and network weight optimization is 135 minutes. The results of the proposed model architecture are presented in Table 1.

Table 1 – Loss function results on subsamples

Sample	$RMSE$, GPa	Metrics $RMSE_{80\%}$, GPa	Metrics $RMSE_{max}$, GPa
Training	0.339	0.386	0.474
Validation	0.386	0.460	0.521
Test	0.412	0.478	0.540

Conclusions. In this work, studies are carried out on the construction of a surrogate model based on a convolutional neural network for approximating a finite element solution of the dispersion-strengthened composite deformation in order to speed up calculations of finding the material microstructure *SSS* and determining the general quality of approximations of this type of problems in mechanics.

To train the neural network, 10,000 variants of the stress-strain state of the parametrized computational model of a composite material sample are analyzed. A neural network based on the U-Net architecture of the encoder-decoder type has been created to predict the distribution of equivalent stresses in the material according to the sample geometry and load values.

Analysis of the results shows:

1) that the value of the network weights after training is still not optimal in terms of minimizing the loss function;

2) the model is still simple to accurately reproduce the *FEM* solution;

3) comparing the speed of *FEM* calculations (which takes 430 minutes) and a trained neural network on 10,000 configurations using a stationary PC. Time advantage up to 70 times for the latter. At the same time, it takes 19 seconds to form the stiffness matrix and calculate one load step. The training of the neural network took 135 minutes. The surrogate model generates a matrix of equivalent stresses simultaneously for 32 samples in 9 seconds.

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