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MODELLING OF FUNCTIONAL PROPERTIES OF SHAPE-MEMORY ALLOYS BY MACHINE LEARNING METHODS

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Summary. *Shape-memory alloys are used in various areas of science and industry due to their unique shape memory effect and superelasticity, caused by martensite and reverse transformations. In this study, it is proposed to model the functional properties of shape memory alloys, namely, the dissipated energy range, strain range and stress range using the methods of machine learning. The modeling is carried ou in the specialized data mining software environment called Orange. There were built five models for each dataset by means of method of neural networks, random forest, gradient boosting, AdaBoost and kNN. The respective regression dependencies are obtained and K fold cross-validation with K=5 is performed. The errors and coefficient for R^2 determination are calculated as the results of modeling by means of the above mentioned machine learning methods for the range of dissipated energy, stresses and strains on the number of loading cycles. For each physical quantity, the best results in terms of method error are obtained for k-nearest neighbors method.*

Key words: *shape-memory alloys, machine learning, regression, k-nearest neighbors, Random Forest, Neural network.*

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Introduction. Shape-memory alloys (SMAs) are very popular due to their unique shape memory effect and superelasticity caused by martensitic and reverse transformations [1]. SMAs are metal alloys that can restore their original shape, memorizing it between two phases of transformations, depending on temperature or magnetic field. They are very simple in application. An alloy can be deformed by applying force and it returns to its original shape or size when heated above certain temperature [2]. Many different types of SMAs are known, for example, Fe–Mn–Si, Cu–Zn–Al, and Cu–Al–N, and each type is used in its own way, although Ni-Ti alloy (trade name Nitinol) is very common due to its stable properties [3]. SMAs are widely used in medicine [4], aerospace industry [5], motor engineering [6], civil engineering [7], etc. During operation, products made on the basis of such alloys are subjected to long-term cyclic loading resulting in premature loss of functional properties, exhaustion of durability and further destruction. Thus, it is necessary to ensure sufficient functional properties and durability of parts and structural elements made of SMA. Therefore, it is important to develop methods of modeling of functional properties and fatigue life, which are based on the revealed regularities of pseudo-elastic behavior and durability of such structural elements, which take into account the influence of stress ratio. Functional properties, durability and residual durability of structural elements can be predicted with high accuracy by machine learning methods, particularly, neural networks (NN), RandomForest, AdaBoost, GradientBoosting, kNN.

Analysis of the available results and investigations. The strength and durability of structural elements were studied, for example, in the investigations of Rampi Ramprasad [8] and Frederic E. Bock [9]. G. M. Seed and G.S. Murphy in 1998 were the first ones in the industry who predicted short cracks by neural networks (NN) [10].

Artificial intelligence methods can be used to model SMA behavior. At present, artificial intelligence methods are intellectually actively used in materials science and fatigue failure mechanics [11, 12].

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Machine learning (ML) is a part of artificial intelligence methods [13], which makes it possible to solve effectively rather complicated problems. It showed excellent results in the field of smart materials modeling [14].

Artificial Intelligence Material Selection (AIMS) framework is developed in paper [15]. This framework is complex program based on various machine learning methods which makes it possible to investigate and find SMAs with desired properties.

NiTiHf alloys that can be used as actuators in space were found in the paper [16]. Seven models constructed by machine learning methods are tested, and the model with the best parameters is selected in order to determine new alloy compositions with predetermined transformation temperature (Ms), temperature hysteresis, and operating output. In this study, the *K*-nearest neighbors method showed the best results in identifying NiTiHf alloys with stable functional properties.

In study [17], the method of SMA behavior modeling, based on NN, is proposed. This NN makes it possible to predict SMA starin and temperature accurately and effectively.

Despite the well-known papers where machine learning methods are applied, the prediction of SMA functional properties by the methods of artificial intelligence itself has not been sufficiently studied and highlighted.

Methods of investigations and discussion of results. Dependences of the ranges of dissipated energy, stresses and deformation on the number of load cycles, obtained in paper [18], are predicted by machine learning methods in Orange 3.34.0 software environment. This program makes it possible to construct flowcharts visually and obtain results in the form of models, numerical data and graphs.

In general, three models were built. The dependences of the corresponding physical value on the number of loading cycles are given to the input of each of them. The number of loading cycles was considered as an independent variable, and physical value as dependent variable. In order to increase the accuracy of the modelling results, the dataset is additionally increased by interpolating the experimental dependences with cubic splines. In total, 599 points were obtained. The sample was divided into two unequal parts. The training sample comprised 66 % of the total dataset. Regression dependencies were built by the methods of random forests, neural networks, gradient boosting, AdaBoost, and the k-nearest neighbors method. Each obtained model was additionally checked by cross-validation method 5 times. Flowchart of the model built in Orange environment is shown in Fig. 1.

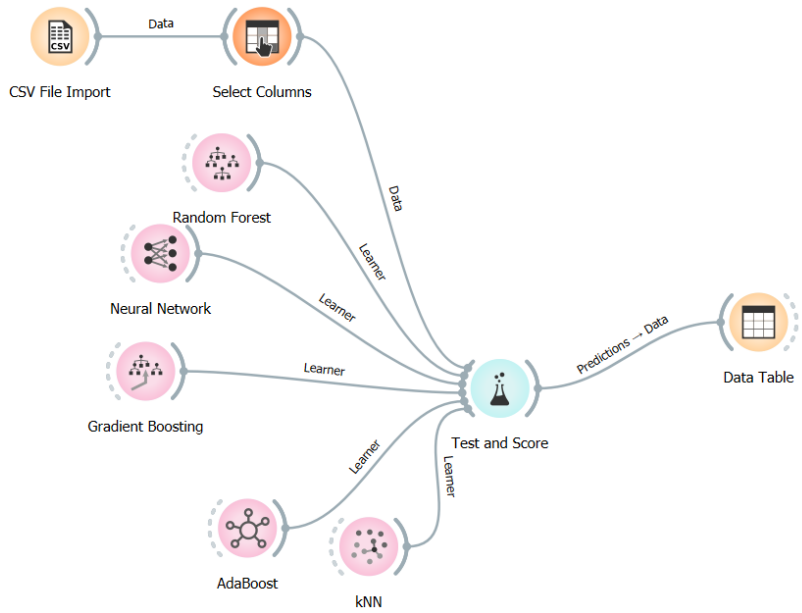

Figure 1. Flowchart diagram of the model built in Orange environment

Tables 1–3 presents the errors of the results and the coefficient of determination obtained by modeling using the machine learning methods for the range of dissipated energy, stresses and strains depending on the number of load cycles, respectively.

Table 1

Errors of the results and the coefficient of determination obtained by modeling using machine learning methods for the range of dissipated energy

Model	MSE	RMSE	MAE	R^2
kNN	0.086	0.294	0.114	1.000
AdaBoost	0.135	0.368	0.179	0.999
RandomForest	0.146	0.381	0.177	0.999
Gradient Boosting	0.150	0.388	0.207	0.999
Neural Network	1.133	1.064	0.493	0.994

For the range of dissipated energy, the smallest mean squared error (MSE) and, accordingly, the RMSE, are obtained by the k-nearest neighbors (kNN) method. AdaBoost, RandomForest, and GradientBoosting methods showed more or less the same results, with MSEs 0.135, 0.146, and 0.150, respectively. Neural network with MSE equal to 1.133 took the last place.

Table 2

Errors of the results and the coefficient of determination obtained by modeling using machine learning methods for the range of strains

Model	MSE	RMSE	MAE	R^2
kNN	0.0005	0.022	0.003	0.908
AdaBoost	0.0005	0.022	0.004	0.907
Random Forest	0.0005	0.022	0.003	0.906
Gradient Boosting	0.001	0.024	0.003	0.885
Neural Network	0.003	0.058	0.035	0.333

For the range of strains, the smallest root mean square error (MSE) and, accordingly, RMSE, are obtained by the k-nearest neighbors (kNN), AdaBoost, and Random Forest methods. GradientBoosting is in the 4th place. The last place is taken by Neural Network with MSE equal to 0.003. Regarding MAE, it turned out to be approximately the same in the models obtained by kNN, AdaBoost, Random Forest, and GradientBoosting.

Table 3

Errors of the results and the coefficient of modeling determination by machine learning methods for the range of stresses

Model	MSE	RMSE	MAE	R^2
kNN	0.006	0.294	0.114	1.000
AdaBoost	0.135	0.368	0.179	0.999
Random Forest	0.152	0.345	0.168	0.999
Gradient Boosting	0.150	0.388	0.207	0.999
Neural Network	1.133	1.064	0.493	0.994

For the stress range, the smallest mean squared error (MSE) and, accordingly, RMSE, were obtained by k-nearest neighbors (kNN) methods. AdaBoost took the second place with MSE result equal to 0.135. RandomForest and GradientBoosting showed more or less the same results. Neural Network with MSE result equal to 1.133 is in the 5th place.

Conclusions. SMA properties, i.e., the range of dissipated energy, strain and stresses were modelled by machine learning methods (kNN, AdaBoost, Random Forest, Gradient Boosting, Neural Network) in Orange software environment. The respective regression dependencies were obtained and cross-validation of the results was carried out 5 times. There were obtained the errors of the results and the coefficient of determination by modeling using machine learning methods for the range of dissipated energy, stresses and strains depending on the number of loading cycles, respectively. For each physical value, the best results in terms of method errors were shown by0 the k-nearest neighbors method.

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МОДЕЛЮВАННЯ ФУНКЦІОНАЛЬНИХ ВЛАСТИВОСТЕЙ СПЛАВІВ З ПАМ'ЯТТЮ ФОРМИ МЕТОДАМИ МАШИННОГО НАВЧАННЯ

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Резюме. *Сплави з пам'яттю форми (СПФ) застосовують у багатьох галузях науки і техніки через їхній унікальний ефект пам'яті форми та суперпружність, котрі спричинено мартенситним та зворотним перетвореннями. У роботі запропоновано моделювати функціональні властивості сплавів з пам'яттю форми, а саме, розмах розсіяної енергії, деформацій та напружень методами машинного навчання. Моделювання здійснювалося у спеціалізованому програмному середовищі аналізу даних Orange. Ця програма дозволяє візуально будувати блок-схеми та отримувати результати у вигляді моделей, числових даних та графіків.*

Загалом побудовано три моделі. На вхід кожної з них подано залежності відповідної фізичної величини від кількості циклів навантаження. Кількість циклів навантаження розглядали як незалежну змінну, а фізичну величину – як залежну змінну. Для збільшення точності результатів моделювання, набір даних додатково збільшили, інтерполювавши експериментальні залежності кубічними сплайнами. Загалом отримали 599 точок. Вибірку поділили на дві нерівні частини. Навчальна вибірка становила 66 % від загальної вибірки. Регресійні залежності будували методами випадкових лісів, нейронних мереж, градієнтного бустінгу, AdaBoost та методом k-найближчих сусідів. Кожну отриману модель додатково тестували методом перехресної перевірки (cross-validation) 5 разів. Для кожного набору даних побудовано п'ять моделей методом нейронних мереж, випадкових лісів, градієнтного бустінгу, AdaBoost та методу k-найближчих сусідів. Отримано відповідні регресійні залежності та здійснено перехресну перевірку результатів 5 разів. Отримано помилки результатів та коефіцієнт детермінації моделюванням зазначеними вище методами машинного навчання для розмаху розсіяної енергії, напружень та деформацій залежно від кількості циклів навантаження відповідно. Для кожної фізичної величини, найліпші результати у термінах помилок методу отримано методом k-найближчих сусідів.

Ключові слова: *сплави з пам'яттю форми, машинне навчання, регресія, метод k-найближчих сусідів, випадковий ліс, нейронна мережа.*

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